



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2026 – 11:01 PM EDT

PDB ID : 4YBB / pdb\_00004ybb  
Title : High-resolution structure of the Escherichia coli ribosome  
Authors : Noeske, J.; Wasserman, M.R.; Terry, D.S.; Altman, R.B.; Blanchard, S.C.;  
Cate, J.H.D.  
Deposited on : 2015-02-18  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

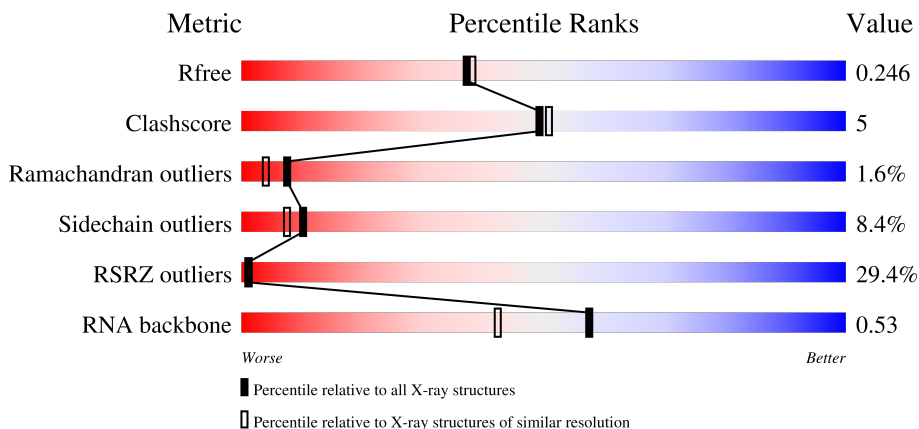
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



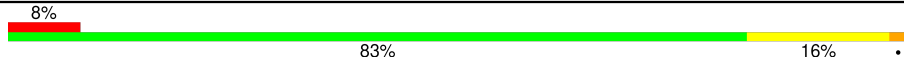

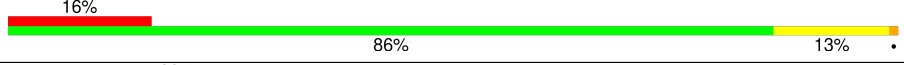

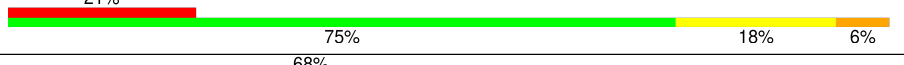

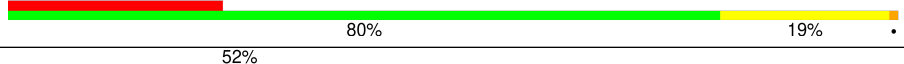







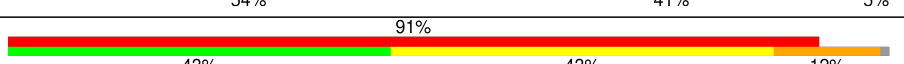
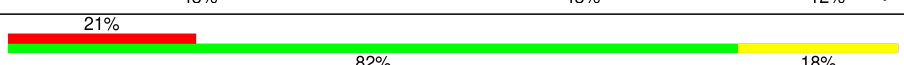

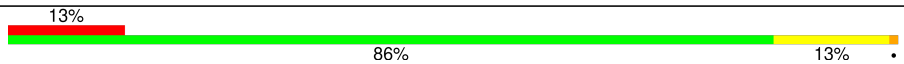

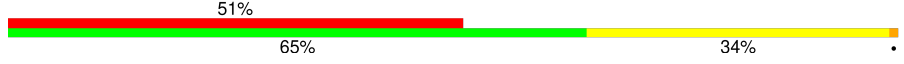

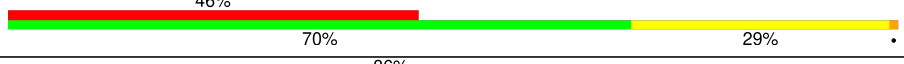
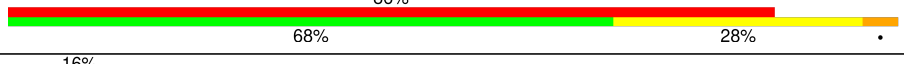


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1534	 73% 22% 5%
1	BA	1534	 6% 70% 24% 6%
2	AB	224	 43% 80% 17%
2	BB	224	 61% 77% 21%

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	60% 61% 23% 15% .
16	AP	82	17% 89% 7% .
16	BP	82	91% 68% 24% 6% .
17	AQ	80	20% 81% 18% .
17	BQ	80	78% 46% 39% 14% .
18	AR	55	22% 82% 18%
18	BR	55	49% 65% 27% 5% .
19	AS	79	46% 76% 22% ..
19	BS	79	76% 66% 20% 10% .
20	AT	86	24% 83% 17%
20	BT	86	80% 63% 27% 8% ..
21	AU	56	38% 77% 21% .
21	BU	56	48% 79% 20% .
22	CA	2904	15% 71% 23% 5%
23	CB	120	82% 13% . .
23	DB	120	88% 11% .
24	CC	271	90% 70% 25% .
24	DC	271	18% 89% 10% .
25	CD	209	85% 78% 18% . .
26	CE	201	85% 73% 21% 6%
26	DE	201	2% 96% .
27	CF	177	62% 68% 29% .
27	DF	177	25% 82% 16% .
28	CG	176	65% 76% 21% .
28	DG	176	9% 88% 11% .

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Mol	Chain	Length	Quality of chain
29	CH	149	67% 66% 26% 7%
29	DH	149	56% 75% 23%
30	CJ	134	72% 72% 24%
30	DJ	134	79% 73% 23%
31	CK	142	73% 77% 18%
31	DK	142	4% 91% 8%
32	CL	123	72% 69% 25% 5%
32	DL	123	2% 82% 16%
33	CM	144	88% 69% 24% 7%
33	DM	144	3% 85% 15%
34	CN	136	81% 85% 11%
34	DN	136	% 88% 10%
35	CO	125	88% 67% 21% 6%
35	DO	125	6% 86% 13%
36	CP	117	56% 69% 26%
36	DP	117	4% 91% 7%
37	CQ	114	79% 81% 18%
37	DQ	114	8% 89% 11%
38	CR	117	78% 77% 21%
38	DR	117	3% 89% 11%
39	CS	103	83% 75% 21%
39	DS	103	2% 87% 13%
40	CT	110	90% 78% 17% 5%
40	DT	110	% 95% 5%
41	CU	93	89% 73% 17% 8%

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Mol	Chain	Length	Quality of chain
41	DU	93	16% 83% 14%
42	CV	102	96% 55% 38% 7%
42	DV	102	13% 87% 11%
43	CW	94	53% 78% 19%
43	DW	94	2% 90% 10%
44	CX	76	83% 82% 16%
44	DX	76	7% 91% 9%
45	CY	77	94% 75% 19% 5%
45	DY	77	16% 92% 8%
46	CZ	62	89% 68% 26% 6%
46	DZ	62	24% 90% 8%
47	C0	58	71% 81% 12% 7%
47	D0	58	9% 91% 7%
48	C1	56	88% 71% 21% 7%
48	D1	56	7% 82% 18%
49	C2	51	57% 69% 29%
49	D2	51	16% 82% 18%
50	C3	46	98% 63% 30%
50	D3	46	2% 83% 17%
51	C4	64	98% 77% 20%
51	D4	64	3% 92% 8%
52	C5	38	95% 71% 21% 8%
52	D5	38	5% 97%
53	DA	2903	2% 78% 18%
54	DD	209	% 88% 12%

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Mol	Chain	Length	Quality of chain
55	DI	135	<p>84% 70% 27% ..</p>

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
56	MG	DA	3137	-	-	-	X
57	PG4	DA	3193	-	-	X	-
57	PG4	DR	202	-	-	X	-
58	MPD	DN	201	-	-	X	-
59	PUT	DA	3223	-	-	X	-
61	PEG	D3	102	-	-	X	-
61	PEG	DP	201	-	-	X	-

## 2 Entry composition [i](#)

There are 69 unique types of molecules in this entry. The entry contains 295060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1534	Total 32930	C 14694	N 6041	O 10661	P 1534	0	0	0
1	BA	1533	Total 32908	C 14684	N 6036	O 10655	P 1533	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	224	Total 1753	C 1109	N 315	O 321	S 8	0	0	0
2	BB	224	Total 1753	C 1109	N 315	O 321	S 8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	Total 1625	C 1028	N 305	O 289	S 3	0	0	0
3	BC	206	Total 1625	C 1028	N 305	O 289	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	205	Total 1643	C 1026	N 315	O 298	S 4	0	0	0
4	BD	205	Total 1643	C 1026	N 315	O 298	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	BJ	98	787	493	150	143	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	117	877	540	174	160	3	0	0	0
11	BK	117	877	540	174	160	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	123	957	591	196	165	5	0	0	0
12	BL	123	957	591	196	165	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	114	884	546	178	157	3	0	0	0
13	BM	114	884	546	178	157	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	100	805	499	164	139	3	0	0	0
14	BN	100	805	499	164	139	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	714	439	144	130	1	0	0	0
15	BO	88	714	439	144	130	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AP	82	Total 649	C 406	N 128	O 114	S 1	0	0	0
16	BP	82	Total 649	C 406	N 128	O 114	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AQ	80	Total 649	C 411	N 121	O 114	S 3	0	0	0
17	BQ	80	Total 649	C 411	N 121	O 114	S 3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	AR	55	Total 456	C 288	N 86	O 82	0	0	0
18	BR	55	Total 456	C 288	N 86	O 82	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	79	Total 638	C 408	N 120	O 108	S 2	0	0	0
19	BS	79	Total 638	C 408	N 120	O 108	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AT	86	Total 670	C 414	N 138	O 115	S 3	0	0	0
20	BT	85	Total 665	C 411	N 137	O 114	S 3	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	2798	U	UNK	conflict	GB 731469900
CA	2800	A	UNK	conflict	GB 731469900

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
23	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
26	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
27	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
28	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			
30	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
32	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
33	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
34	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
35	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CP	116	Total	C	N	O		0	0	0
			892	552	178	162				
36	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
37	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	CR	117	Total	C	N	O	0	0	0
			947	604	192	151			
38	DR	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
39	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
40	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	CV	102	Total	C	N	O	0	0	0
			780	492	146	142			
42	DV	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
43	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
44	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
45	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
46	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
48	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
49	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
50	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
51	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
52	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 53 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	DA	2897	62361	27827	11476	20154	2904	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	2798	U	UNK	conflict	GB 731469900
DA	2800	A	UNK	conflict	GB 731469900

- Molecule 54 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	DD	209	1576	986	290	296	4	0	1	0

- Molecule 55 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	DI	135	1023	649	179	192	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

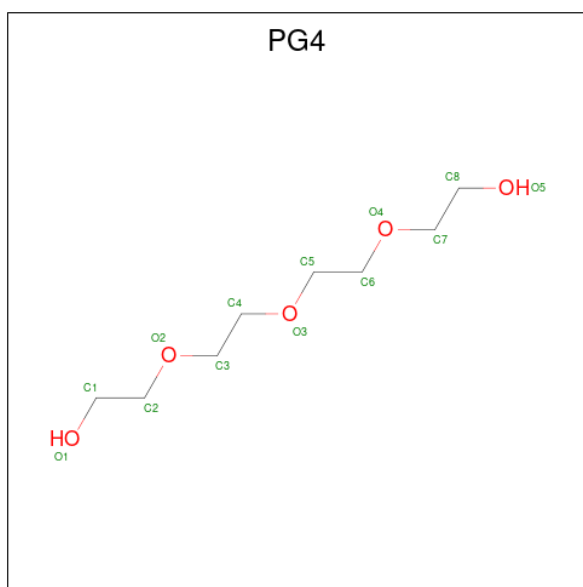
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	70	Total 70	Mg 70	0	0
56	BA	41	Total 41	Mg 41	0	0
56	CA	155	Total 155	Mg 155	0	0
56	CB	3	Total 3	Mg 3	0	0
56	C3	1	Total 1	Mg 1	0	0

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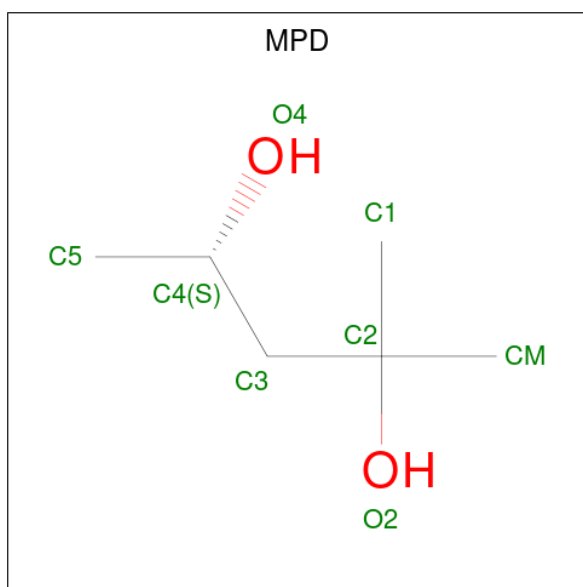
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DA	183	Total Mg 183 183	0	0
56	DB	9	Total Mg 9 9	0	0
56	DR	1	Total Mg 1 1	0	0

- Molecule 57 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



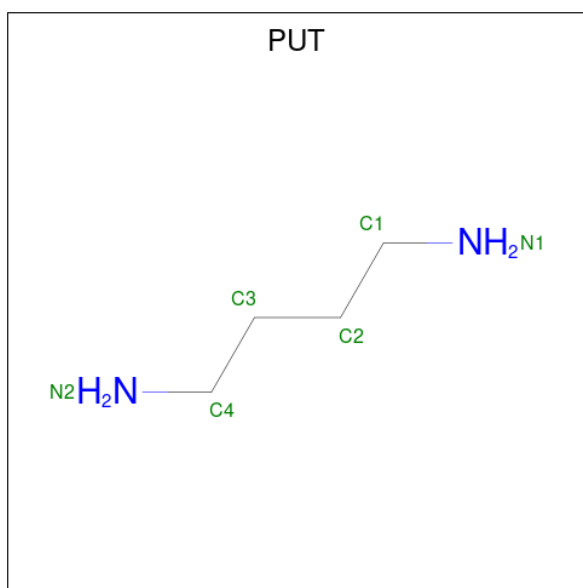
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C O 13 8 5	0	0
57	BA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DQ	1	Total C O 13 8 5	0	0
57	DR	1	Total C O 13 8 5	0	0
57	DS	1	Total C O 13 8 5	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	1	Total C O 8 6 2	0	0
58	AA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DA	1	Total C O 8 6 2	0	0
58	DE	1	Total C O 8 6 2	0	0
58	DE	1	Total C O 8 6 2	0	0
58	DK	1	Total C O 8 6 2	0	0
58	DN	1	Total C O 8 6 2	0	0
58	DS	1	Total C O 8 6 2	0	0
58	DT	1	Total C O 8 6 2	0	0
58	DT	1	Total C O 8 6 2	0	0

- Molecule 59 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	1	Total C N 6 4 2	0	0
59	AA	1	Total C N 6 4 2	0	0
59	AA	1	Total C N 6 4 2	0	0
59	AA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0

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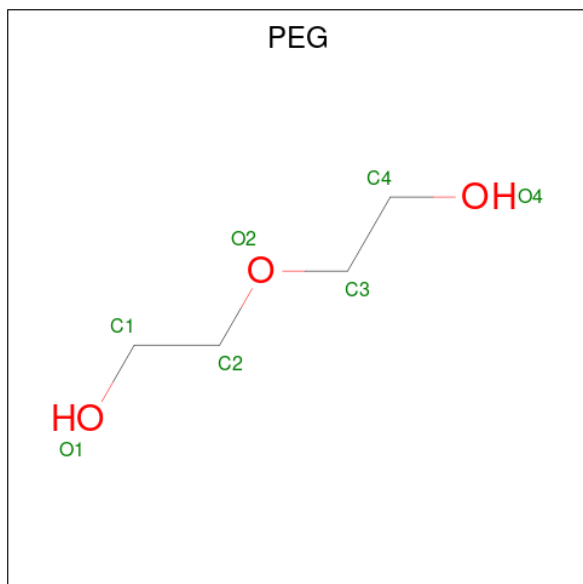
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DM	1	Total	C	N	0	0
			6	4	2		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AB	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0	0
			1	1		
60	D5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



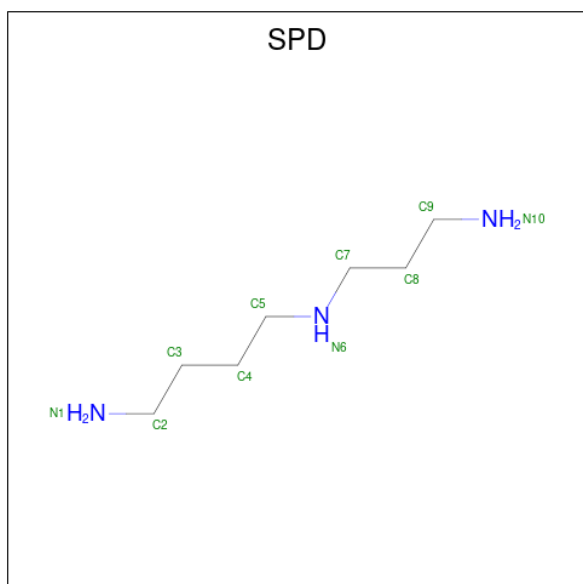
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DL	1	Total C O 7 4 3	0	0
61	DP	1	Total C O 7 4 3	0	0
61	DQ	1	Total C O 7 4 3	0	0
61	D3	1	Total C O 7 4 3	0	0

- Molecule 62 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



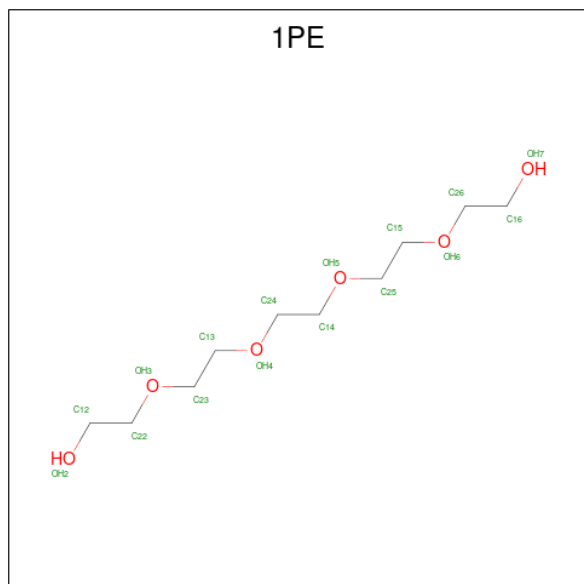
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0

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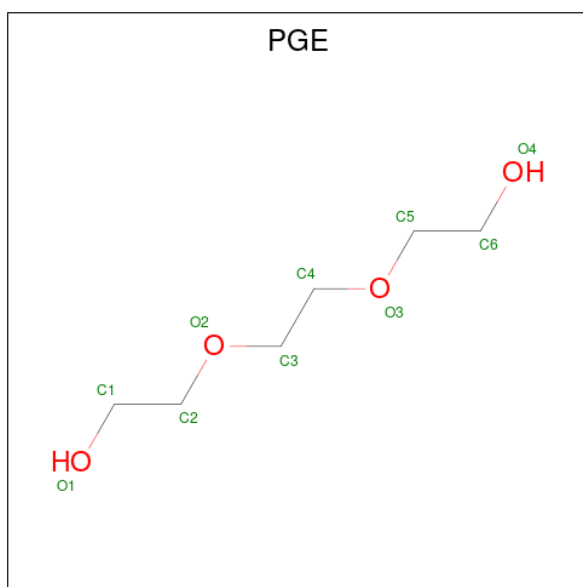
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 63 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



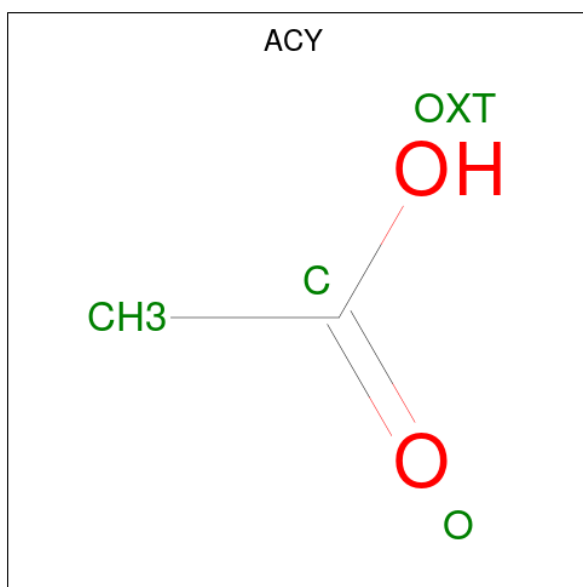
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DA	1	Total	C	O	0	0
			16	10	6		
63	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 64 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



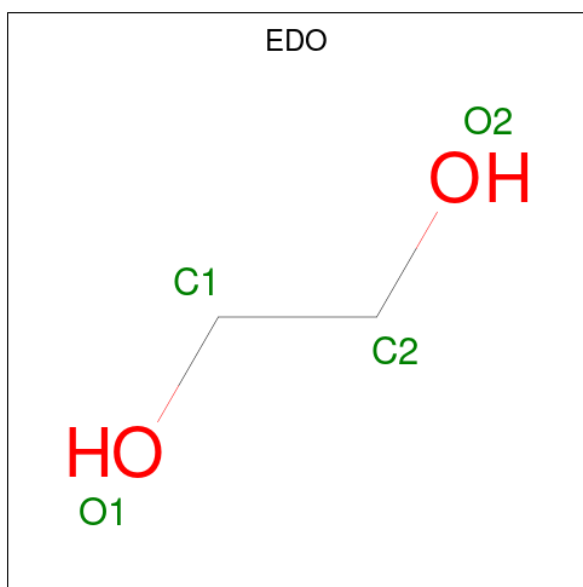
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DS	1	Total C O 10 6 4	0	0
64	DU	1	Total C O 10 6 4	0	0
64	D1	1	Total C O 10 6 4	0	0
64	D3	1	Total C O 10 6 4	0	0

- Molecule 65 is ACETIC ACID (CCD ID: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C O 4 2 2	0	0
65	DA	1	Total C O 4 2 2	0	0
65	DA	1	Total C O 4 2 2	0	0

- Molecule 66 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



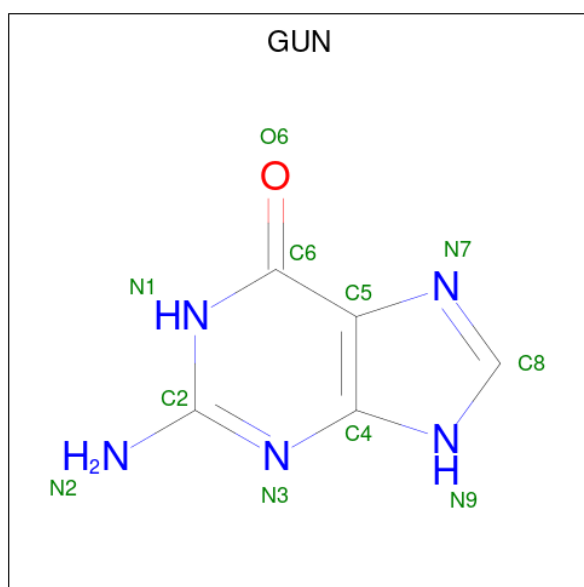
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 4 2 2	0	0

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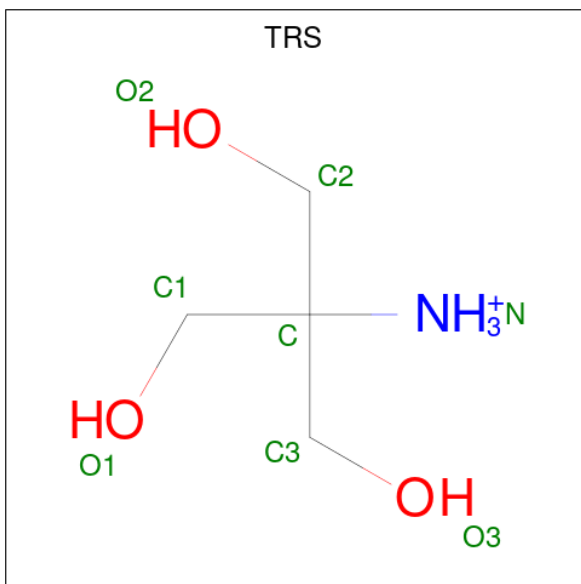
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0
66	DB	1	Total C O 4 2 2	0	0
66	DB	1	Total C O 4 2 2	0	0
66	DB	1	Total C O 4 2 2	0	0
66	DR	1	Total C O 4 2 2	0	0
66	D0	1	Total C O 4 2 2	0	0
66	D1	1	Total C O 4 2 2	0	0

- Molecule 67 is GUANINE (CCD ID: GUN) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
67	DA	1	11	5	5	1	0	0

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
68	DA	1	8	4	1	3	0	0

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
69	AA	509	509	509	0	0
69	AC	6	6	6	0	0
69	AD	2	2	2	0	0
69	AE	5	5	5	0	0
69	AF	1	1	1	0	0
69	AG	1	1	1	0	0
69	AH	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AJ	2	Total 2	O 2	0	0
69	AK	6	Total 6	O 6	0	0
69	AL	10	Total 10	O 10	0	0
69	AM	4	Total 4	O 4	0	0
69	AN	6	Total 6	O 6	0	0
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	2	Total 2	O 2	0	0
69	BA	286	Total 286	O 286	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	2	Total 2	O 2	0	0
69	BL	5	Total 5	O 5	0	0
69	BN	3	Total 3	O 3	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	3	Total 3	O 3	0	0
69	BT	5	Total 5	O 5	0	0
69	BU	2	Total 2	O 2	0	0
69	CA	692	Total 692	O 692	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CB	13	Total 13	O 13	0	0
69	CC	8	Total 8	O 8	0	0
69	CD	6	Total 6	O 6	0	0
69	CE	6	Total 6	O 6	0	0
69	CK	1	Total 1	O 1	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	5	Total 5	O 5	0	0
69	CO	1	Total 1	O 1	0	0
69	CS	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	2	Total 2	O 2	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	C3	2	Total 2	O 2	0	0
69	C4	1	Total 1	O 1	0	0
69	DA	4815	Total 4815	O 4815	0	0
69	DB	209	Total 209	O 209	0	0
69	DC	106	Total 106	O 106	0	0
69	DD	103	Total 103	O 103	0	0
69	DE	62	Total 62	O 62	0	0
69	DF	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	59	Total 59	O 59	0	0
69	DL	45	Total 45	O 45	0	0
69	DM	67	Total 67	O 67	0	0
69	DN	74	Total 74	O 74	0	0
69	DO	42	Total 42	O 42	0	0
69	DP	37	Total 37	O 37	0	0
69	DQ	27	Total 27	O 27	0	0
69	DR	67	Total 67	O 67	0	0
69	DS	50	Total 50	O 50	0	0
69	DT	61	Total 61	O 61	0	0
69	DU	19	Total 19	O 19	0	0
69	DV	22	Total 22	O 22	0	0
69	DW	32	Total 32	O 32	0	0
69	DX	30	Total 30	O 30	0	0
69	DY	10	Total 10	O 10	0	0
69	DZ	8	Total 8	O 8	0	0
69	D0	25	Total 25	O 25	0	0
69	D1	47	Total 47	O 47	0	0
69	D2	9	Total 9	O 9	0	0

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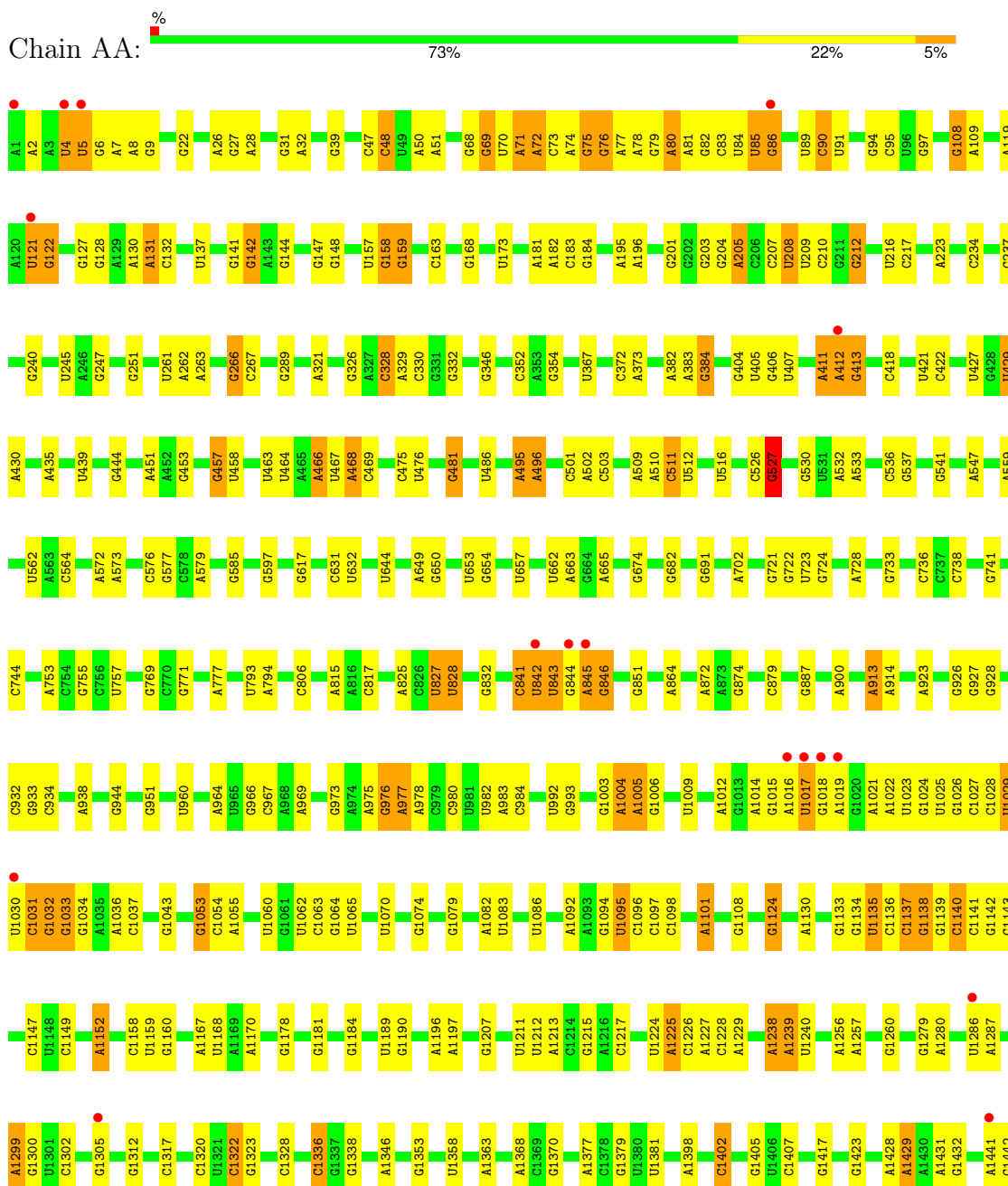
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
69	D3	25	Total 25	O 25	0	0
69	D4	38	Total 38	O 38	0	0
69	D5	14	Total 14	O 14	0	0

### 3 Residue-property plots

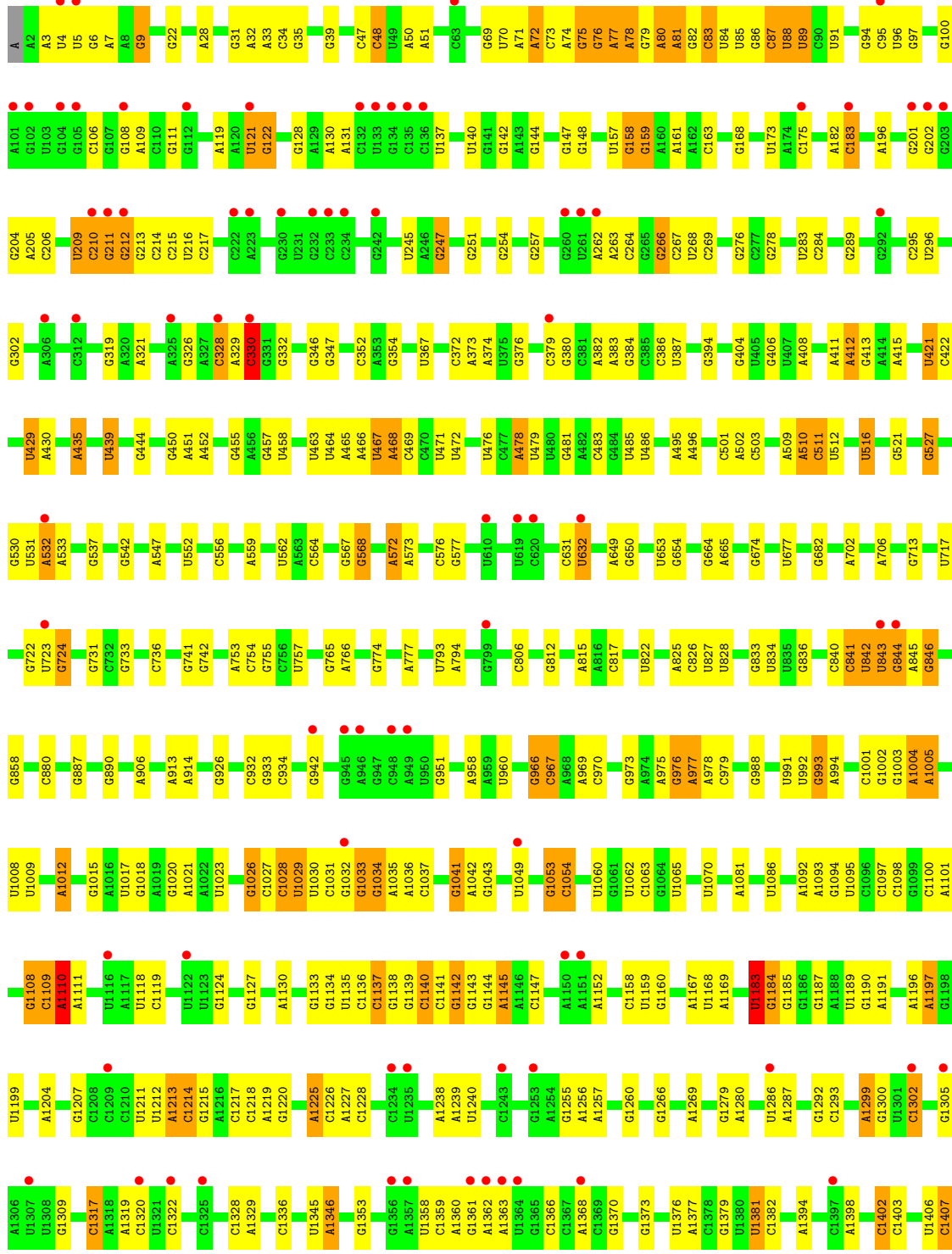
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

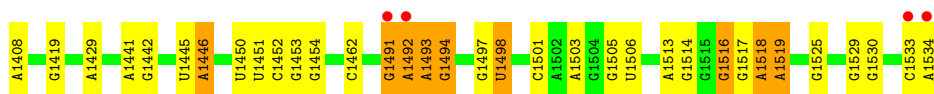
#### • Molecule 1: 16S rRNA



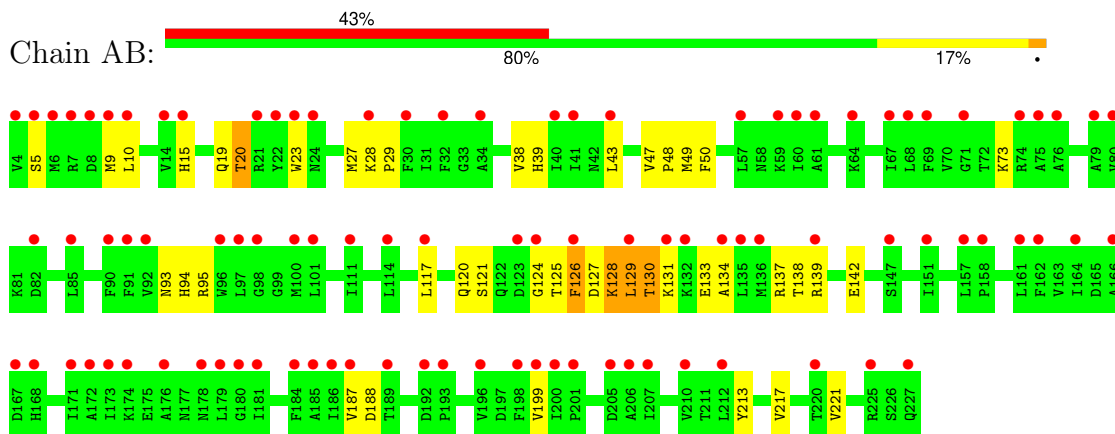


● Molecule 1: 16S rRNA

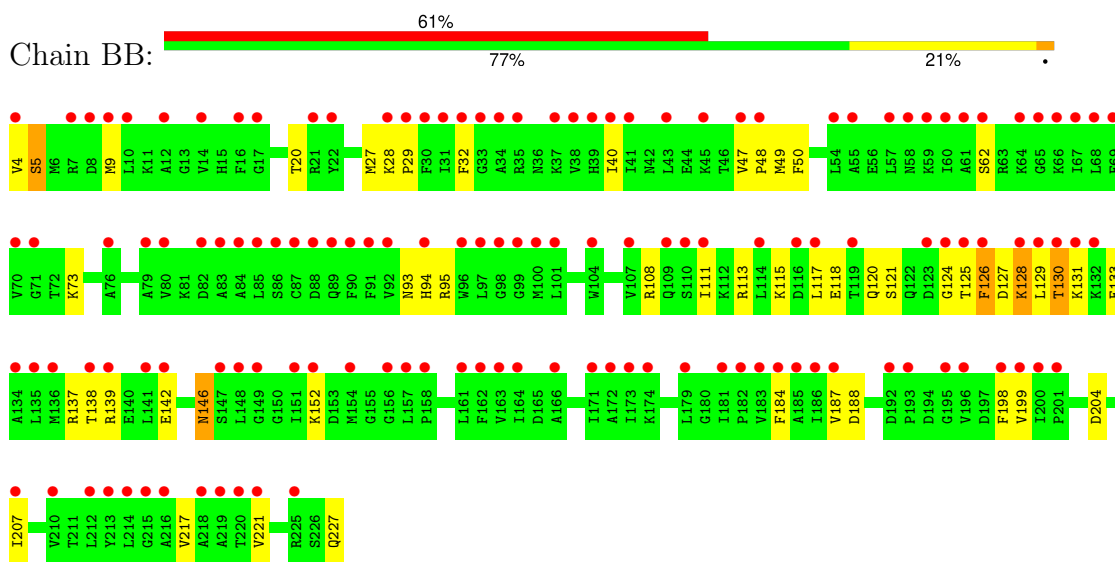




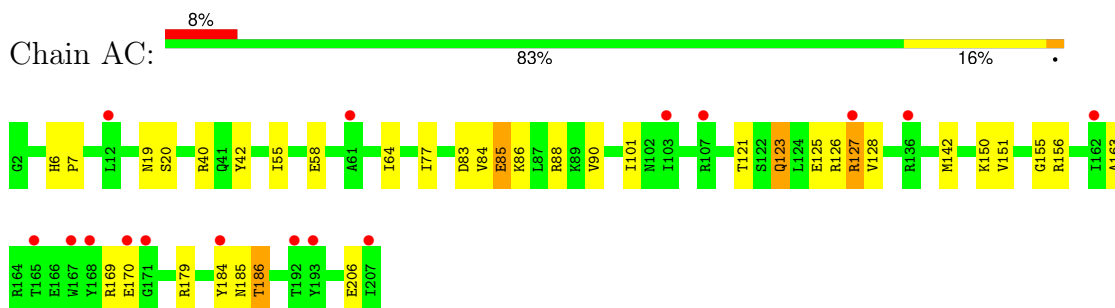
- Molecule 2: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S2

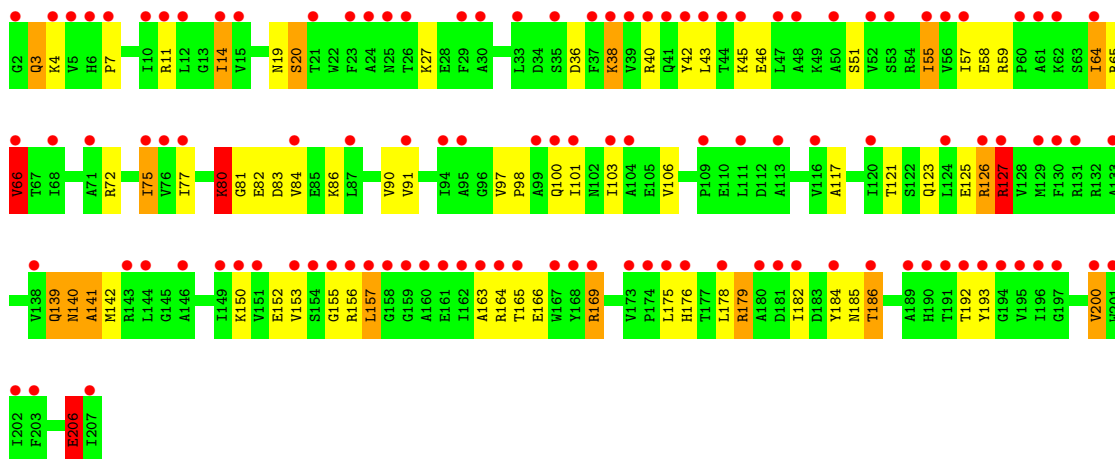


- Molecule 3: 30S ribosomal protein S3

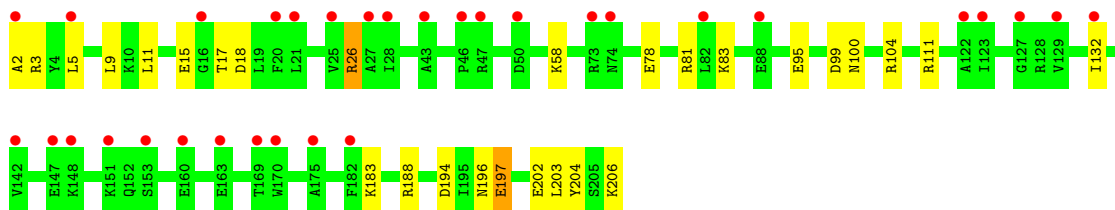
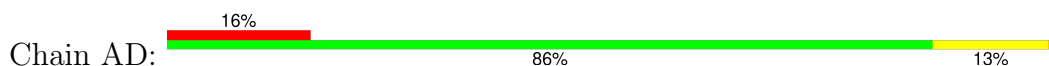


- Molecule 3: 30S ribosomal protein S3

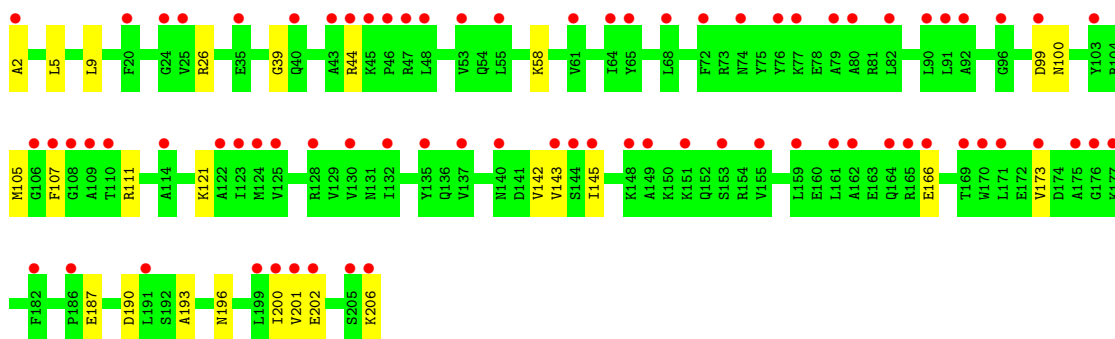
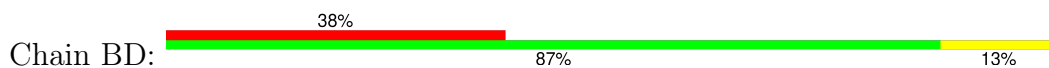




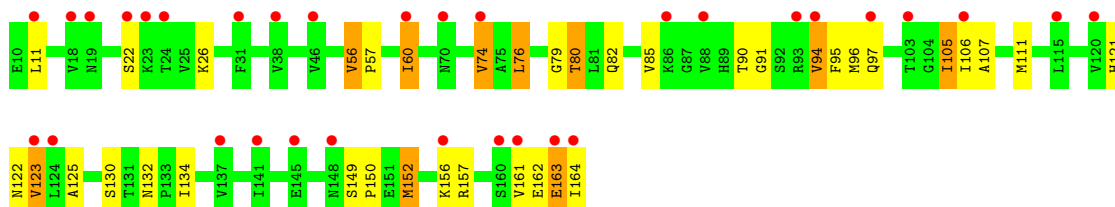
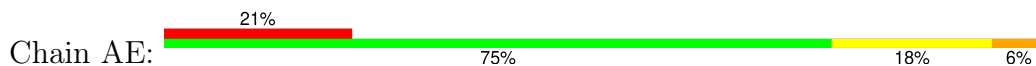
- Molecule 4: 30S ribosomal protein S4



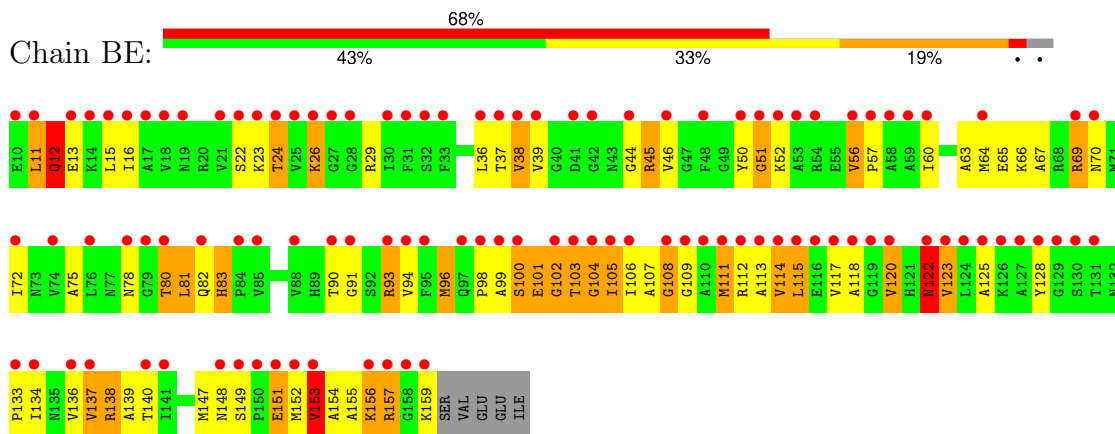
- Molecule 4: 30S ribosomal protein S4



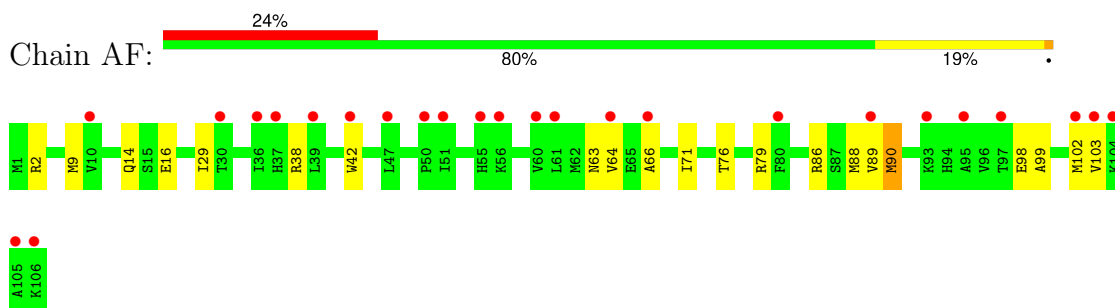
- Molecule 5: 30S ribosomal protein S5



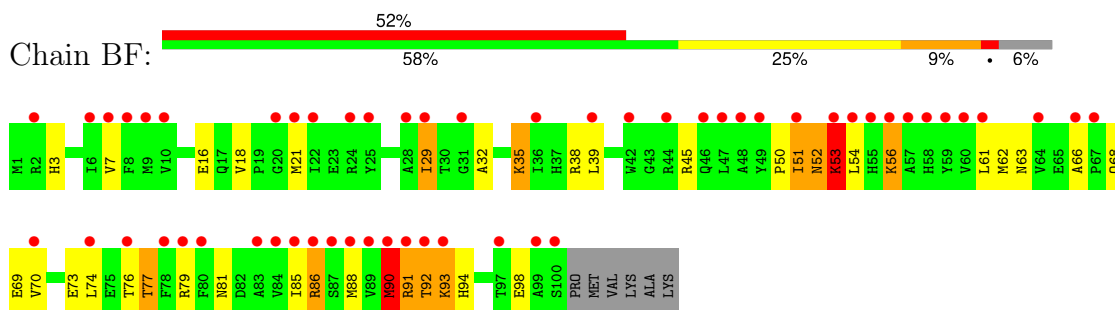
- Molecule 5: 30S ribosomal protein S5



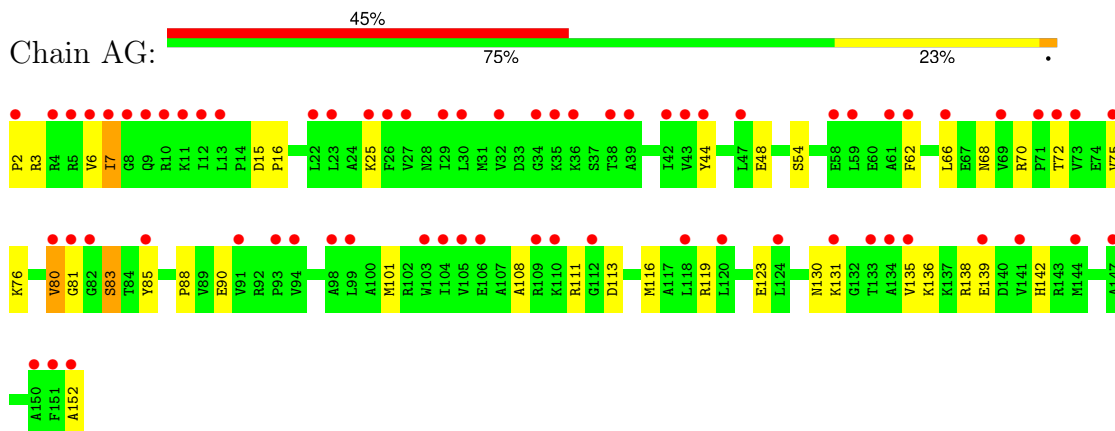
- Molecule 6: 30S ribosomal protein S6



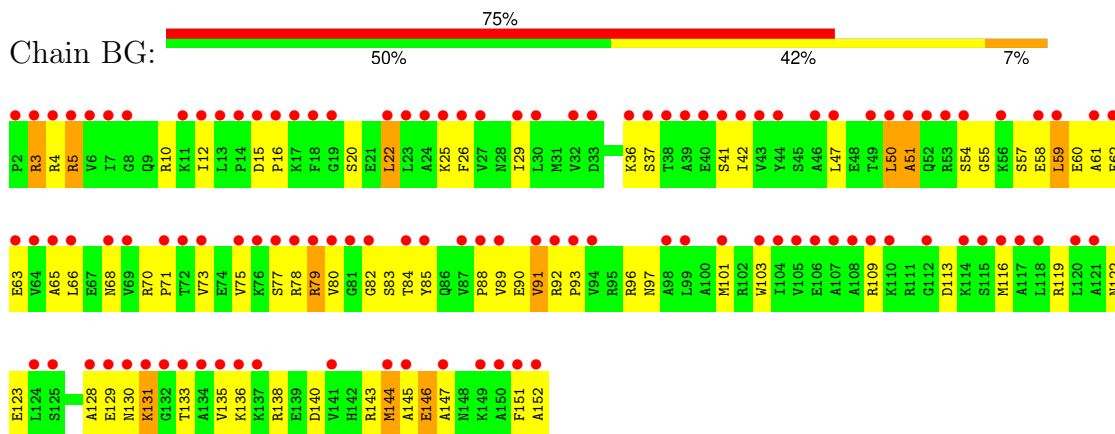
- Molecule 6: 30S ribosomal protein S6



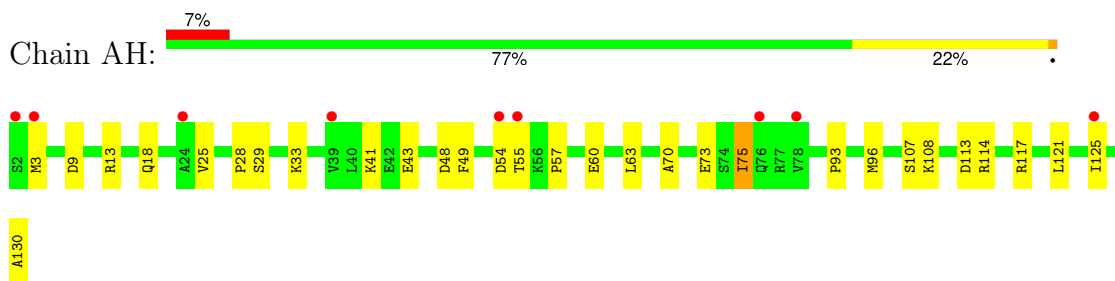
- Molecule 7: 30S ribosomal protein S7



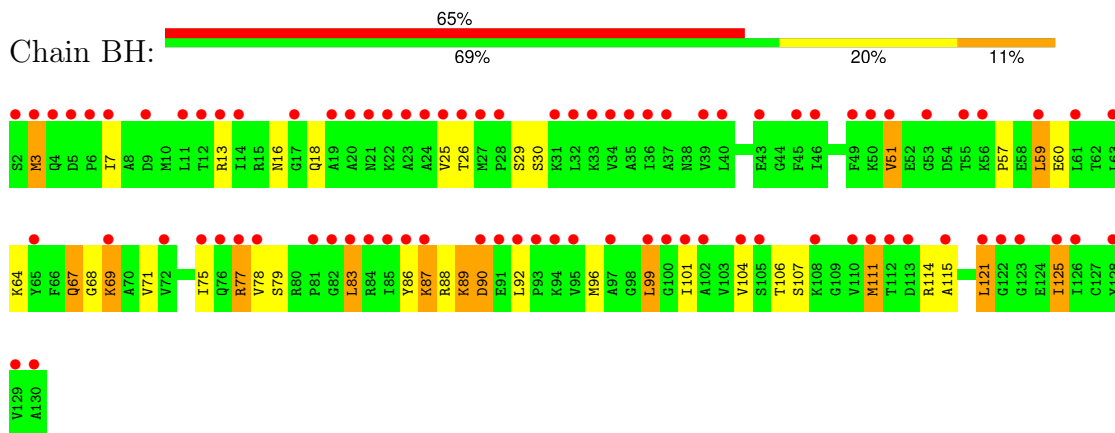
- Molecule 7: 30S ribosomal protein S7



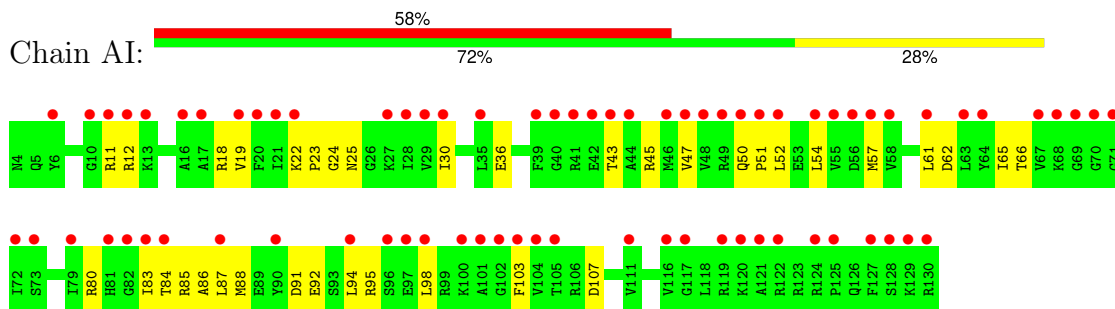
- Molecule 8: 30S ribosomal protein S8



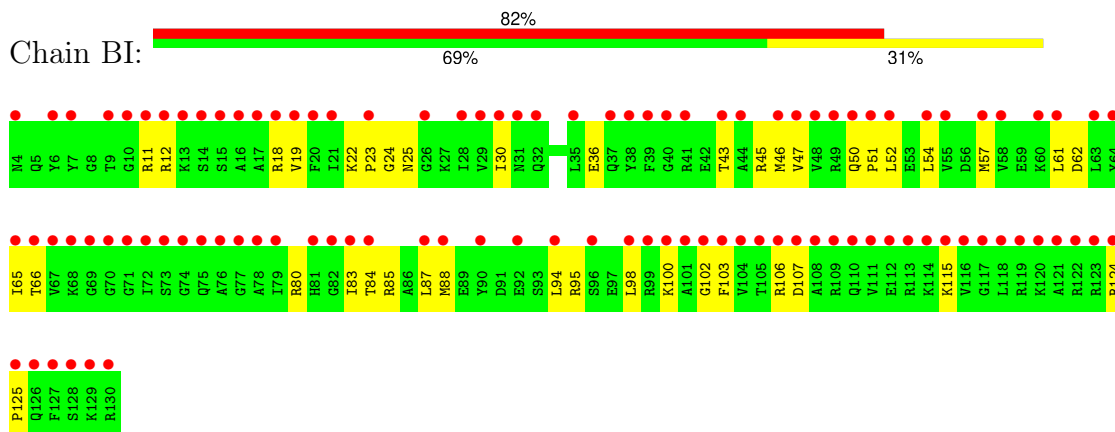
- Molecule 8: 30S ribosomal protein S8



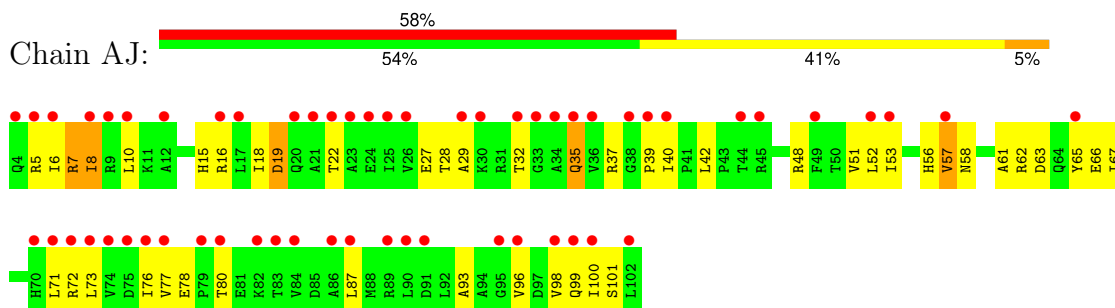
- Molecule 9: 30S ribosomal protein S9



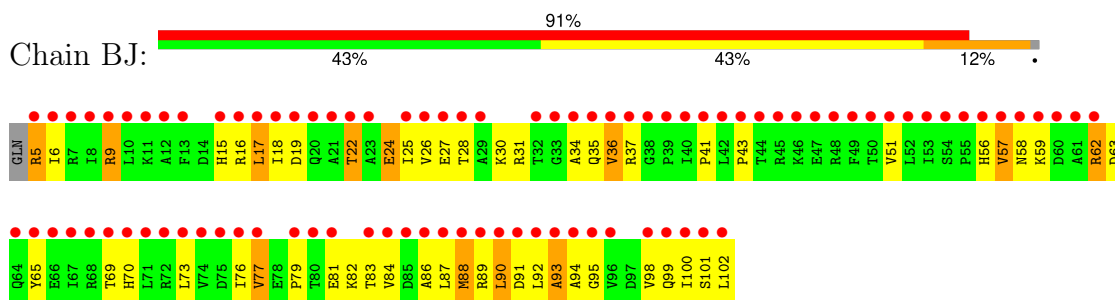
- Molecule 9: 30S ribosomal protein S9



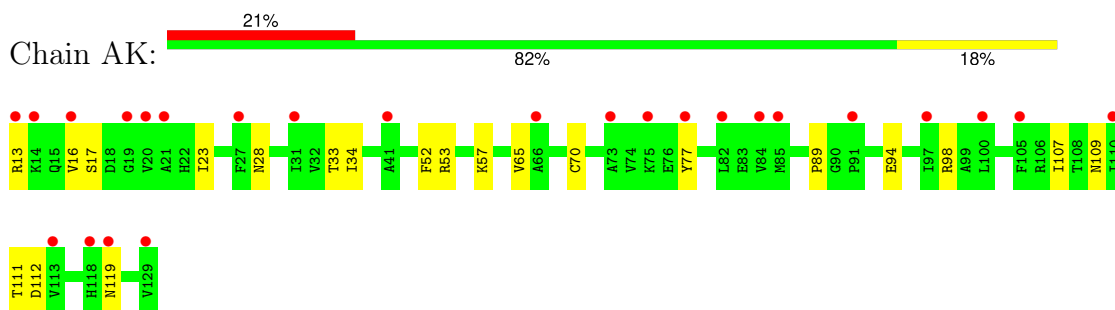
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

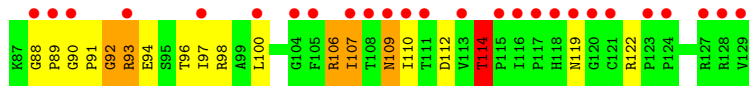
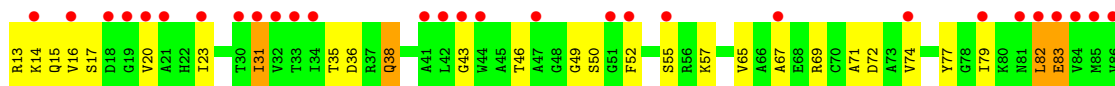


- Molecule 11: 30S ribosomal protein S11

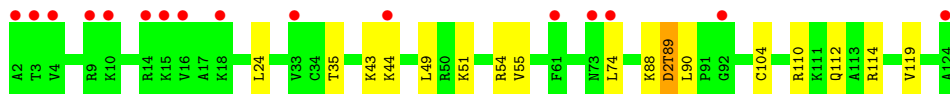
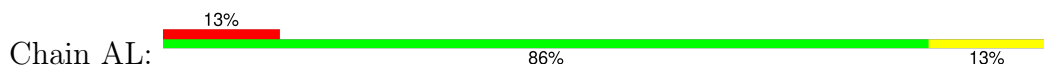


- Molecule 11: 30S ribosomal protein S11

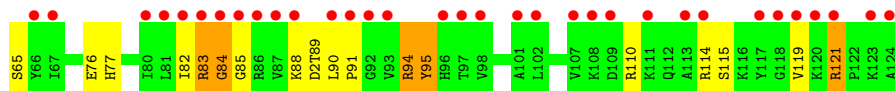
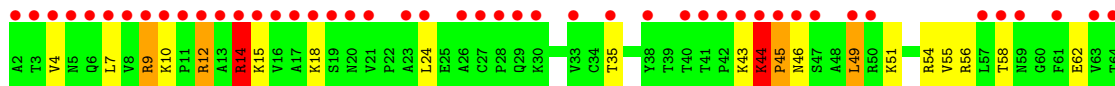




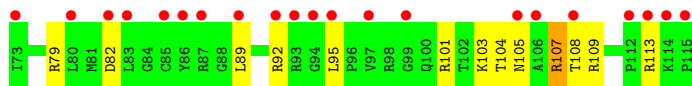
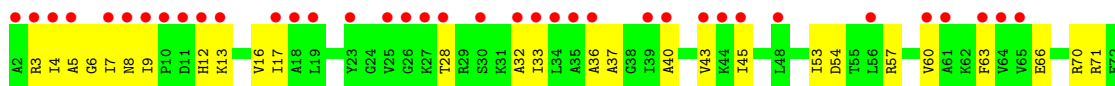
- Molecule 12: 30S ribosomal protein S12



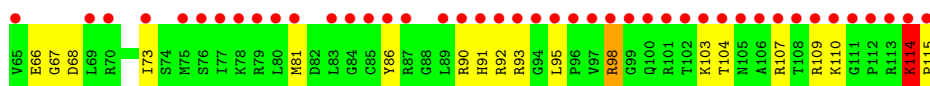
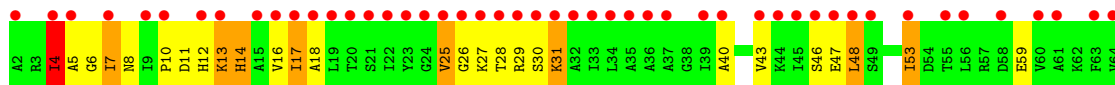
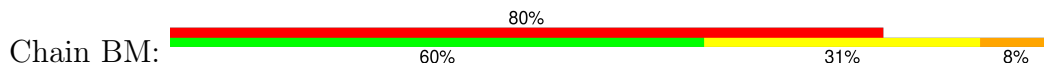
- Molecule 12: 30S ribosomal protein S12



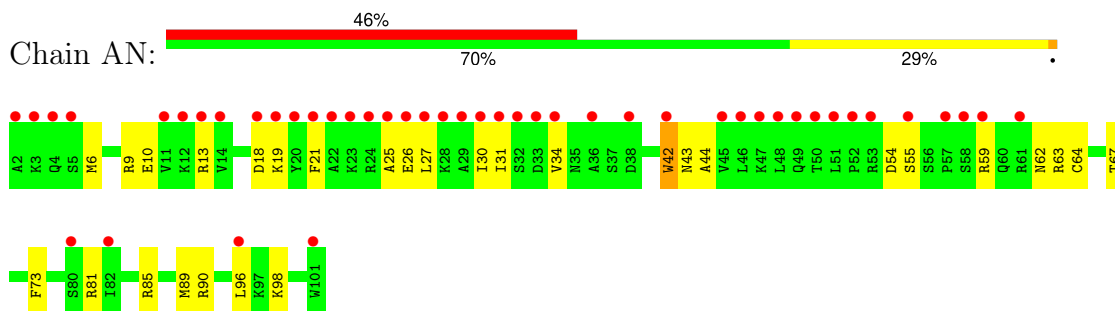
- Molecule 13: 30S ribosomal protein S13



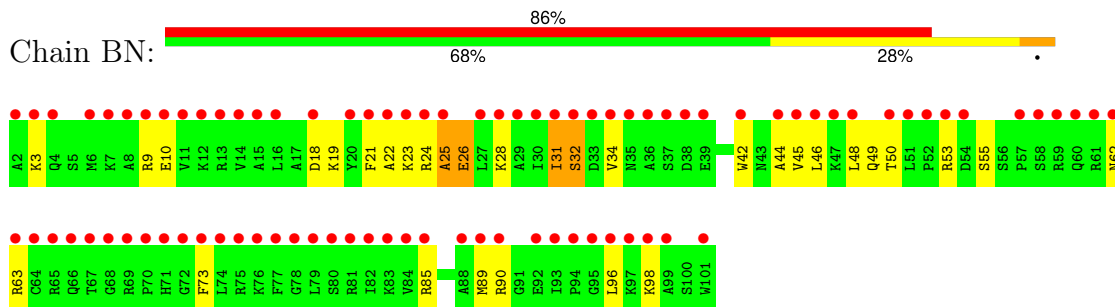
- Molecule 13: 30S ribosomal protein S13



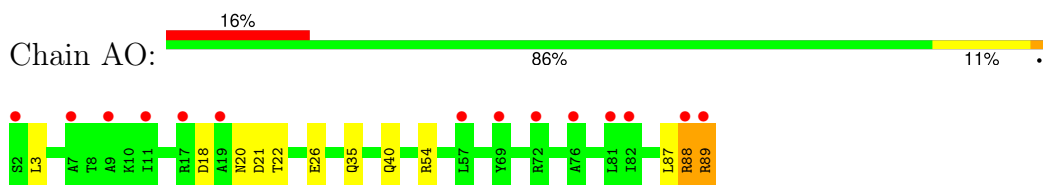
- Molecule 14: 30S ribosomal protein S14



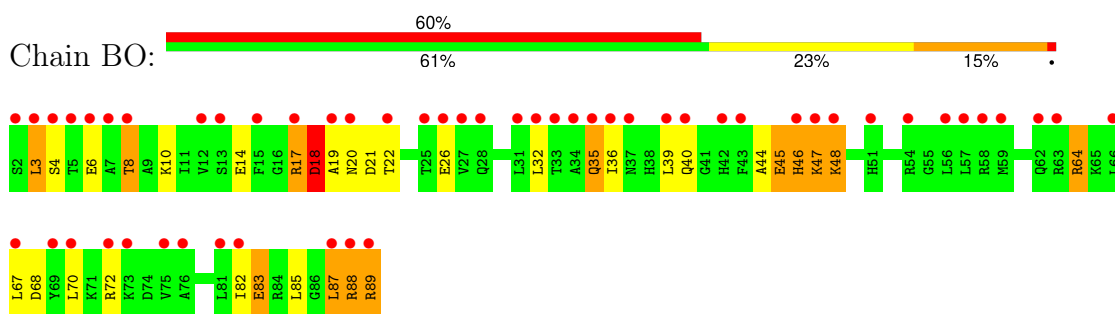
- Molecule 14: 30S ribosomal protein S14



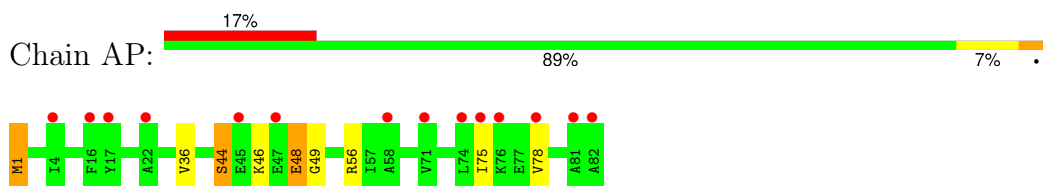
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

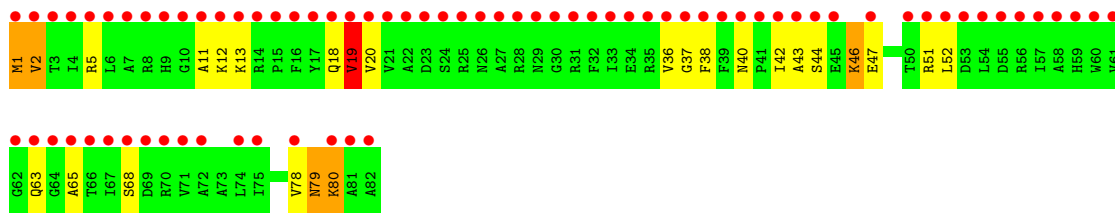


- Molecule 16: 30S ribosomal protein S16

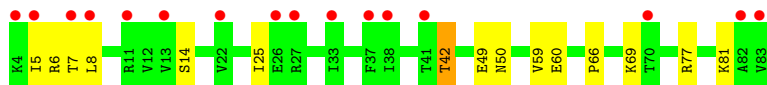
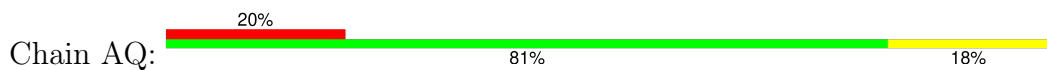


- Molecule 16: 30S ribosomal protein S16

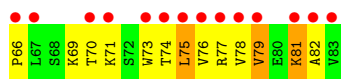
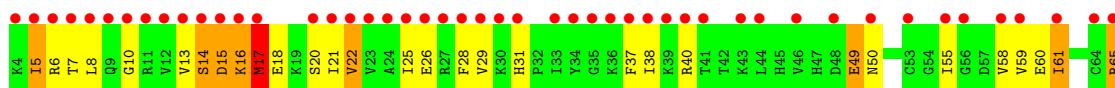
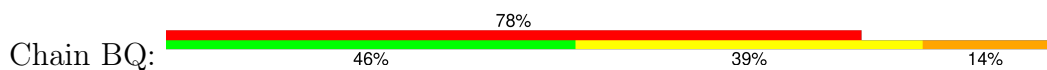




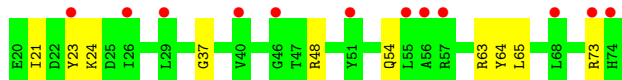
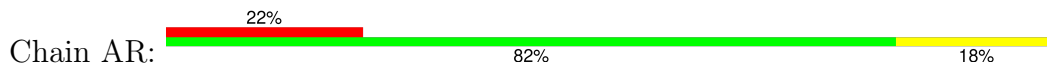
- Molecule 17: 30S ribosomal protein S17



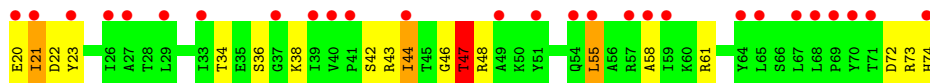
- Molecule 17: 30S ribosomal protein S17



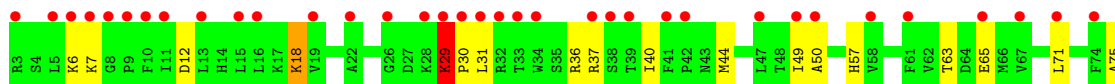
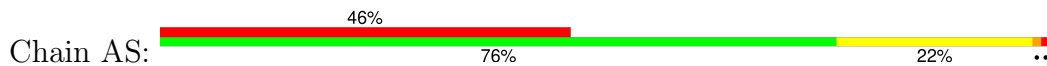
- Molecule 18: 30S ribosomal protein S18

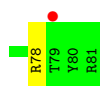


- Molecule 18: 30S ribosomal protein S18

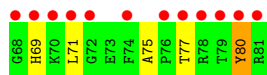
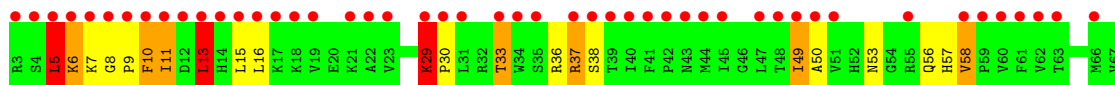
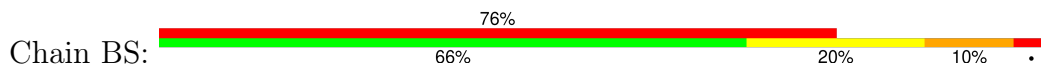


- Molecule 19: 30S ribosomal protein S19

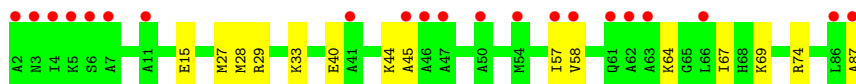
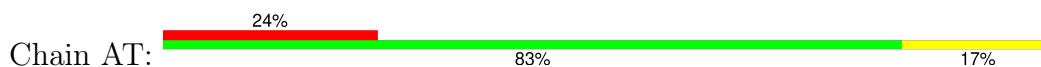




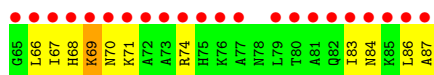
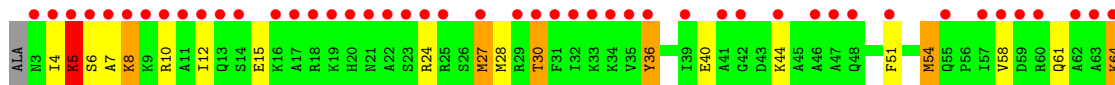
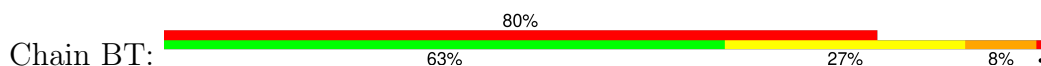
- Molecule 19: 30S ribosomal protein S19



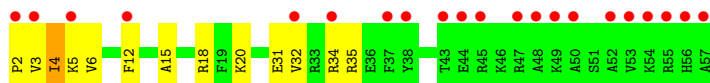
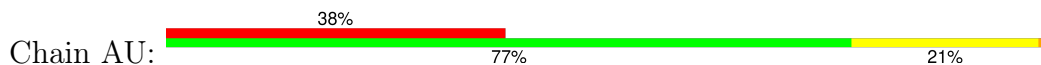
- Molecule 20: 30S ribosomal protein S20



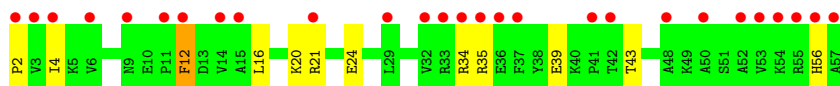
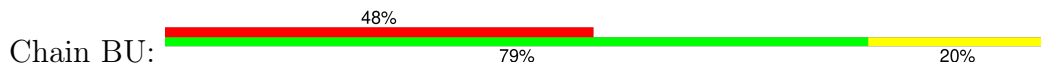
- Molecule 20: 30S ribosomal protein S20



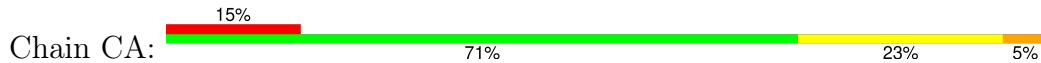
- Molecule 21: 30S ribosomal protein S21

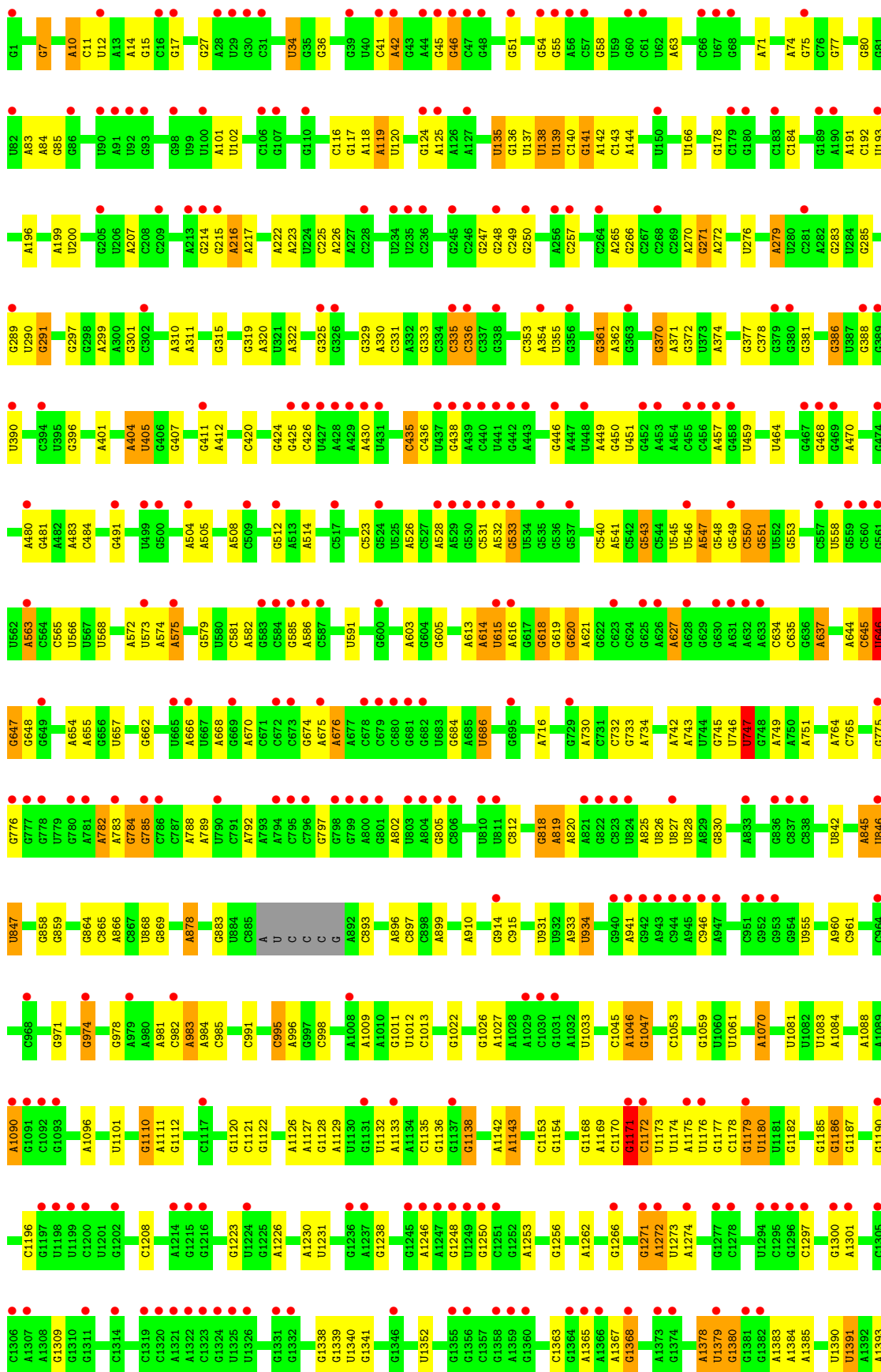


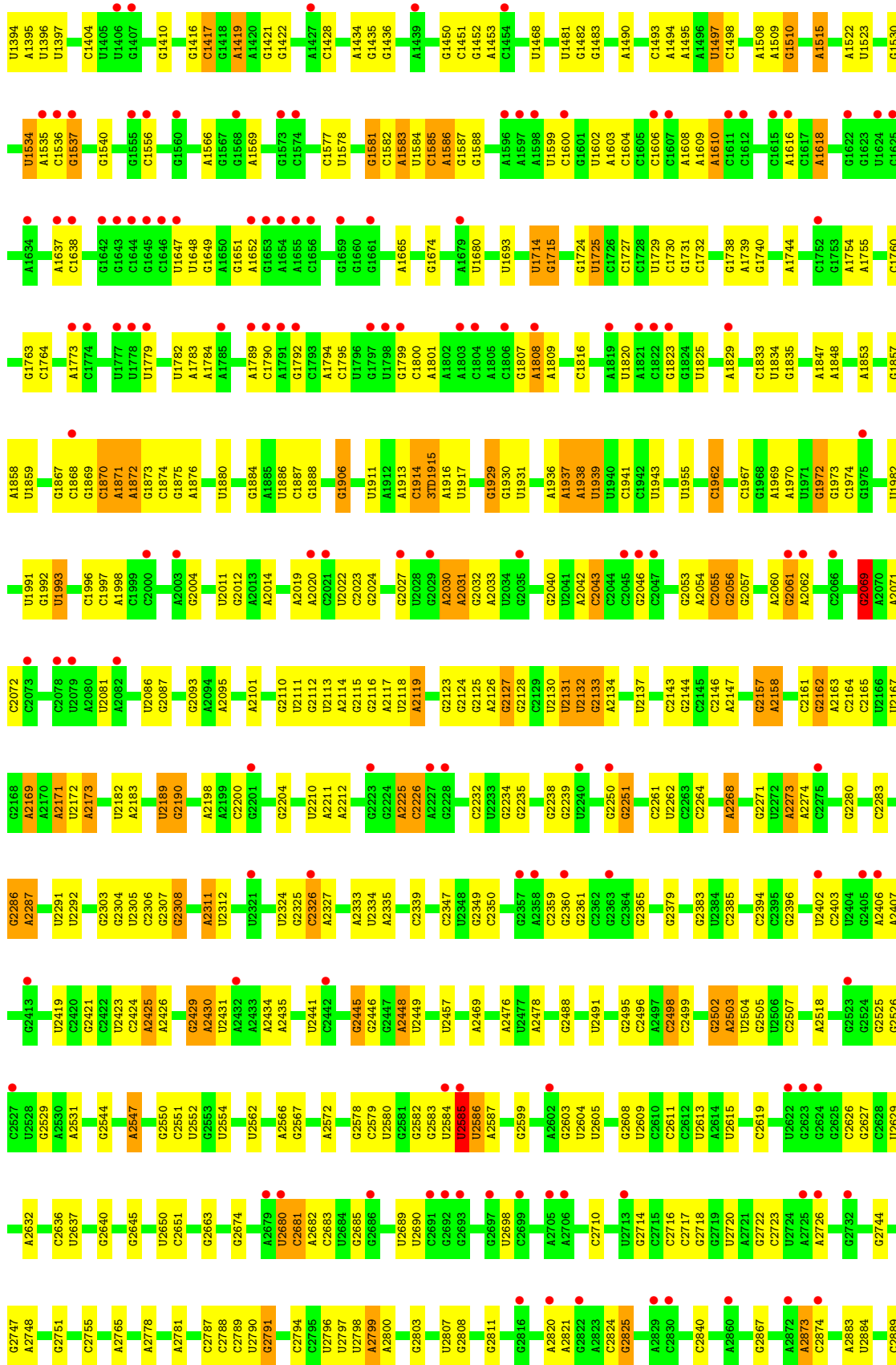
- Molecule 21: 30S ribosomal protein S21

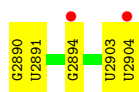


- Molecule 22: 23S rRNA

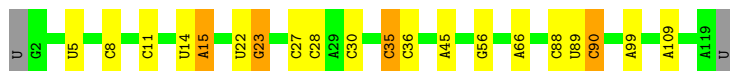
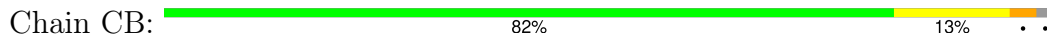




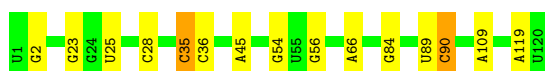




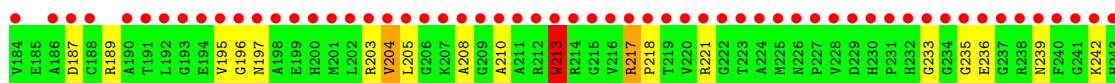
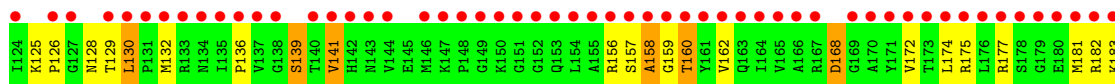
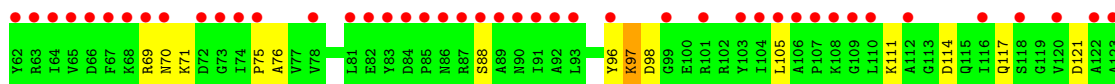
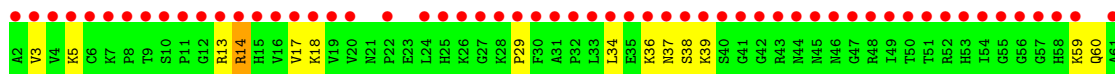
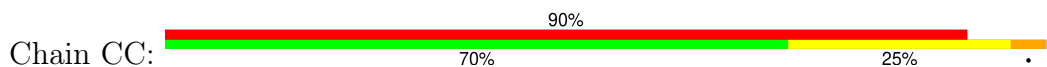
- Molecule 23: 5S rRNA



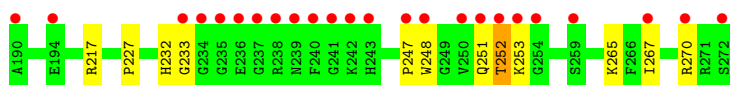
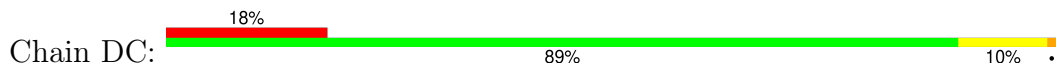
- Molecule 23: 5S rRNA



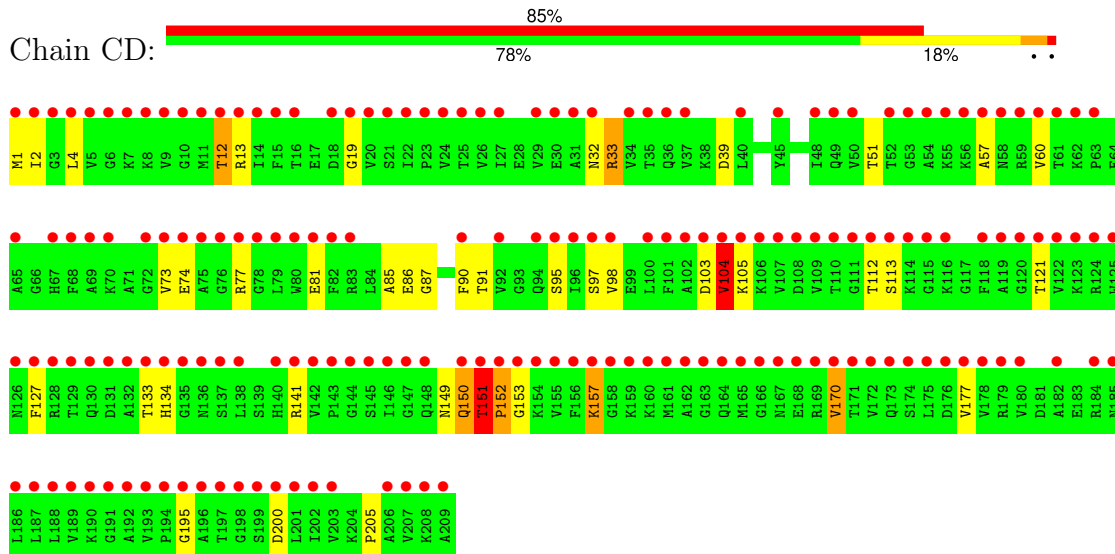
- Molecule 24: 50S ribosomal protein L2



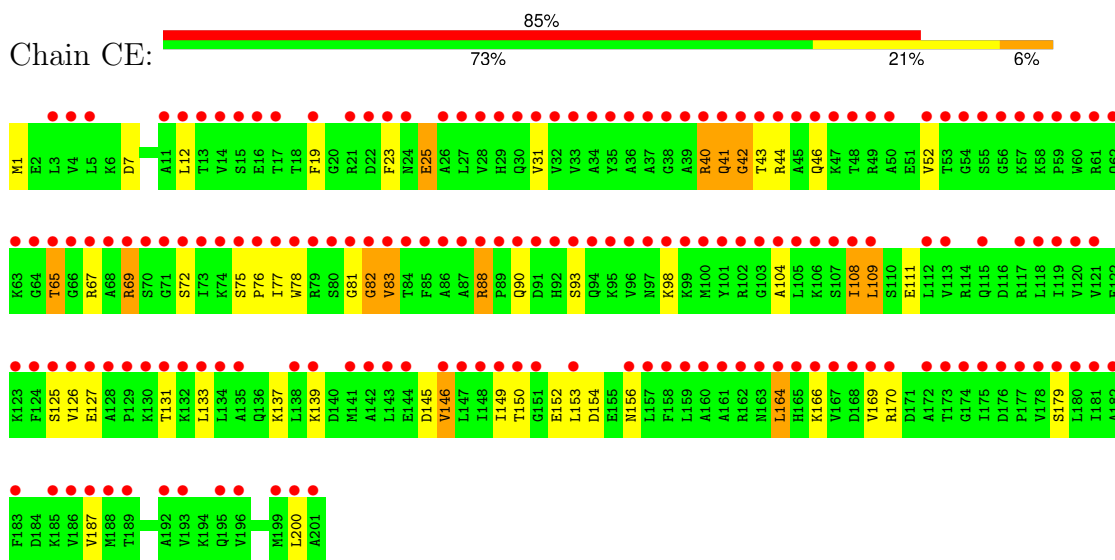
- Molecule 24: 50S ribosomal protein L2



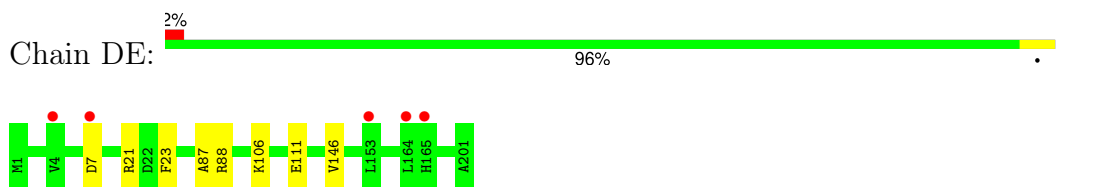
• Molecule 25: 50S ribosomal protein L3



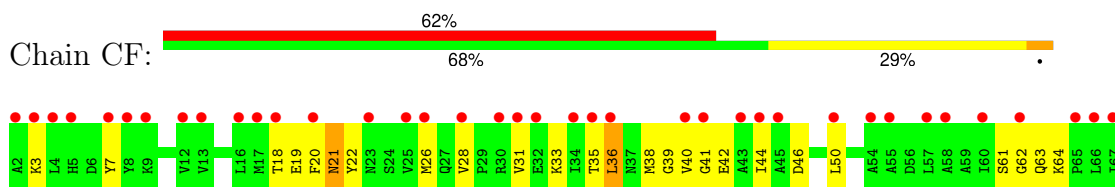
• Molecule 26: 50S ribosomal protein L4

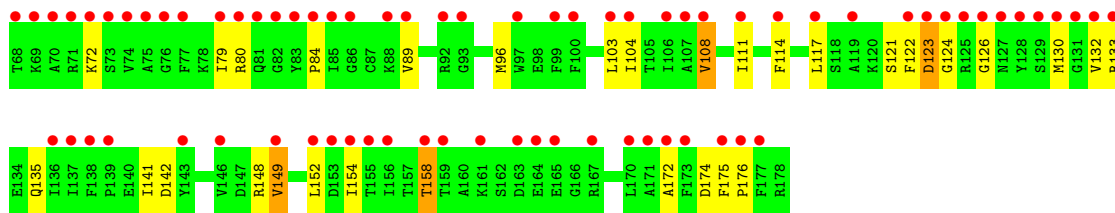


• Molecule 26: 50S ribosomal protein L4

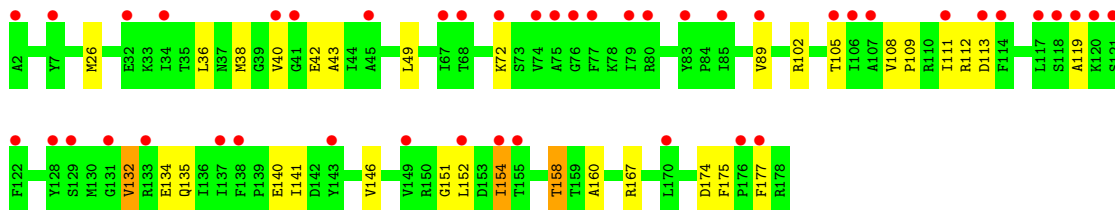
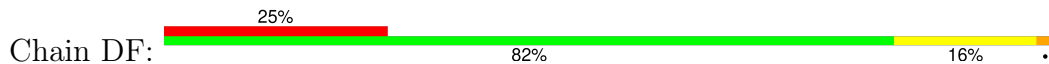


• Molecule 27: 50S ribosomal protein L5

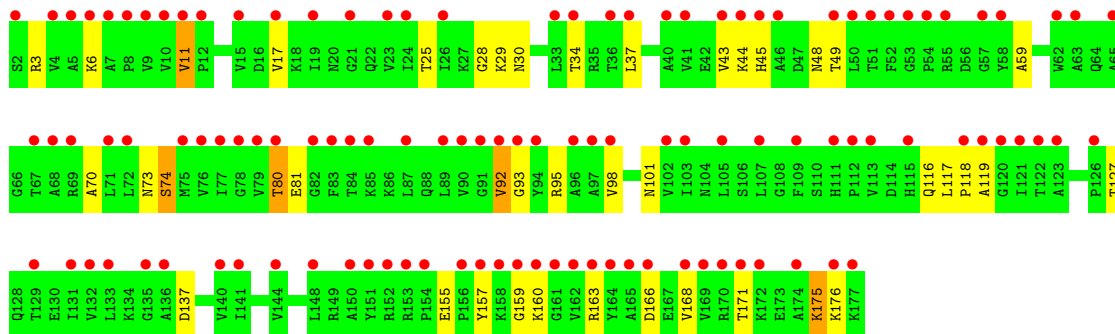
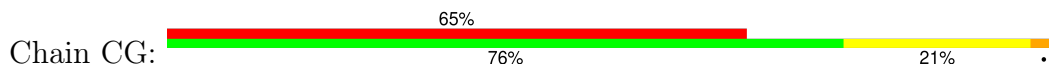




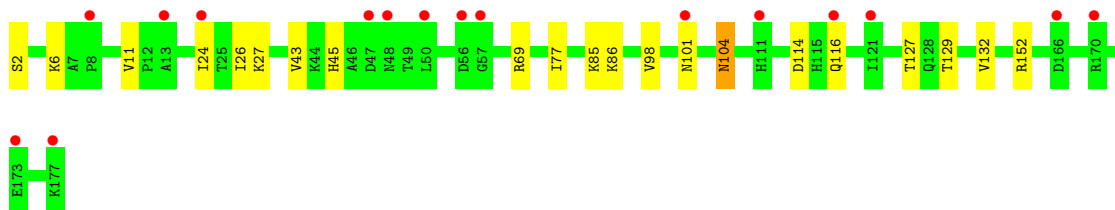
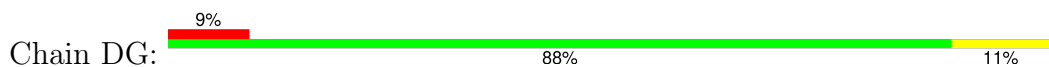
● Molecule 27: 50S ribosomal protein L5



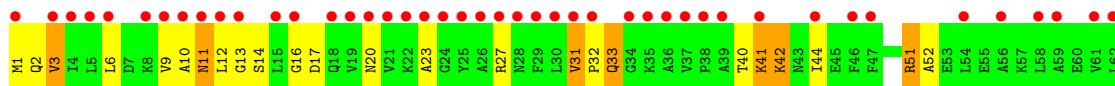
● Molecule 28: 50S ribosomal protein L6

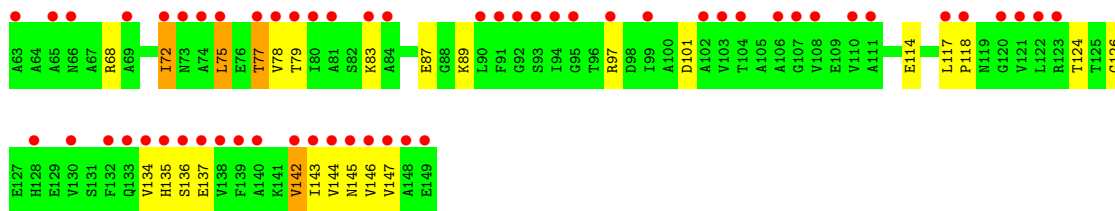


● Molecule 28: 50S ribosomal protein L6

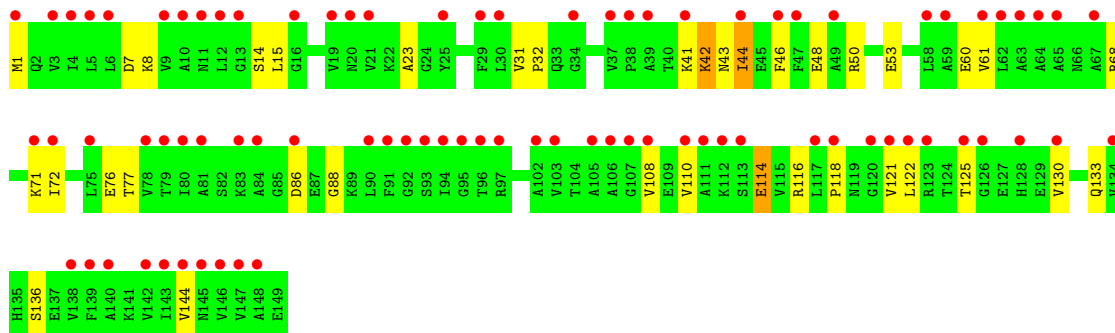
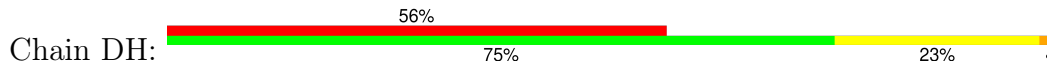


● Molecule 29: 50S ribosomal protein L9

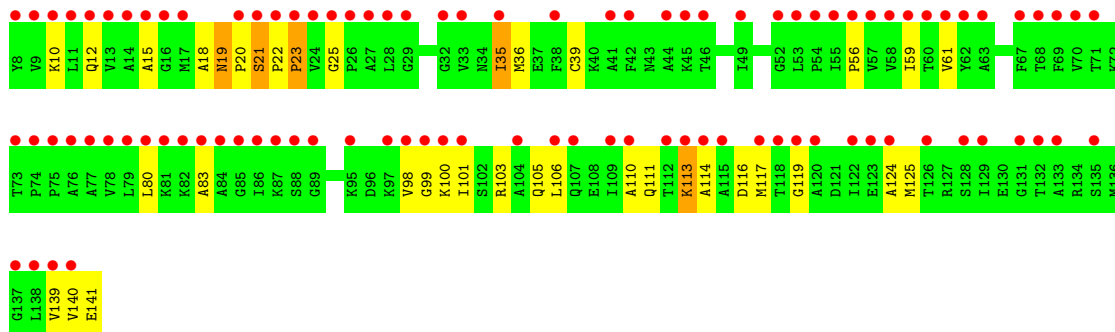
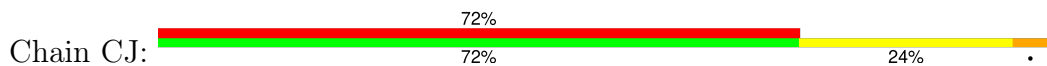




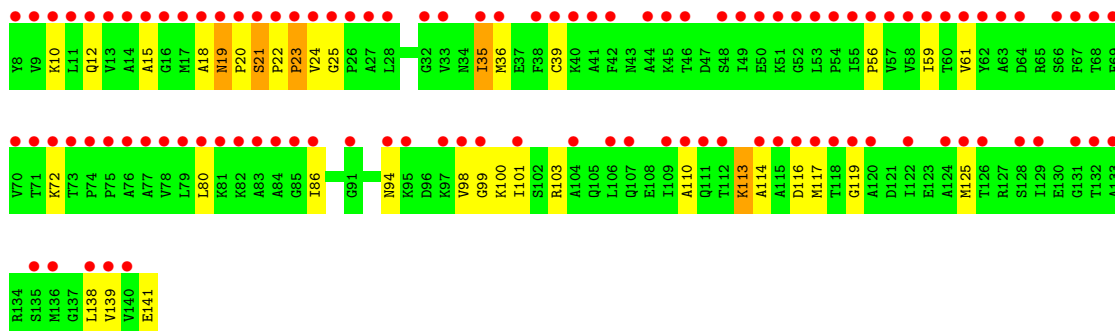
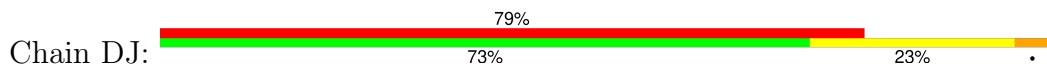
● Molecule 29: 50S ribosomal protein L9



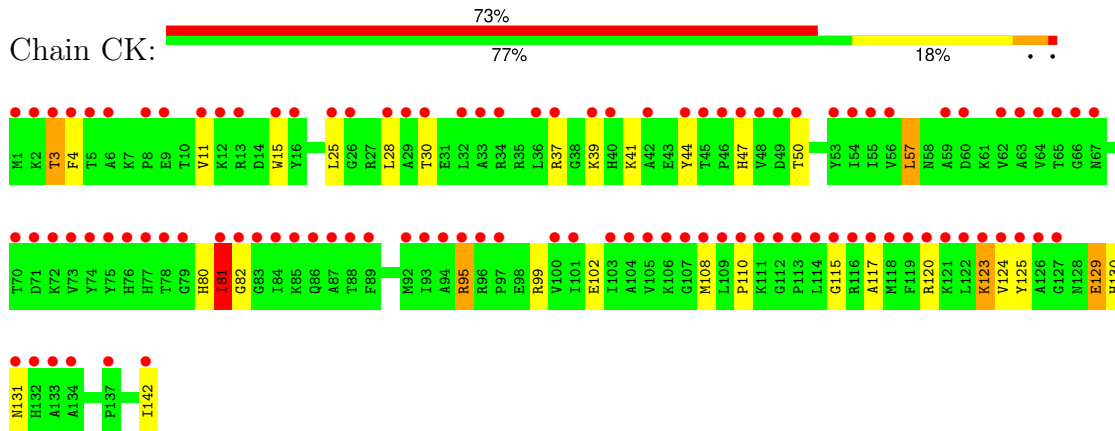
● Molecule 30: 50S ribosomal protein L11



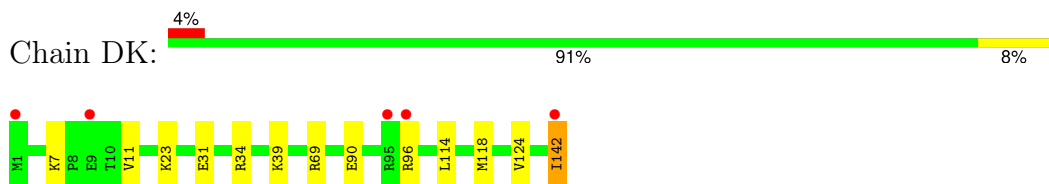
● Molecule 30: 50S ribosomal protein L11



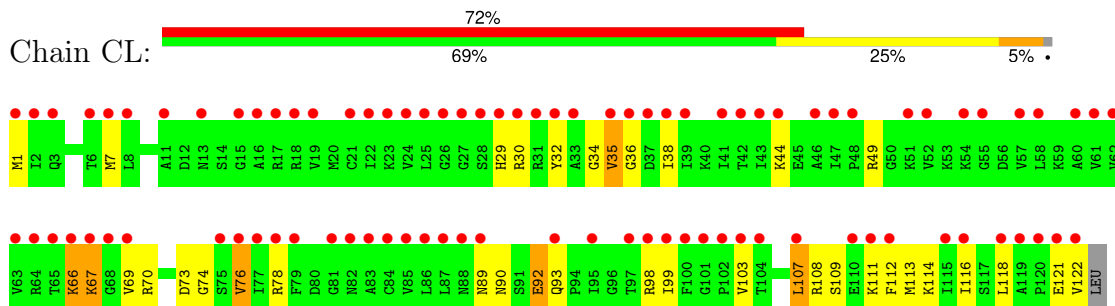
- Molecule 31: 50S ribosomal protein L13



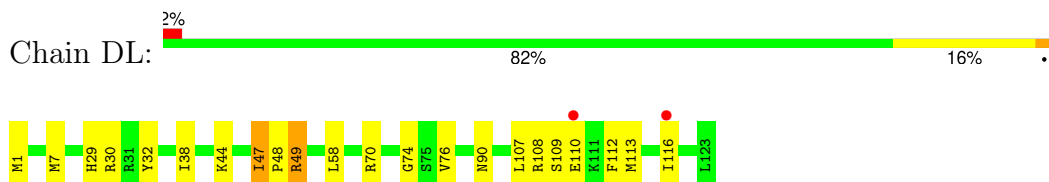
- Molecule 31: 50S ribosomal protein L13



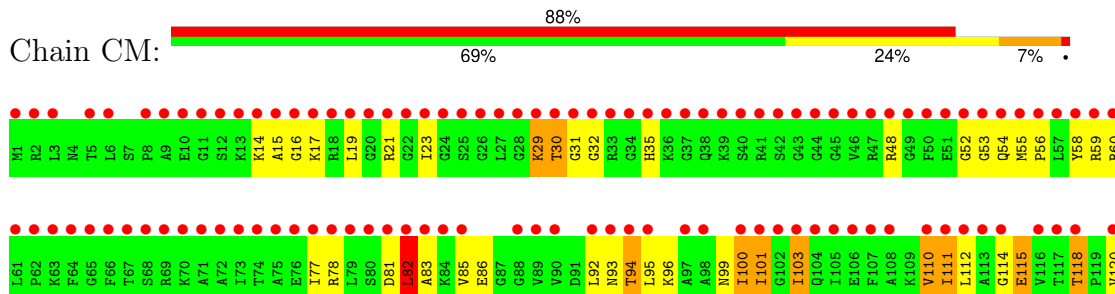
- Molecule 32: 50S ribosomal protein L14

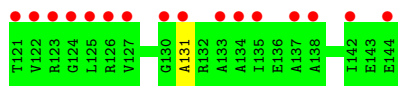


- Molecule 32: 50S ribosomal protein L14

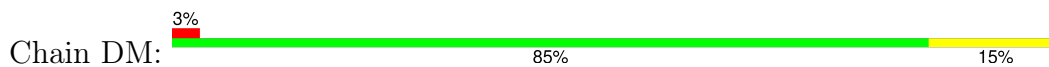


- Molecule 33: 50S ribosomal protein L15

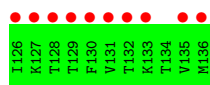
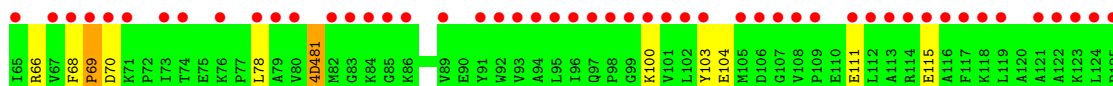
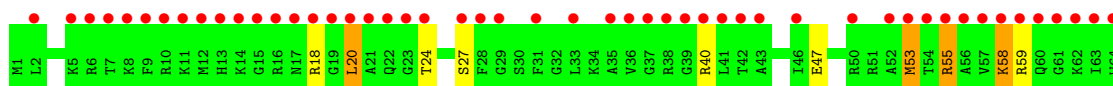
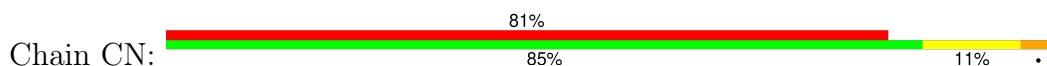




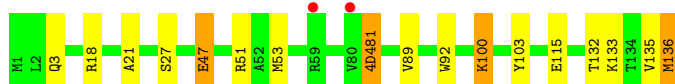
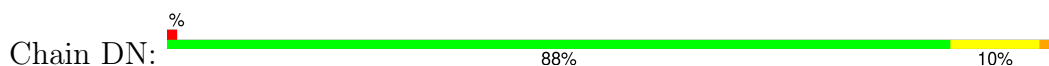
- Molecule 33: 50S ribosomal protein L15



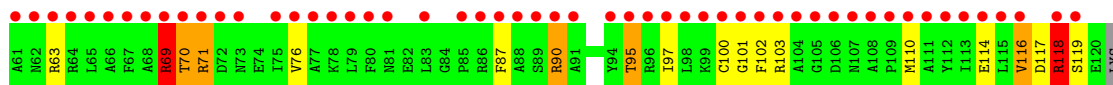
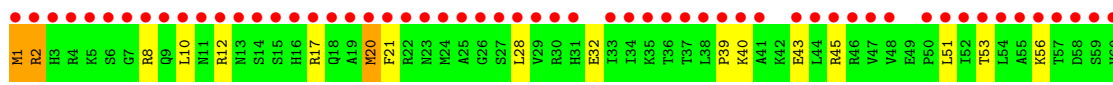
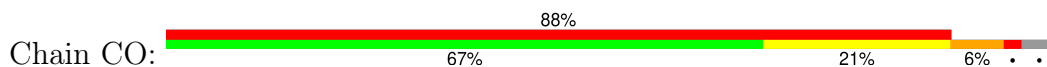
- Molecule 34: 50S ribosomal protein L16



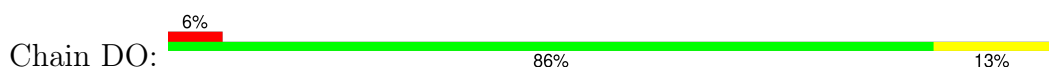
- Molecule 34: 50S ribosomal protein L16

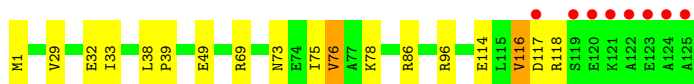


- Molecule 35: 50S ribosomal protein L17

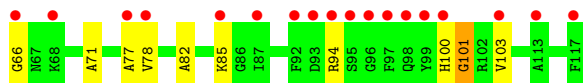
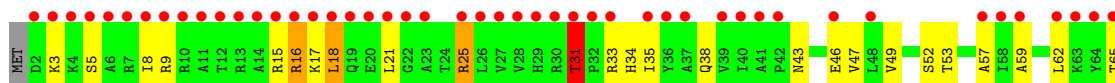


- Molecule 35: 50S ribosomal protein L17

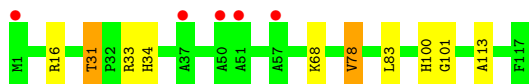




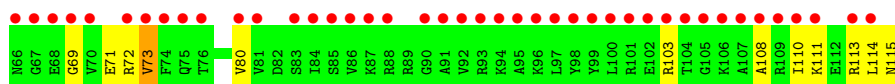
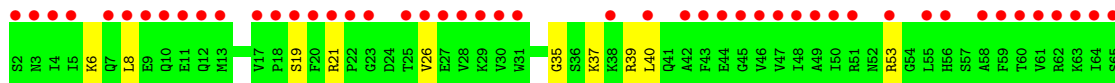
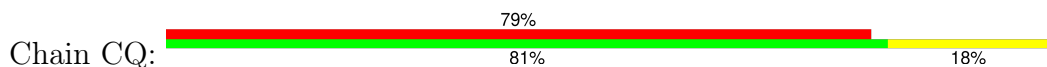
- Molecule 36: 50S ribosomal protein L18



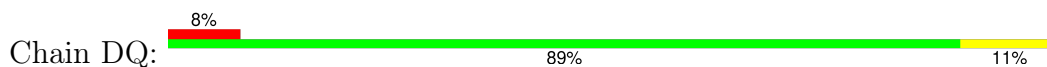
- Molecule 36: 50S ribosomal protein L18



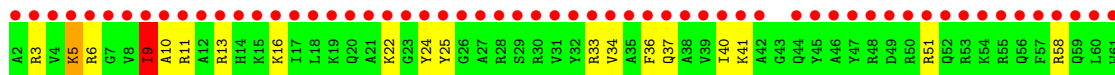
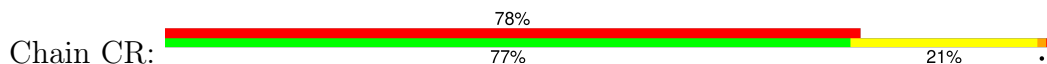
- Molecule 37: 50S ribosomal protein L19

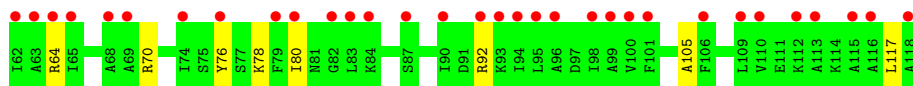


- Molecule 37: 50S ribosomal protein L19

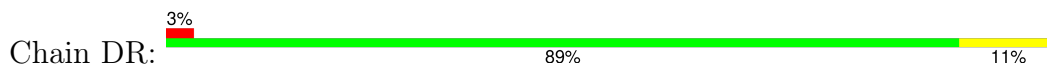


- Molecule 38: 50S ribosomal protein L20

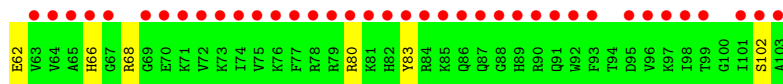
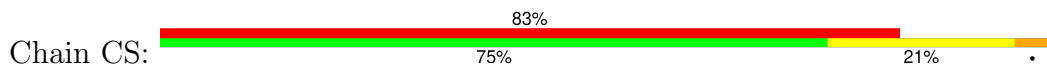




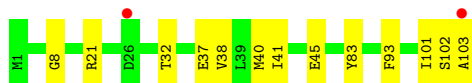
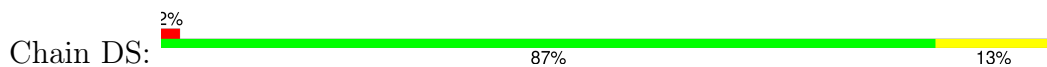
- Molecule 38: 50S ribosomal protein L20



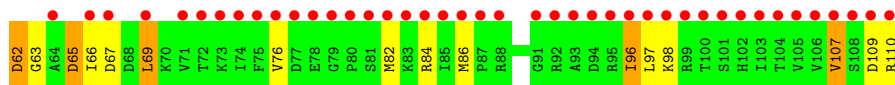
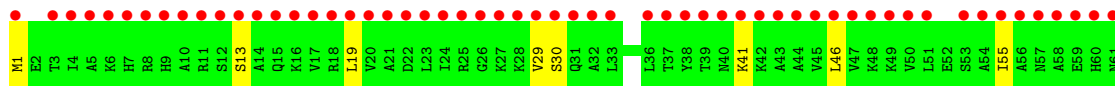
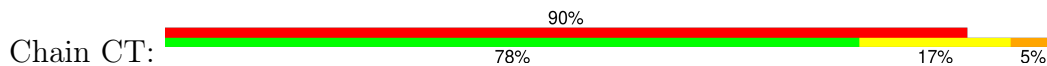
- Molecule 39: 50S ribosomal protein L21



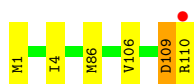
- Molecule 39: 50S ribosomal protein L21



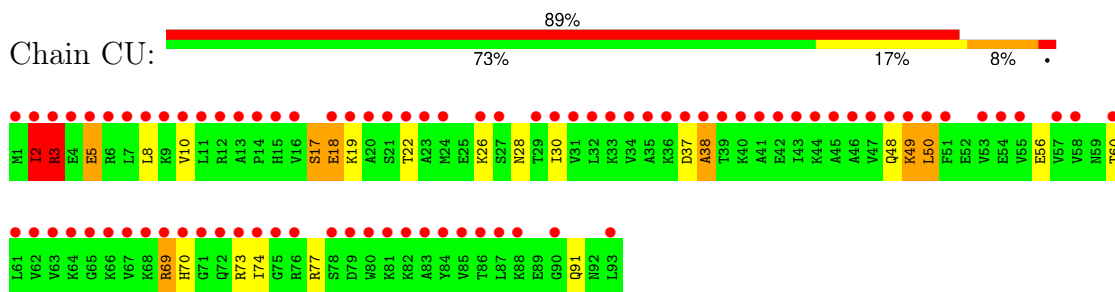
- Molecule 40: 50S ribosomal protein L22



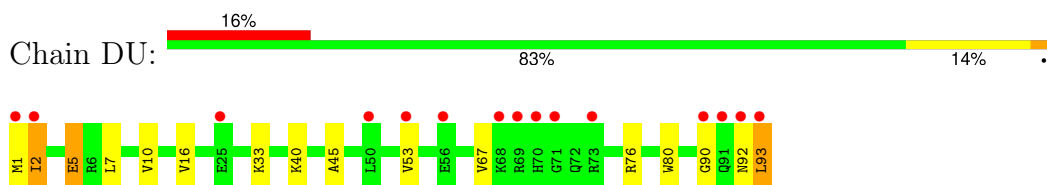
- Molecule 40: 50S ribosomal protein L22



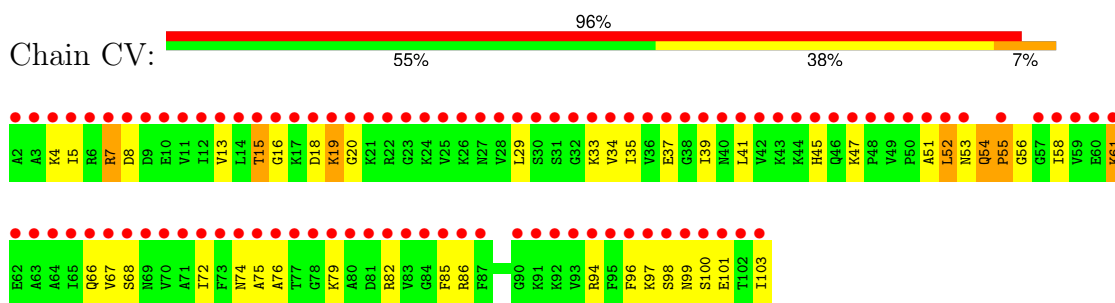
- Molecule 41: 50S ribosomal protein L23



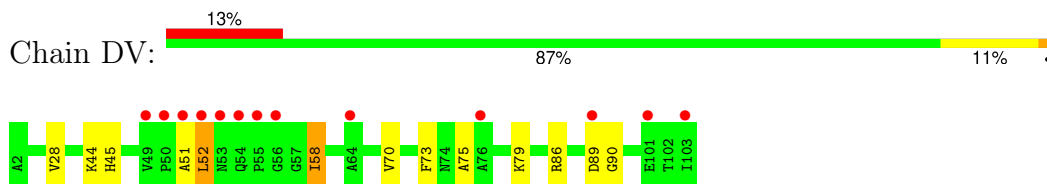
- Molecule 41: 50S ribosomal protein L23



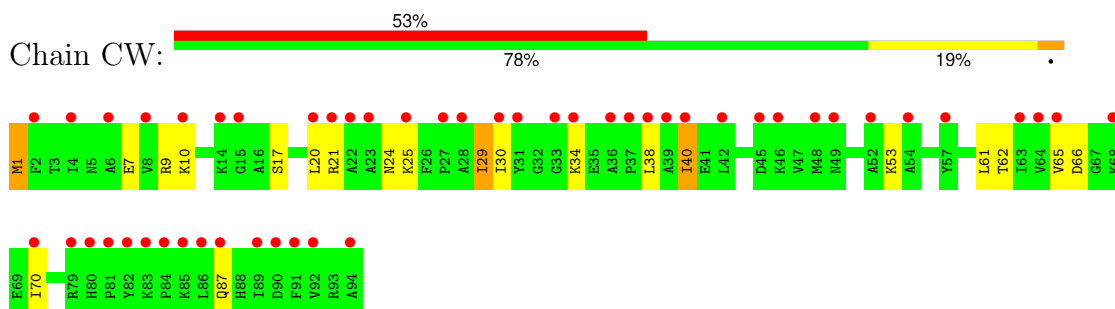
- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25

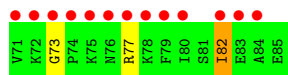
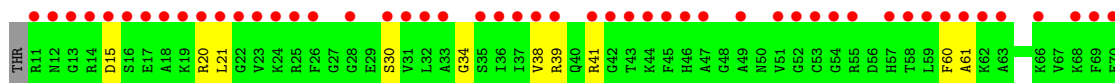
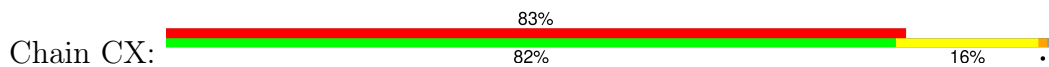


- Molecule 43: 50S ribosomal protein L25

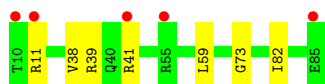
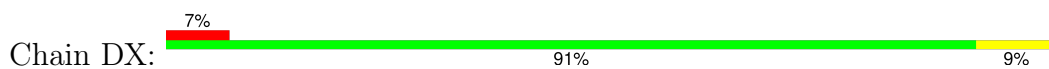




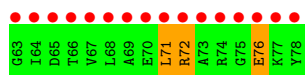
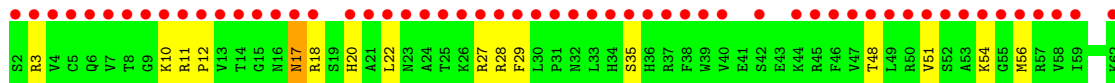
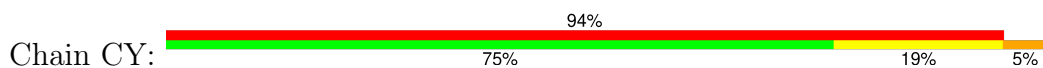
- Molecule 44: 50S ribosomal protein L27



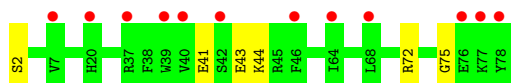
- Molecule 44: 50S ribosomal protein L27



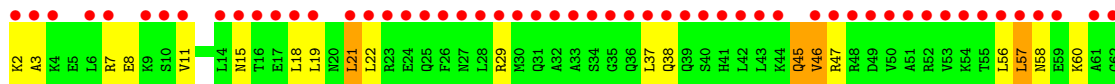
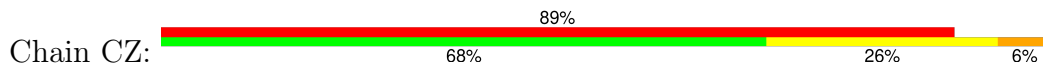
- Molecule 45: 50S ribosomal protein L28



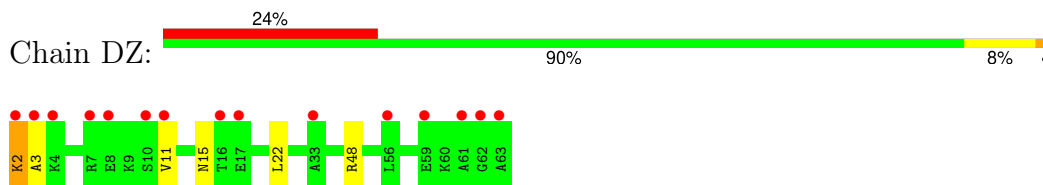
- Molecule 45: 50S ribosomal protein L28



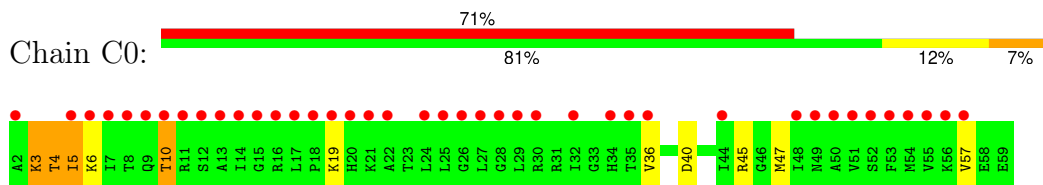
- Molecule 46: 50S ribosomal protein L29



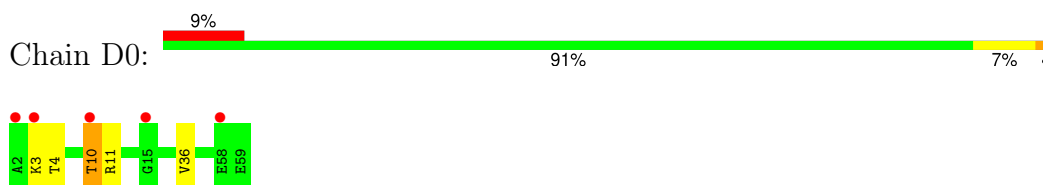
- Molecule 46: 50S ribosomal protein L29



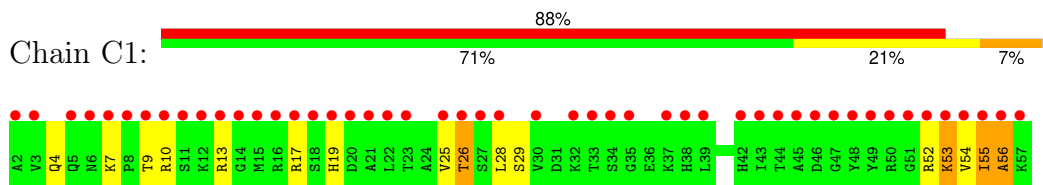
- Molecule 47: 50S ribosomal protein L30



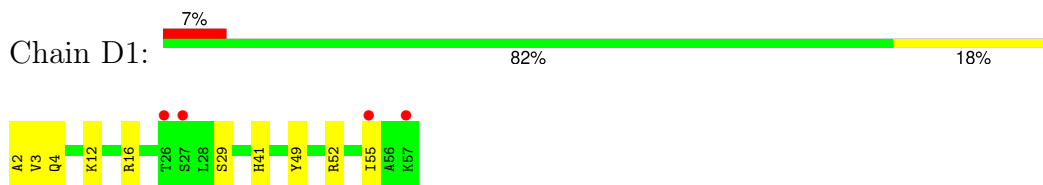
- Molecule 47: 50S ribosomal protein L30



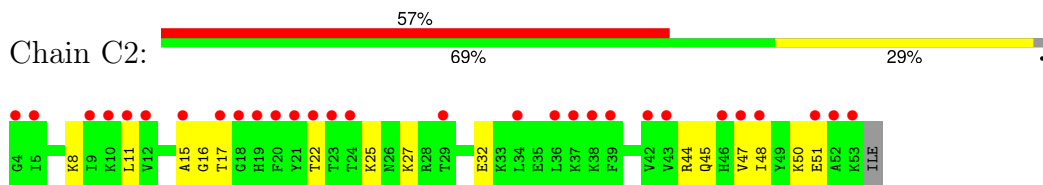
- Molecule 48: 50S ribosomal protein L32



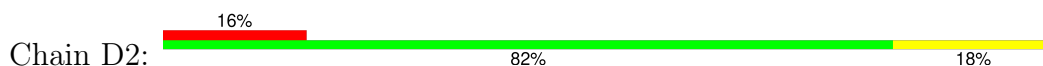
- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33

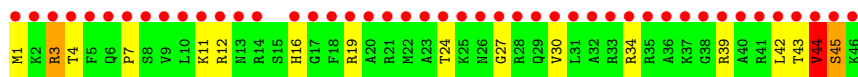


- Molecule 49: 50S ribosomal protein L33

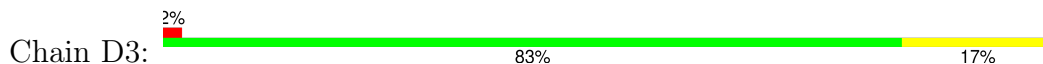




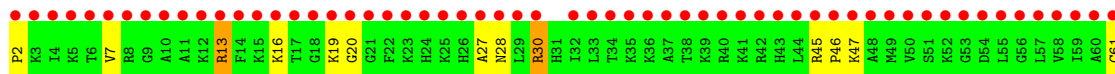
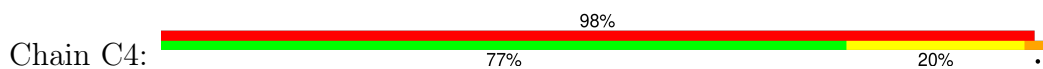
- Molecule 50: 50S ribosomal protein L34



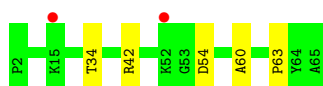
- Molecule 50: 50S ribosomal protein L34



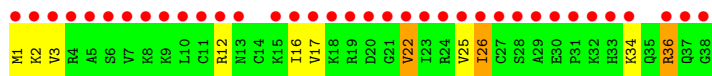
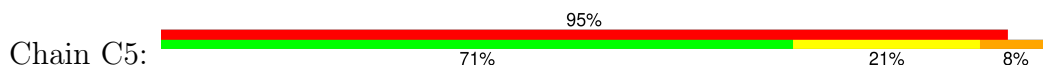
- Molecule 51: 50S ribosomal protein L35



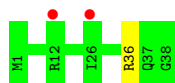
- Molecule 51: 50S ribosomal protein L35



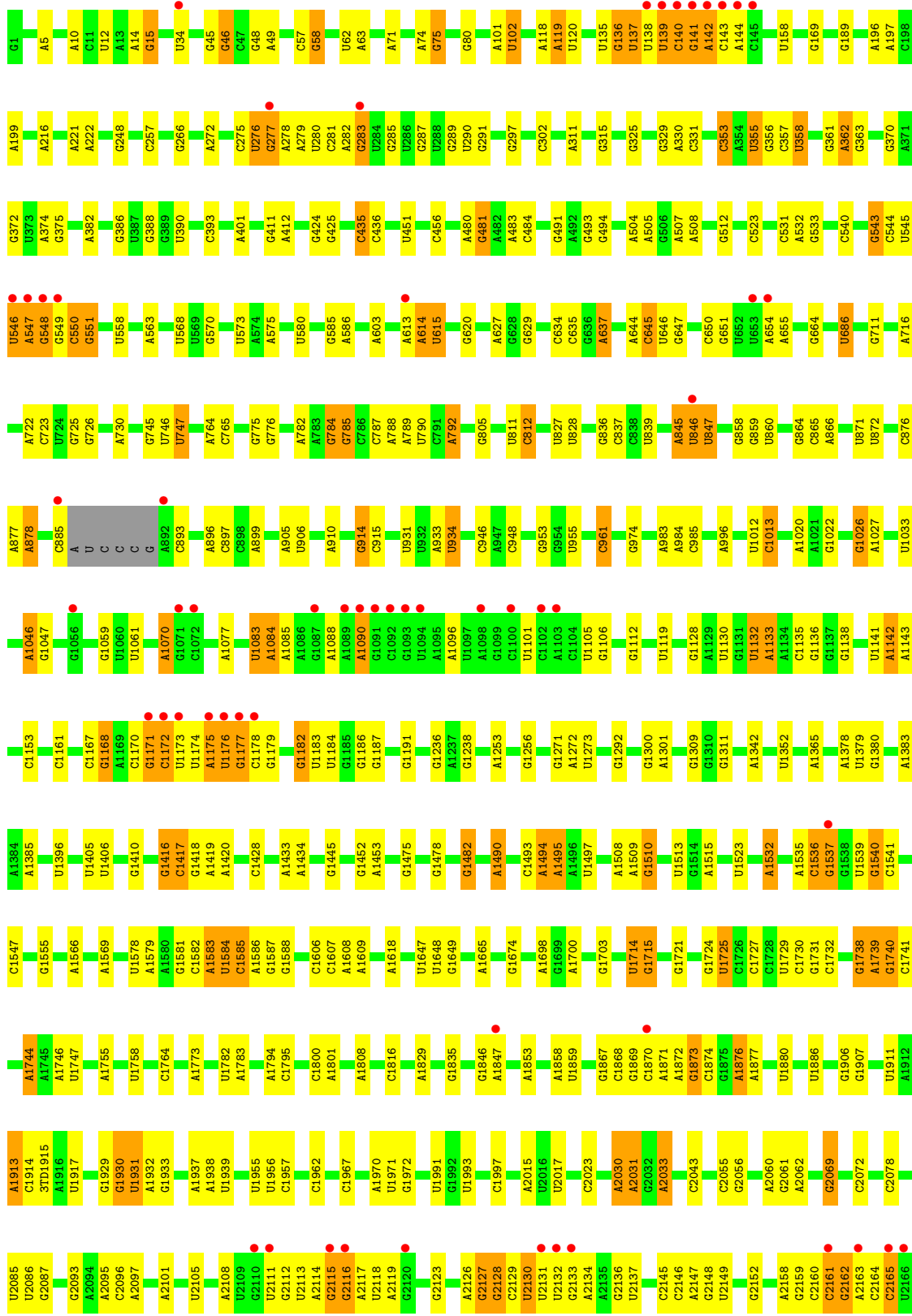
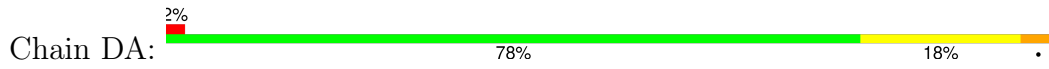
- Molecule 52: 50S ribosomal protein L36

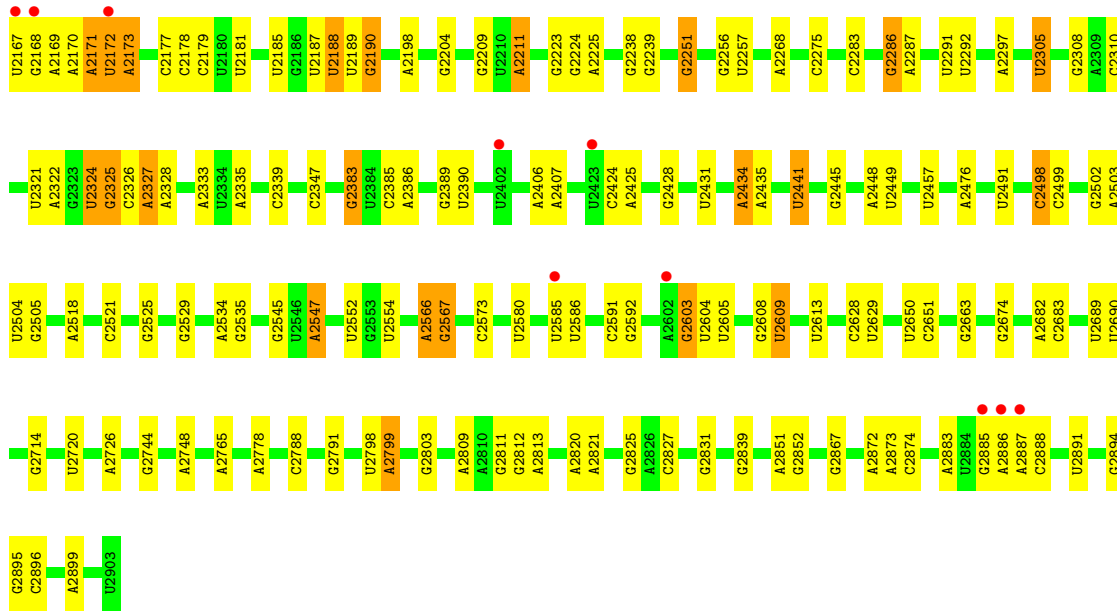


- Molecule 52: 50S ribosomal protein L36

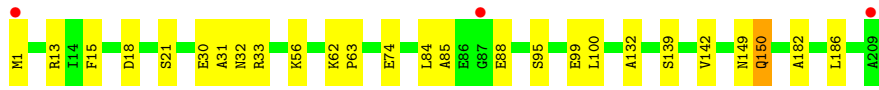
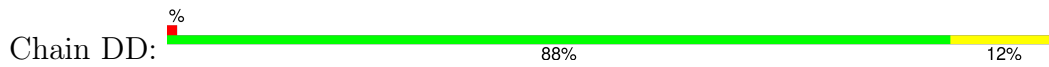


● Molecule 53: 23S rRNA

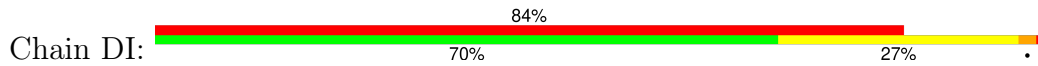




● Molecule 54: 50S ribosomal protein L3



● Molecule 55: 50S ribosomal protein L10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.17Å 433.89Å 624.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.39 – 2.10 69.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (69.39-2.10) 93.0 (69.39-2.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.10Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.218 , 0.234 0.235 , 0.246	Depositor DCC
$R_{free}$ test set	10048 reflections (0.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	295060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: OMG, 2MA, MA6, SPD, TRS, OMC, PSU, 6MZ, PEG, 4OC, ZN, 1MG, PUT, H2U, 3TD, 2MG, MG, 5MC, MPD, GUN, 5MU, ACY, MEQ, D2T, EDO, OMU, 1PE, 4D4, G7M, PG4, PGE, UR3

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	0.32	0/36593	0.48	0/57081
1	BA	0.30	1/36568 (0.0%)	0.58	8/57042 (0.0%)
2	AB	0.48	0/1784	0.82	1/2403 (0.0%)
2	BB	0.48	0/1784	0.92	1/2403 (0.0%)
3	AC	0.47	0/1652	0.80	0/2225
3	BC	0.57	0/1652	1.12	10/2225 (0.4%)
4	AD	0.46	0/1665	0.76	0/2227
4	BD	0.54	0/1665	0.78	0/2227
5	AE	0.59	0/1157	0.88	2/1557 (0.1%)
5	BE	0.75	0/1118	1.49	16/1504 (1.1%)
6	AF	0.51	0/881	0.82	1/1189 (0.1%)
6	BF	0.65	0/835	1.18	4/1128 (0.4%)
7	AG	0.44	0/1196	0.78	0/1602
7	BG	0.56	0/1196	1.26	8/1602 (0.5%)
8	AH	0.55	0/989	0.84	0/1326
8	BH	0.54	0/989	1.12	6/1326 (0.5%)
9	AI	0.48	0/1034	0.84	0/1375
9	BI	0.42	0/1034	0.88	2/1375 (0.1%)
10	AJ	0.66	0/806	0.90	0/1089
10	BJ	0.90	0/797	0.92	2/1077 (0.2%)
11	AK	0.50	0/893	0.77	0/1205
11	BK	0.60	0/893	1.22	10/1205 (0.8%)
12	AL	0.59	0/960	0.79	0/1286
12	BL	0.64	0/960	1.16	8/1286 (0.6%)
13	AM	0.49	0/893	0.85	0/1193
13	BM	0.54	0/893	1.34	9/1193 (0.8%)
14	AN	0.54	0/817	0.86	1/1088 (0.1%)
14	BN	0.61	0/817	1.03	6/1088 (0.6%)
15	AO	0.51	0/722	0.71	0/964
15	BO	0.57	0/722	1.12	3/964 (0.3%)
16	AP	0.52	0/659	0.85	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	BP	0.64	0/659	1.18	4/884 (0.5%)
17	AQ	0.55	0/658	0.83	1/881 (0.1%)
17	BQ	0.59	0/658	1.12	3/881 (0.3%)
18	AR	0.49	0/463	0.77	0/621
18	BR	0.63	0/463	1.28	2/621 (0.3%)
19	AS	0.47	0/653	0.82	2/877 (0.2%)
19	BS	0.53	0/653	1.22	6/877 (0.7%)
20	AT	0.52	0/676	0.83	0/895
20	BT	0.56	0/671	1.29	6/888 (0.7%)
21	AU	0.58	0/472	0.78	0/627
21	BU	0.53	0/472	0.80	0/627
22	CA	0.29	0/69165	0.57	17/107896 (0.0%)
23	CB	0.24	0/2828	0.49	0/4410
23	DB	0.44	0/2872	0.56	0/4478
24	CC	0.53	0/2122	1.03	9/2852 (0.3%)
24	DC	0.73	0/2122	0.91	2/2852 (0.1%)
25	CD	0.55	0/1586	1.00	2/2134 (0.1%)
26	CE	0.51	0/1571	1.04	5/2113 (0.2%)
26	DE	0.74	0/1571	0.86	1/2113 (0.0%)
27	CF	0.48	0/1435	1.10	5/1926 (0.3%)
27	DF	0.59	0/1435	0.86	0/1926
28	CG	0.52	0/1343	0.76	0/1816
28	DG	0.65	0/1343	0.87	0/1816
29	CH	0.48	0/1121	0.82	1/1515 (0.1%)
29	DH	0.51	0/1121	0.82	1/1515 (0.1%)
30	CJ	0.68	0/993	0.96	3/1341 (0.2%)
30	DJ	0.71	0/993	1.01	3/1341 (0.2%)
31	CK	0.46	0/1152	0.78	0/1551
31	DK	0.89	0/1152	0.93	0/1551
32	CL	0.48	0/947	0.93	1/1268 (0.1%)
32	DL	0.83	0/955	1.00	3/1279 (0.2%)
33	CM	0.56	0/1062	1.34	13/1413 (0.9%)
33	DM	0.81	0/1062	0.91	1/1413 (0.1%)
34	CN	0.43	0/1081	0.90	0/1443
34	DN	0.80	0/1092	0.90	2/1457 (0.1%)
35	CO	0.51	0/973	1.11	4/1301 (0.3%)
35	DO	0.90	0/1006	1.00	0/1345
36	CP	0.49	0/902	1.11	7/1209 (0.6%)
36	DP	0.64	0/910	0.85	1/1219 (0.1%)
37	CQ	0.47	0/929	0.97	2/1242 (0.2%)
37	DQ	0.79	0/929	0.85	0/1242
38	CR	0.51	1/960 (0.1%)	0.92	0/1278
38	DR	0.94	1/960 (0.1%)	0.93	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	CS	0.48	0/829	1.05	6/1107 (0.5%)
39	DS	0.89	0/829	0.88	0/1107
40	CT	0.53	0/864	1.08	2/1156 (0.2%)
40	DT	0.94	0/864	0.90	0/1156
41	CU	0.53	0/745	1.20	6/994 (0.6%)
41	DU	0.76	0/745	0.97	1/994 (0.1%)
42	CV	0.56	0/788	1.19	2/1051 (0.2%)
42	DV	0.69	0/788	0.91	0/1051
43	CW	0.39	0/766	0.85	0/1025
43	DW	0.77	0/766	0.83	0/1025
44	CX	0.46	0/576	0.91	2/762 (0.3%)
44	DX	0.86	0/598	0.91	2/790 (0.3%)
45	CY	0.47	0/635	0.93	1/848 (0.1%)
45	DY	0.75	0/635	0.87	0/848
46	CZ	0.43	0/502	1.05	1/667 (0.1%)
46	DZ	0.61	0/502	0.84	0/667
47	C0	0.48	0/453	0.98	1/605 (0.2%)
47	D0	0.90	0/467	0.85	0/623
48	C1	0.52	0/450	1.03	2/599 (0.3%)
48	D1	0.87	0/450	0.92	0/599
49	C2	0.54	0/416	0.95	0/554
49	D2	0.71	0/421	0.86	0/561
50	C3	0.58	0/380	1.07	0/498
50	D3	0.85	0/380	0.99	0/498
51	C4	0.51	0/513	1.04	0/676
51	D4	0.78	0/513	0.86	0/676
52	C5	0.54	0/303	1.18	2/397 (0.5%)
52	D5	0.84	0/303	0.91	0/397
53	DA	0.56	0/69295	0.65	1/108100 (0.0%)
54	DD	0.92	1/1576 (0.1%)	0.97	3/2119 (0.1%)
55	DI	0.51	0/1037	0.90	1/1402 (0.1%)
All	All	0.48	4/309204 (0.0%)	0.71	239/462103 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BA	0	1
6	BF	0	1
24	DC	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	CD	0	1
30	CJ	0	1
30	DJ	0	1
32	CL	0	1
47	C0	0	1
47	D0	0	1
55	DI	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	CR	9	ILE	CA-CB	6.38	1.62	1.54
38	DR	42	ALA	CA-CB	-5.63	1.44	1.53
54	DD	132	ALA	CA-CB	-5.20	1.44	1.53
1	BA	1498	UR3	O3'-P	5.15	1.61	1.56

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BE	104	GLY	N-CA-C	13.54	137.28	112.37
33	CM	101	ILE	N-CA-C	11.91	124.33	112.90
33	CM	52	GLY	N-CA-C	-11.27	94.98	112.45
41	CU	3	ARG	N-CA-C	-10.66	90.52	108.75
33	CM	103	ILE	N-CA-C	9.97	123.51	111.05

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BA	702	A	Sidechain
6	BF	90	MET	Peptide
25	CD	151	THR	Peptide
30	CJ	98	VAL	Peptide
32	CL	34	GLY	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	193	0
1	BA	32908	0	16580	237	0
2	AB	1753	0	1780	29	0
2	BB	1753	0	1780	30	0
3	AC	1625	0	1696	16	0
3	BC	1625	0	1696	36	0
4	AD	1643	0	1707	20	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	33	0
5	BE	1105	0	1148	66	0
6	AF	862	0	864	16	0
6	BF	817	0	808	24	0
7	AG	1182	0	1238	24	0
7	BG	1182	0	1238	36	0
8	AH	979	0	1031	20	0
8	BH	979	0	1031	21	0
9	AI	1022	0	1070	29	0
9	BI	1022	0	1070	26	0
10	AJ	796	0	836	40	0
10	BJ	787	0	828	21	0
11	AK	877	0	887	14	0
11	BK	877	0	887	29	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	22	0
13	AM	884	0	941	33	0
13	BM	884	0	941	27	0
14	AN	805	0	844	30	0
14	BN	805	0	844	43	0
15	AO	714	0	734	8	0
15	BO	714	0	734	25	0
16	AP	649	0	666	6	0
16	BP	649	0	666	11	0
17	AQ	649	0	691	8	0
17	BQ	649	0	691	22	0
18	AR	456	0	478	9	0
18	BR	456	0	478	13	0
19	AS	638	0	665	16	0
19	BS	638	0	665	29	0
20	AT	670	0	719	14	0
20	BT	665	0	714	13	0
21	AU	465	0	491	9	0
21	BU	465	0	491	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CA	62229	0	31319	415	0
23	CB	2529	0	1281	12	0
23	DB	2569	0	1301	10	0
24	CC	2083	0	2154	41	0
24	DC	2083	0	2154	18	0
25	CD	1565	0	1616	34	0
26	CE	1552	0	1619	28	0
26	DE	1552	0	1619	3	0
27	CF	1411	0	1444	22	0
27	DF	1411	0	1444	21	0
28	CG	1323	0	1371	9	0
28	DG	1323	0	1371	7	0
29	CH	1110	0	1148	15	0
29	DH	1110	0	1148	15	0
30	CJ	979	0	1028	27	0
30	DJ	979	0	1028	30	0
31	CK	1129	0	1162	17	0
31	DK	1129	0	1162	6	0
32	CL	938	0	1012	27	0
32	DL	946	0	1023	13	0
33	CM	1053	0	1129	33	0
33	DM	1053	0	1129	11	0
34	CN	1075	0	1155	9	0
34	DN	1092	0	1179	13	0
35	CO	960	0	1000	21	0
35	DO	993	0	1034	10	0
36	CP	892	0	923	15	0
36	DP	900	0	935	9	0
37	CQ	917	0	962	7	0
37	DQ	917	0	962	9	0
38	CR	947	0	1019	25	0
38	DR	947	0	1019	13	0
39	CS	816	0	839	10	0
39	DS	816	0	839	7	0
40	CT	857	0	922	8	0
40	DT	857	0	922	3	0
41	CU	739	0	807	19	0
41	DU	739	0	807	17	0
42	CV	780	0	831	27	0
42	DV	780	0	831	5	0
43	CW	753	0	780	8	0
43	DW	753	0	780	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	CX	569	0	581	7	0
44	DX	591	0	606	4	0
45	CY	625	0	652	11	0
45	DY	625	0	652	3	0
46	CZ	501	0	531	10	0
46	DZ	501	0	531	4	0
47	C0	449	0	488	3	0
47	D0	463	0	504	1	0
48	C1	444	0	458	12	0
48	D1	444	0	458	6	0
49	C2	409	0	440	7	0
49	D2	414	0	442	7	0
50	C3	377	0	418	14	0
50	D3	377	0	418	10	0
51	C4	504	0	572	10	0
51	D4	504	0	572	5	0
52	C5	302	0	340	8	0
52	D5	302	0	340	0	0
53	DA	62361	0	31381	309	0
54	DD	1576	0	1627	18	0
55	DI	1023	0	1052	24	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	C3	1	0	0	0	0
56	CA	155	0	0	0	0
56	CB	3	0	0	0	0
56	DA	183	0	0	0	0
56	DB	9	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	2	0
57	DA	26	0	36	8	0
57	DQ	13	0	18	3	0
57	DR	13	0	18	10	0
57	DS	13	0	18	2	0
58	AA	16	0	28	0	0
58	DA	40	0	70	5	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	6	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AA	24	0	48	1	0
59	DA	66	0	132	16	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D3	7	0	10	5	0
61	DA	42	0	60	3	0
61	DL	7	0	10	0	0
61	DP	7	0	10	4	0
61	DQ	7	0	10	1	0
62	DA	40	0	76	7	0
63	DA	32	0	44	4	0
64	D1	10	0	14	0	0
64	D3	10	0	14	0	0
64	DA	50	0	70	3	0
64	DS	10	0	14	0	0
64	DU	10	0	14	1	0
65	DA	12	0	9	1	0
66	D0	4	0	6	0	0
66	D1	4	0	6	0	0
66	DA	24	0	36	11	0
66	DB	12	0	18	1	0
66	DR	4	0	6	0	0
67	DA	11	0	5	1	0
68	DA	8	0	12	0	0
69	AA	509	0	0	9	0
69	AC	6	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	2	0
69	AS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AT	2	0	0	0	0
69	AU	2	0	0	0	0
69	BA	286	0	0	16	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	2	0	0	0	0
69	BL	5	0	0	1	0
69	BN	3	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	1	0
69	BT	5	0	0	0	0
69	BU	2	0	0	0	0
69	C3	2	0	0	1	0
69	C4	1	0	0	0	0
69	CA	692	0	0	56	0
69	CB	13	0	0	1	0
69	CC	8	0	0	0	0
69	CD	6	0	0	0	0
69	CE	6	0	0	2	0
69	CK	1	0	0	0	0
69	CL	1	0	0	1	0
69	CM	5	0	0	0	0
69	CO	1	0	0	0	0
69	CS	1	0	0	0	0
69	CU	2	0	0	1	0
69	CV	2	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	25	0	0	0	0
69	D1	47	0	0	3	0
69	D2	9	0	0	1	0
69	D3	25	0	0	0	0
69	D4	38	0	0	2	0
69	D5	14	0	0	0	0
69	DA	4815	0	0	46	0
69	DB	209	0	0	2	0
69	DC	106	0	0	2	0
69	DD	103	0	0	1	0
69	DE	62	0	0	0	0
69	DF	14	0	0	1	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DK	59	0	0	1	0
69	DL	45	0	0	1	0
69	DM	67	0	0	0	0
69	DN	74	0	0	0	0
69	DO	42	0	0	1	0
69	DP	37	0	0	1	0
69	DQ	27	0	0	2	0
69	DR	67	0	0	1	0
69	DS	50	0	0	1	0
69	DT	61	0	0	0	0
69	DU	19	0	0	0	0
69	DV	22	0	0	0	0
69	DW	32	0	0	0	0
69	DX	30	0	0	2	0
69	DY	10	0	0	1	0
69	DZ	8	0	0	0	0
All	All	295060	0	194384	2516	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 5.

The worst 5 of 2516 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)
14:BN:26:GLU:OE2	14:BN:26:GLU:N	1.97	0.96
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.44	0.94
14:AN:64:CYS:SG	69:AN:204:HOH:O	2.25	0.94
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.50	0.94
22:CA:1652:A:OP1	35:CO:8:ARG:NH2	2.04	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	209 (94%)	11 (5%)	2 (1%)	14	10
2	BB	222/224 (99%)	209 (94%)	11 (5%)	2 (1%)	14	10
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	24	22
3	BC	204/206 (99%)	186 (91%)	10 (5%)	8 (4%)	2	0
4	AD	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
4	BD	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
5	AE	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
5	BE	148/155 (96%)	122 (82%)	14 (10%)	12 (8%)	1	0
6	AF	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	3	1
7	AG	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	18	15
7	BG	149/151 (99%)	131 (88%)	15 (10%)	3 (2%)	6	2
8	AH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
8	BH	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	12
9	AI	125/127 (98%)	111 (89%)	13 (10%)	1 (1%)	16	12
9	BI	125/127 (98%)	111 (89%)	13 (10%)	1 (1%)	16	12
10	AJ	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	12	9
10	BJ	96/99 (97%)	63 (66%)	22 (23%)	11 (12%)	0	0
11	AK	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
11	BK	115/117 (98%)	100 (87%)	11 (10%)	4 (4%)	3	1
12	AL	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
12	BL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	7	3
13	AM	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	4	1
13	BM	112/114 (98%)	95 (85%)	10 (9%)	7 (6%)	1	0
14	AN	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
14	BN	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
15	AO	86/88 (98%)	80 (93%)	3 (4%)	3 (4%)	3	1
15	BO	86/88 (98%)	79 (92%)	2 (2%)	5 (6%)	1	0
16	AP	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	9	6
16	BP	80/82 (98%)	66 (82%)	11 (14%)	3 (4%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
17	BQ	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	1	0
18	AR	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	6	3
18	BR	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	3
19	AS	77/79 (98%)	69 (90%)	7 (9%)	1 (1%)	9	6
19	BS	77/79 (98%)	65 (84%)	9 (12%)	3 (4%)	2	0
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	77 (93%)	3 (4%)	3 (4%)	2	1
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
24	CC	269/271 (99%)	251 (93%)	15 (6%)	3 (1%)	11	8
24	DC	269/271 (99%)	253 (94%)	15 (6%)	1 (0%)	30	28
25	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	9	5
26	CE	199/201 (99%)	186 (94%)	9 (4%)	4 (2%)	6	2
26	DE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	CF	175/177 (99%)	155 (89%)	14 (8%)	6 (3%)	3	1
27	DF	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
28	CG	174/176 (99%)	135 (78%)	33 (19%)	6 (3%)	3	1
28	DG	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
29	CH	147/149 (99%)	116 (79%)	22 (15%)	9 (6%)	1	0
29	DH	147/149 (99%)	129 (88%)	16 (11%)	2 (1%)	9	5
30	CJ	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	3	1
30	DJ	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	3	1
31	CK	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	9	5
31	DK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
32	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	16	12
32	DL	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	12
33	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	2	0
33	DM	142/144 (99%)	138 (97%)	3 (2%)	1 (1%)	18	15
34	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	12
34	DN	134/136 (98%)	128 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	CO	118/125 (94%)	110 (93%)	5 (4%)	3 (2%)	4	1
35	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
36	CP	114/117 (97%)	105 (92%)	4 (4%)	5 (4%)	2	0
36	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	CQ	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	14	10
37	DQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
38	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
38	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
39	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	1
39	DS	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	CT	108/110 (98%)	101 (94%)	4 (4%)	3 (3%)	4	1
40	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	CU	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	3	1
41	DU	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	11	8
42	CV	100/102 (98%)	81 (81%)	11 (11%)	8 (8%)	1	0
42	DV	100/102 (98%)	96 (96%)	3 (3%)	1 (1%)	12	9
43	CW	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
43	DW	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
44	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
44	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
45	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
45	DY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
46	CZ	60/62 (97%)	52 (87%)	5 (8%)	3 (5%)	1	0
46	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
47	C0	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	6	3
47	D0	57/58 (98%)	54 (95%)	2 (4%)	1 (2%)	6	3
48	C1	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	2	1
48	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
49	C2	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	5	2
49	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
50	C3	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
51	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
52	C5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	D5	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
54	DD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
55	DI	133/135 (98%)	107 (80%)	19 (14%)	7 (5%)	1	0
All	All	11407/11629 (98%)	10507 (92%)	713 (6%)	187 (2%)	7	4

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	130	THR
3	AC	127	ARG
9	AI	25	ASN
10	AJ	57	VAL
13	AM	5	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	181 (97%)	5 (3%)	39	45
2	BB	186/186 (100%)	179 (96%)	7 (4%)	29	32
3	AC	170/170 (100%)	160 (94%)	10 (6%)	18	16
3	BC	170/170 (100%)	140 (82%)	30 (18%)	2	1
4	AD	172/172 (100%)	165 (96%)	7 (4%)	27	29
4	BD	172/172 (100%)	167 (97%)	5 (3%)	37	42
5	AE	118/118 (100%)	108 (92%)	10 (8%)	10	7
5	BE	113/118 (96%)	88 (78%)	25 (22%)	1	0
6	AF	92/92 (100%)	88 (96%)	4 (4%)	26	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BF	87/92 (95%)	71 (82%)	16 (18%)	1	1
7	AG	124/124 (100%)	118 (95%)	6 (5%)	23	23
7	BG	124/124 (100%)	99 (80%)	25 (20%)	1	0
8	AH	104/104 (100%)	101 (97%)	3 (3%)	37	42
8	BH	104/104 (100%)	86 (83%)	18 (17%)	2	1
9	AI	105/105 (100%)	102 (97%)	3 (3%)	37	42
9	BI	105/105 (100%)	102 (97%)	3 (3%)	37	42
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	11	8
10	BJ	86/87 (99%)	64 (74%)	22 (26%)	0	0
11	AK	90/90 (100%)	87 (97%)	3 (3%)	33	37
11	BK	90/90 (100%)	79 (88%)	11 (12%)	5	2
12	AL	102/102 (100%)	97 (95%)	5 (5%)	22	22
12	BL	102/102 (100%)	85 (83%)	17 (17%)	2	1
13	AM	92/92 (100%)	88 (96%)	4 (4%)	26	27
13	BM	92/92 (100%)	78 (85%)	14 (15%)	3	1
14	AN	83/83 (100%)	83 (100%)	0	100	100
14	BN	83/83 (100%)	81 (98%)	2 (2%)	43	49
15	AO	76/76 (100%)	73 (96%)	3 (4%)	28	31
15	BO	76/76 (100%)	63 (83%)	13 (17%)	2	1
16	AP	65/65 (100%)	62 (95%)	3 (5%)	24	25
16	BP	65/65 (100%)	54 (83%)	11 (17%)	2	1
17	AQ	74/74 (100%)	70 (95%)	4 (5%)	20	18
17	BQ	74/74 (100%)	55 (74%)	19 (26%)	0	0
18	AR	48/48 (100%)	48 (100%)	0	100	100
18	BR	48/48 (100%)	44 (92%)	4 (8%)	10	8
19	AS	70/70 (100%)	69 (99%)	1 (1%)	59	67
19	BS	70/70 (100%)	59 (84%)	11 (16%)	2	1
20	AT	65/65 (100%)	63 (97%)	2 (3%)	35	39
20	BT	65/65 (100%)	50 (77%)	15 (23%)	1	0
21	AU	48/48 (100%)	46 (96%)	2 (4%)	26	28
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	CC	216/216 (100%)	190 (88%)	26 (12%)	5	3
24	DC	216/216 (100%)	210 (97%)	6 (3%)	38	43
25	CD	164/164 (100%)	150 (92%)	14 (8%)	10	7
26	CE	165/165 (100%)	144 (87%)	21 (13%)	4	2
26	DE	165/165 (100%)	164 (99%)	1 (1%)	78	86
27	CF	148/148 (100%)	127 (86%)	21 (14%)	3	1
27	DF	148/148 (100%)	141 (95%)	7 (5%)	23	24
28	CG	137/137 (100%)	112 (82%)	25 (18%)	2	1
28	DG	137/137 (100%)	128 (93%)	9 (7%)	15	13
29	CH	114/114 (100%)	89 (78%)	25 (22%)	1	0
29	DH	114/114 (100%)	101 (89%)	13 (11%)	5	3
30	CJ	104/104 (100%)	99 (95%)	5 (5%)	23	23
30	DJ	104/104 (100%)	98 (94%)	6 (6%)	18	16
31	CK	116/116 (100%)	104 (90%)	12 (10%)	7	4
31	DK	116/116 (100%)	112 (97%)	4 (3%)	32	35
32	CL	103/104 (99%)	95 (92%)	8 (8%)	11	9
32	DL	104/104 (100%)	101 (97%)	3 (3%)	37	42
33	CM	103/103 (100%)	96 (93%)	7 (7%)	14	12
33	DM	103/103 (100%)	100 (97%)	3 (3%)	37	42
34	CN	108/108 (100%)	94 (87%)	14 (13%)	4	2
34	DN	109/108 (101%)	103 (94%)	6 (6%)	19	18
35	CO	100/102 (98%)	86 (86%)	14 (14%)	3	2
35	DO	102/102 (100%)	98 (96%)	4 (4%)	28	31
36	CP	86/87 (99%)	74 (86%)	12 (14%)	3	2
36	DP	87/87 (100%)	85 (98%)	2 (2%)	44	51
37	CQ	99/99 (100%)	88 (89%)	11 (11%)	6	3
37	DQ	99/99 (100%)	94 (95%)	5 (5%)	21	21
38	CR	89/89 (100%)	82 (92%)	7 (8%)	11	9
38	DR	89/89 (100%)	87 (98%)	2 (2%)	45	53
39	CS	84/84 (100%)	74 (88%)	10 (12%)	5	3
39	DS	84/84 (100%)	79 (94%)	5 (6%)	17	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	CT	93/93 (100%)	79 (85%)	14 (15%)	3	1
40	DT	93/93 (100%)	91 (98%)	2 (2%)	45	53
41	CU	80/80 (100%)	66 (82%)	14 (18%)	2	1
41	DU	80/80 (100%)	76 (95%)	4 (5%)	22	22
42	CV	83/83 (100%)	70 (84%)	13 (16%)	2	1
42	DV	83/83 (100%)	78 (94%)	5 (6%)	17	15
43	CW	78/78 (100%)	65 (83%)	13 (17%)	2	1
43	DW	78/78 (100%)	74 (95%)	4 (5%)	21	21
44	CX	56/58 (97%)	52 (93%)	4 (7%)	13	11
44	DX	58/58 (100%)	56 (97%)	2 (3%)	32	35
45	CY	67/67 (100%)	58 (87%)	9 (13%)	4	2
45	DY	67/67 (100%)	66 (98%)	1 (2%)	57	65
46	CZ	54/54 (100%)	46 (85%)	8 (15%)	3	1
46	DZ	54/54 (100%)	53 (98%)	1 (2%)	50	58
47	C0	48/48 (100%)	41 (85%)	7 (15%)	3	1
47	D0	49/48 (102%)	47 (96%)	2 (4%)	27	29
48	C1	47/47 (100%)	42 (89%)	5 (11%)	6	4
48	D1	47/47 (100%)	45 (96%)	2 (4%)	26	27
49	C2	45/46 (98%)	42 (93%)	3 (7%)	15	12
49	D2	45/46 (98%)	44 (98%)	1 (2%)	45	53
50	C3	38/38 (100%)	33 (87%)	5 (13%)	4	2
50	D3	38/38 (100%)	37 (97%)	1 (3%)	40	46
51	C4	51/51 (100%)	47 (92%)	4 (8%)	11	9
51	D4	51/51 (100%)	51 (100%)	0	100	100
52	C5	34/34 (100%)	31 (91%)	3 (9%)	9	7
52	D5	34/34 (100%)	33 (97%)	1 (3%)	37	42
54	DD	163/163 (100%)	161 (99%)	2 (1%)	63	72
55	DI	103/103 (100%)	100 (97%)	3 (3%)	37	42
All	All	9461/9478 (100%)	8665 (92%)	796 (8%)	10	7

5 of 796 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	CH	6	LEU
38	CR	13	ARG
29	CH	83	LYS
29	CH	3	VAL
34	CN	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
26	CE	46	GLN
40	CT	31	GLN
33	DM	35	HIS
26	CE	115	GLN
37	CQ	15	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	259 (16%)	9 (0%)
1	BA	1532/1534 (99%)	269 (17%)	10 (0%)
22	CA	2896/2904 (99%)	424 (14%)	32 (1%)
23	CB	117/120 (97%)	11 (9%)	0
23	DB	119/120 (99%)	8 (6%)	0
53	DA	2887/2903 (99%)	384 (13%)	26 (0%)
All	All	9084/9115 (99%)	1355 (14%)	77 (0%)

5 of 1355 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	28	A

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	DA	846	U
53	DA	2130	U
53	DA	984	A

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Mol	Chain	Res	Type
53	DA	1647	U
53	DA	2585	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	D2T	BL	89	12	8,9,10	0.95	0	6,11,13	2.18	3 (50%)
22	PSU	CA	1911	22	18,21,22	1.12	2 (11%)	21,30,33	1.83	4 (19%)
1	2MG	AA	1516	1	23,26,27	1.19	3 (13%)	33,38,41	2.23	10 (30%)
22	PSU	CA	2457	22	18,21,22	1.05	2 (11%)	21,30,33	2.03	5 (23%)
53	G7M	DA	2069	53	23,26,27	1.47	4 (17%)	34,39,42	1.66	5 (14%)
53	PSU	DA	2457	53	18,21,22	0.86	1 (5%)	21,30,33	1.53	3 (14%)
1	PSU	BA	516	1	18,21,22	1.02	2 (11%)	21,30,33	1.83	5 (23%)
1	2MG	BA	966	1	23,26,27	1.27	3 (13%)	33,38,41	2.27	5 (15%)
22	5MU	CA	747	22	19,22,23	1.31	4 (21%)	27,32,35	2.36	6 (22%)
1	4OC	BA	1402	1	20,23,24	0.81	0	25,32,35	1.07	2 (8%)
53	OMU	DA	2552	53	19,22,23	1.21	3 (15%)	25,31,34	1.85	6 (24%)
1	UR3	AA	1498	1	19,22,23	0.97	1 (5%)	26,32,35	1.90	5 (19%)
54	MEQ	DD	150[A]	54	8,9,10	0.94	0	5,10,12	1.38	2 (40%)
1	2MG	AA	1207	1	23,26,27	1.27	5 (21%)	33,38,41	2.17	8 (24%)
53	PSU	DA	955	53	18,21,22	1.15	1 (5%)	21,30,33	1.61	3 (14%)
53	2MG	DA	2445	53	23,26,27	1.32	2 (8%)	33,38,41	2.12	8 (24%)
53	PSU	DA	2580	53	18,21,22	0.81	1 (5%)	21,30,33	1.60	6 (28%)
22	6MZ	CA	2030	22	22,25,26	1.60	4 (18%)	29,36,39	2.25	11 (37%)
53	5MC	DA	1962	53	19,22,23	1.48	3 (15%)	26,32,35	1.34	5 (19%)
1	5MC	AA	967	1	19,22,23	1.53	2 (10%)	26,32,35	1.12	3 (11%)
22	5MU	CA	1939	22	19,22,23	1.34	3 (15%)	27,32,35	2.10	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	OMG	DA	2251	53	23,26,27	1.18	3 (13%)	32,38,41	1.95	7 (21%)
1	UR3	BA	1498	1	19,22,23	1.04	1 (5%)	26,32,35	1.73	3 (11%)
1	MA6	AA	1518	1	23,26,27	1.50	5 (21%)	33,38,41	1.98	8 (24%)
22	2MG	CA	2445	22	23,26,27	1.27	3 (13%)	33,38,41	2.17	8 (24%)
1	MA6	BA	1519	1	23,26,27	1.43	5 (21%)	33,38,41	2.24	12 (36%)
53	3TD	DA	1915	53	19,22,23	1.61	3 (15%)	23,32,35	2.18	3 (13%)
53	5MU	DA	1939	53	19,22,23	1.38	4 (21%)	27,32,35	1.99	7 (25%)
22	PSU	CA	2605	22	18,21,22	0.97	2 (11%)	21,30,33	2.00	4 (19%)
53	H2U	DA	2449	53	18,21,22	1.31	2 (11%)	19,30,33	1.51	4 (21%)
34	4D4	DN	81[A]	-	9,11,12	2.10	2 (22%)	7,13,15	0.93	0
1	5MC	BA	1407	1	19,22,23	1.92	2 (10%)	26,32,35	1.14	3 (11%)
53	PSU	DA	2604	53	18,21,22	1.05	1 (5%)	21,30,33	1.75	5 (23%)
53	PSU	DA	2605	53	18,21,22	0.97	1 (5%)	21,30,33	1.78	3 (14%)
22	G7M	CA	2069	22	23,26,27	1.51	3 (13%)	34,39,42	1.75	5 (14%)
22	PSU	CA	955	22	18,21,22	0.98	1 (5%)	21,30,33	1.81	3 (14%)
12	D2T	AL	89	12	8,9,10	2.48	2 (25%)	6,11,13	1.57	2 (33%)
53	6MZ	DA	2030	53	22,25,26	1.41	6 (27%)	29,36,39	2.16	12 (41%)
53	PSU	DA	1911	53	18,21,22	1.00	1 (5%)	21,30,33	1.90	4 (19%)
1	2MG	BA	1516	1	23,26,27	1.27	4 (17%)	33,38,41	2.37	12 (36%)
1	5MC	AA	1407	1	19,22,23	1.91	2 (10%)	26,32,35	1.14	2 (7%)
53	PSU	DA	1917	53	18,21,22	1.04	2 (11%)	21,30,33	1.90	5 (23%)
53	2MA	DA	2503	56,53	22,25,26	1.26	5 (22%)	32,37,40	2.39	9 (28%)
22	PSU	CA	1917	22	18,21,22	1.08	1 (5%)	21,30,33	1.69	4 (19%)
1	MA6	AA	1519	1	23,26,27	1.43	5 (21%)	33,38,41	2.07	10 (30%)
22	PSU	CA	2504	22	18,21,22	1.07	2 (11%)	21,30,33	1.96	5 (23%)
22	OMG	CA	2251	22	23,26,27	1.19	1 (4%)	32,38,41	2.01	7 (21%)
1	4OC	AA	1402	1	20,23,24	0.78	0	25,32,35	0.97	1 (4%)
53	PSU	DA	2504	53	18,21,22	0.91	0	21,30,33	1.64	3 (14%)
54	MEQ	DD	150[B]	54	8,9,10	1.24	1 (12%)	5,10,12	1.03	0
22	3TD	CA	1915	22	19,22,23	1.61	3 (15%)	23,32,35	2.14	5 (21%)
53	1MG	DA	745	53	23,26,27	1.14	3 (13%)	33,39,42	1.74	6 (18%)
53	5MU	DA	747	53	19,22,23	1.48	4 (21%)	27,32,35	2.33	6 (22%)
1	G7M	BA	527	1	23,26,27	1.56	3 (13%)	34,39,42	1.79	4 (11%)
22	OMC	CA	2498	22,56	19,22,23	0.80	0	25,31,34	0.87	1 (4%)
22	2MG	CA	1835	22	23,26,27	1.29	4 (17%)	33,38,41	2.14	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	4D4	CN	81	34	9,11,12	2.16	2 (22%)	7,13,15	0.69	0
53	6MZ	DA	1618	53	22,25,26	1.55	5 (22%)	29,36,39	2.11	10 (34%)
53	OMC	DA	2498	56,53	19,22,23	0.91	1 (5%)	25,31,34	1.08	1 (4%)
22	1MG	CA	745	22	23,26,27	1.26	3 (13%)	33,39,42	1.86	5 (15%)
22	PSU	CA	2580	22	18,21,22	1.07	2 (11%)	21,30,33	1.99	6 (28%)
22	5MC	CA	1962	22	19,22,23	1.68	3 (15%)	26,32,35	1.19	2 (7%)
22	6MZ	CA	1618	22	22,25,26	1.57	3 (13%)	29,36,39	2.31	11 (37%)
53	2MG	DA	1835	53	23,26,27	1.03	2 (8%)	33,38,41	2.57	11 (33%)
22	PSU	CA	746	22,56	18,21,22	1.24	1 (5%)	21,30,33	2.06	5 (23%)
34	4D4	DN	81[B]	-	9,11,12	2.02	2 (22%)	7,13,15	0.74	0
1	PSU	AA	516	56,1	18,21,22	0.96	2 (11%)	21,30,33	2.02	4 (19%)
1	2MG	AA	966	1	23,26,27	1.24	2 (8%)	33,38,41	2.12	8 (24%)
1	2MG	BA	1207	1	23,26,27	1.20	3 (13%)	33,38,41	2.26	8 (24%)
53	PSU	DA	746	56,53	18,21,22	1.25	4 (22%)	21,30,33	2.22	5 (23%)
1	MA6	BA	1518	1	23,26,27	1.47	5 (21%)	33,38,41	2.07	8 (24%)
1	5MC	BA	967	1	19,22,23	1.72	3 (15%)	26,32,35	1.07	2 (7%)
22	OMU	CA	2552	22	19,22,23	1.17	2 (10%)	25,31,34	1.81	5 (20%)
22	2MA	CA	2503	22	22,25,26	1.68	4 (18%)	32,37,40	2.27	9 (28%)
1	G7M	AA	527	1	23,26,27	1.44	5 (21%)	34,39,42	1.84	5 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	D2T	BL	89	12	-	4/7/12/14	-
22	PSU	CA	1911	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
22	PSU	CA	2457	22	-	0/7/25/26	0/2/2/2
53	G7M	DA	2069	53	-	2/7/25/26	0/3/3/3
53	PSU	DA	2457	53	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
22	5MU	CA	747	22	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	3/9/29/30	0/2/2/2
53	OMU	DA	2552	53	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
54	MEQ	DD	150[A]	54	-	2/8/9/11	-
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
53	PSU	DA	955	53	-	0/7/25/26	0/2/2/2
53	2MG	DA	2445	53	-	0/9/27/28	0/3/3/3
53	PSU	DA	2580	53	-	0/7/25/26	0/2/2/2
22	6MZ	CA	2030	22	-	2/9/27/28	0/3/3/3
53	5MC	DA	1962	53	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	5MU	CA	1939	22	-	0/7/25/26	0/2/2/2
53	OMG	DA	2251	53	-	0/9/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
22	2MG	CA	2445	22	-	0/9/27/28	0/3/3/3
1	MA6	BA	1519	1	-	2/11/29/30	0/3/3/3
53	3TD	DA	1915	53	-	0/7/25/26	0/2/2/2
53	5MU	DA	1939	53	-	0/7/25/26	0/2/2/2
22	PSU	CA	2605	22	-	0/7/25/26	0/2/2/2
53	H2U	DA	2449	53	-	0/7/38/39	0/2/2/2
34	4D4	DN	81[A]	-	-	0/11/12/14	-
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
53	PSU	DA	2604	53	-	0/7/25/26	0/2/2/2
53	PSU	DA	2605	53	-	0/7/25/26	0/2/2/2
22	G7M	CA	2069	22	-	1/7/25/26	0/3/3/3
22	PSU	CA	955	22	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
53	6MZ	DA	2030	53	-	2/9/27/28	0/3/3/3
53	PSU	DA	1911	53	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
53	PSU	DA	1917	53	-	0/7/25/26	0/2/2/2
53	2MA	DA	2503	56,53	-	1/7/25/26	0/3/3/3
22	PSU	CA	1917	22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	1/11/29/30	0/3/3/3
22	PSU	CA	2504	22	-	0/7/25/26	0/2/2/2
22	OMG	CA	2251	22	-	1/9/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
53	PSU	DA	2504	53	-	0/7/25/26	0/2/2/2
54	MEQ	DD	150[B]	54	-	4/8/9/11	-
22	3TD	CA	1915	22	-	2/7/25/26	0/2/2/2
53	1MG	DA	745	53	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	5MU	DA	747	53	-	1/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/7/25/26	0/3/3/3
22	OMC	CA	2498	22,56	-	0/9/27/28	0/2/2/2
22	2MG	CA	1835	22	-	2/9/27/28	0/3/3/3
34	4D4	CN	81	34	-	6/11/12/14	-
53	6MZ	DA	1618	53	-	0/9/27/28	0/3/3/3
53	OMC	DA	2498	56,53	-	1/9/27/28	0/2/2/2
22	1MG	CA	745	22	-	0/7/25/26	0/3/3/3
22	PSU	CA	2580	22	-	0/7/25/26	0/2/2/2
22	5MC	CA	1962	22	-	0/7/25/26	0/2/2/2
22	6MZ	CA	1618	22	-	0/9/27/28	0/3/3/3
53	2MG	DA	1835	53	-	0/9/27/28	0/3/3/3
22	PSU	CA	746	22,56	-	2/7/25/26	0/2/2/2
34	4D4	DN	81[B]	-	-	5/11/12/14	-
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
53	PSU	DA	746	56,53	-	2/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	1/11/29/30	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
22	OMU	CA	2552	22	-	1/9/27/28	0/2/2/2
22	2MA	CA	2503	22	-	1/7/25/26	0/3/3/3
1	G7M	AA	527	1	-	0/7/25/26	0/3/3/3

The worst 5 of 187 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1407	5MC	C5-C4	7.09	1.49	1.44
1	AA	1407	5MC	C5-C4	7.02	1.49	1.44
1	BA	967	5MC	C5-C4	6.25	1.48	1.44
22	CA	1962	5MC	C5-C4	6.12	1.48	1.44
12	AL	89	D2T	CB-CA	5.75	1.56	1.54

The worst 5 of 395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1915	3TD	N1-C2-N3	8.35	122.20	116.13
53	DA	1835	2MG	C2-N3-C4	8.25	122.32	112.00
22	CA	1915	3TD	N1-C2-N3	7.77	121.78	116.13
1	BA	966	2MG	C2-N3-C4	7.48	121.36	112.00
53	DA	2503	2MA	C5-C4-N3	-7.35	119.44	127.18

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	N1-C2-N2-CM2
1	AA	966	2MG	N3-C2-N2-CM2
1	BA	527	G7M	O4'-C4'-C5'-O5'
12	BL	89	D2T	CA-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1

There are no ring outliers.

32 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BA	516	PSU	1	0
1	BA	966	2MG	1	0
22	CA	747	5MU	1	0
1	BA	1402	4OC	2	0
54	DD	150[A]	MEQ	2	0
22	CA	2030	6MZ	2	0
22	CA	1939	5MU	1	0
53	DA	2251	OMG	2	0
1	BA	1498	UR3	1	0
1	AA	1518	MA6	2	0
22	CA	2445	2MG	2	0
1	BA	1519	MA6	4	0
34	DN	81[A]	4D4	1	0
1	BA	1407	5MC	2	0
22	CA	2069	G7M	1	0
12	AL	89	D2T	1	0
53	DA	2030	6MZ	2	0
1	BA	1516	2MG	1	0
1	AA	1519	MA6	3	0
22	CA	2251	OMG	1	0
1	AA	1402	4OC	1	0
54	DD	150[B]	MEQ	1	0
22	CA	1915	3TD	4	0
22	CA	2498	OMC	2	0
34	CN	81	4D4	1	0
53	DA	2498	OMC	2	0
22	CA	1962	5MC	1	0
22	CA	1618	6MZ	1	0
1	BA	1518	MA6	2	0
1	BA	967	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	CA	2503	2MA	3	0
1	AA	527	G7M	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 546 ligands modelled in this entry, 466 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
59	PUT	DA	3188	-	5,5,5	0.19	0	4,4,4	0.27	0
61	PEG	DA	3219	-	6,6,6	1.03	0	5,5,5	0.44	0
66	EDO	DA	3210	-	3,3,3	0.30	0	2,2,2	0.51	0
62	SPD	DA	3187	-	9,9,9	0.42	0	8,8,8	0.93	0
59	PUT	AA	1673	-	5,5,5	0.22	0	4,4,4	0.48	0
61	PEG	DA	3201	-	6,6,6	1.04	0	5,5,5	0.49	0
64	PGE	D1	102	-	9,9,9	1.05	0	8,8,8	0.31	0
64	PGE	DS	201	-	9,9,9	0.96	0	8,8,8	0.31	0
59	PUT	DA	3213	-	5,5,5	0.26	0	4,4,4	0.20	0
59	PUT	DA	3206	-	5,5,5	0.28	0	4,4,4	0.51	0
61	PEG	AL	201	-	6,6,6	0.96	0	5,5,5	0.45	0
62	SPD	DA	3183	-	9,9,9	0.42	0	8,8,8	0.77	0
58	MPD	DS	203	-	7,7,7	1.01	1 (14%)	9,10,10	0.60	0
57	PG4	DA	3217	-	12,12,12	0.74	0	11,11,11	0.54	0
64	PGE	DA	3226	-	9,9,9	0.97	0	8,8,8	0.26	0
64	PGE	DA	3215	-	9,9,9	0.94	0	8,8,8	0.30	0
58	MPD	DA	3208	-	7,7,7	0.53	0	9,10,10	0.37	0
66	EDO	D1	101	-	3,3,3	0.25	0	2,2,2	0.45	0
59	PUT	AA	1672	-	5,5,5	0.21	0	4,4,4	0.54	0
64	PGE	D3	101	-	9,9,9	0.92	0	8,8,8	0.37	0
66	EDO	DA	3198	-	3,3,3	0.33	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	PUT	DA	3214	-	5,5,5	0.23	0	4,4,4	0.42	0
61	PEG	DA	3227	-	6,6,6	0.97	0	5,5,5	0.42	0
64	PGE	DA	3218	-	9,9,9	0.84	0	8,8,8	0.38	0
58	MPD	DE	302	-	7,7,7	0.53	0	9,10,10	0.58	0
57	PG4	DQ	202	-	12,12,12	0.67	0	11,11,11	0.56	0
58	MPD	DA	3205	-	7,7,7	0.77	0	9,10,10	1.15	1 (11%)
67	GUN	DA	3212	-	12,12,12	1.65	2 (16%)	15,17,17	3.23	9 (60%)
58	MPD	DA	3190	-	7,7,7	0.67	0	9,10,10	0.68	0
66	EDO	DA	3209	-	3,3,3	0.35	0	2,2,2	0.34	0
66	EDO	D0	101	-	3,3,3	0.34	0	2,2,2	0.46	0
68	TRS	DA	3221	-	7,7,7	0.38	0	9,9,9	0.80	0
59	PUT	DA	3224	-	5,5,5	0.25	0	4,4,4	0.71	0
59	PUT	DA	3189	-	5,5,5	0.30	0	4,4,4	0.41	0
64	PGE	DA	3204	-	9,9,9	0.97	0	8,8,8	0.55	0
65	ACY	DA	3191	-	3,3,3	0.91	0	3,3,3	0.80	0
66	EDO	DA	3194	-	3,3,3	0.29	0	2,2,2	0.49	0
64	PGE	DU	101	-	9,9,9	0.97	0	8,8,8	0.43	0
66	EDO	DB	210	-	3,3,3	0.27	0	2,2,2	0.76	0
58	MPD	DN	201	-	7,7,7	0.54	0	9,10,10	0.91	0
61	PEG	DA	3200	-	6,6,6	1.07	0	5,5,5	0.53	0
62	SPD	DA	3207	-	9,9,9	0.50	0	8,8,8	0.65	0
57	PG4	DR	202	-	12,12,12	0.84	0	11,11,11	0.43	0
59	PUT	DA	3184	-	5,5,5	0.29	0	4,4,4	0.30	0
61	PEG	DA	3228	-	6,6,6	1.05	0	5,5,5	0.18	0
57	PG4	AA	1670	-	12,12,12	0.81	0	11,11,11	0.41	0
58	MPD	DT	201	-	7,7,7	0.86	1 (14%)	9,10,10	1.09	0
59	PUT	DA	3223	-	5,5,5	0.32	0	4,4,4	0.42	0
66	EDO	DR	203	-	3,3,3	0.29	0	2,2,2	0.42	0
58	MPD	DK	201	-	7,7,7	0.55	0	9,10,10	0.75	0
58	MPD	AA	1671	-	7,7,7	0.55	0	9,10,10	0.61	0
58	MPD	AA	1676	-	7,7,7	0.72	0	9,10,10	0.62	0
59	PUT	DA	3222	-	5,5,5	0.22	0	4,4,4	0.41	0
61	PEG	DP	201	-	6,6,6	0.98	0	5,5,5	0.41	0
57	PG4	BA	1642	-	12,12,12	0.80	0	11,11,11	0.43	0
59	PUT	DM	201	-	5,5,5	0.27	0	4,4,4	0.66	0
63	1PE	DA	3203	-	15,15,15	0.66	0	14,14,14	0.32	0
59	PUT	DA	3220	-	5,5,5	0.19	0	4,4,4	0.46	0
58	MPD	DA	3192	-	7,7,7	0.41	0	9,10,10	1.38	1 (11%)
64	PGE	DA	3186	-	9,9,9	0.94	0	8,8,8	0.30	0
59	PUT	AA	1674	-	5,5,5	0.21	0	4,4,4	0.52	0
57	PG4	DA	3193	-	12,12,12	0.79	0	11,11,11	0.59	0
61	PEG	D3	102	-	6,6,6	1.00	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	MPD	DA	3211	-	7,7,7	0.53	0	9,10,10	0.95	1 (11%)
58	MPD	DE	301	-	7,7,7	0.64	0	9,10,10	0.73	0
66	EDO	DB	211	-	3,3,3	0.35	0	2,2,2	0.52	0
61	PEG	DL	201	-	6,6,6	0.87	0	5,5,5	0.55	0
59	PUT	AA	1675	-	5,5,5	0.28	0	4,4,4	0.33	0
66	EDO	DA	3197	-	3,3,3	0.26	0	2,2,2	0.57	0
66	EDO	DA	3216	-	3,3,3	0.36	0	2,2,2	0.39	0
66	EDO	DB	212	-	3,3,3	0.32	0	2,2,2	0.48	0
62	SPD	DA	3225	-	9,9,9	0.56	0	8,8,8	1.10	1 (12%)
65	ACY	DA	3196	-	3,3,3	1.00	0	3,3,3	0.86	0
63	1PE	DA	3185	-	15,15,15	0.55	0	14,14,14	0.49	0
61	PEG	DA	3199	-	6,6,6	0.92	0	5,5,5	0.58	0
59	PUT	DA	3195	-	5,5,5	0.25	0	4,4,4	0.38	0
57	PG4	DS	202	-	12,12,12	0.76	0	11,11,11	0.32	0
65	ACY	DA	3202	-	3,3,3	0.95	0	3,3,3	0.64	0
58	MPD	DT	202	-	7,7,7	0.54	0	9,10,10	0.58	0
61	PEG	DQ	201	-	6,6,6	1.01	0	5,5,5	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3188	-	-	0/3/3/3	-
61	PEG	DA	3219	-	-	1/4/4/4	-
66	EDO	DA	3210	-	-	0/1/1/1	-
62	SPD	DA	3187	-	-	0/7/7/7	-
59	PUT	AA	1673	-	-	0/3/3/3	-
61	PEG	DA	3201	-	-	3/4/4/4	-
64	PGE	D1	102	-	-	1/7/7/7	-
64	PGE	DS	201	-	-	2/7/7/7	-
59	PUT	DA	3213	-	-	0/3/3/3	-
59	PUT	DA	3206	-	-	1/3/3/3	-
61	PEG	AL	201	-	-	2/4/4/4	-
62	SPD	DA	3183	-	-	3/7/7/7	-
58	MPD	DS	203	-	-	0/5/5/5	-
57	PG4	DA	3217	-	-	5/10/10/10	-
64	PGE	DA	3226	-	-	4/7/7/7	-
64	PGE	DA	3215	-	-	3/7/7/7	-
58	MPD	DA	3208	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	EDO	D1	101	-	-	0/1/1/1	-
59	PUT	AA	1672	-	-	0/3/3/3	-
64	PGE	D3	101	-	-	3/7/7/7	-
66	EDO	DA	3198	-	-	0/1/1/1	-
59	PUT	DA	3214	-	-	1/3/3/3	-
61	PEG	DA	3227	-	-	3/4/4/4	-
64	PGE	DA	3218	-	-	3/7/7/7	-
58	MPD	DE	302	-	-	1/5/5/5	-
57	PG4	DQ	202	-	-	0/10/10/10	-
58	MPD	DA	3205	-	-	4/5/5/5	-
67	GUN	DA	3212	-	-	-	0/2/2/2
58	MPD	DA	3190	-	-	2/5/5/5	-
66	EDO	DA	3209	-	-	1/1/1/1	-
66	EDO	D0	101	-	-	1/1/1/1	-
68	TRS	DA	3221	-	-	6/9/9/9	-
59	PUT	DA	3224	-	-	0/3/3/3	-
59	PUT	DA	3189	-	-	0/3/3/3	-
64	PGE	DA	3204	-	-	5/7/7/7	-
66	EDO	DA	3194	-	-	0/1/1/1	-
64	PGE	DU	101	-	-	2/7/7/7	-
66	EDO	DB	210	-	-	1/1/1/1	-
58	MPD	DN	201	-	-	3/5/5/5	-
61	PEG	DA	3200	-	-	2/4/4/4	-
62	SPD	DA	3207	-	-	5/7/7/7	-
57	PG4	DR	202	-	-	5/10/10/10	-
59	PUT	DA	3184	-	-	1/3/3/3	-
61	PEG	DA	3228	-	-	1/4/4/4	-
57	PG4	AA	1670	-	-	6/10/10/10	-
58	MPD	DT	201	-	-	1/5/5/5	-
59	PUT	DA	3223	-	-	1/3/3/3	-
66	EDO	DR	203	-	-	1/1/1/1	-
58	MPD	DK	201	-	-	1/5/5/5	-
58	MPD	AA	1671	-	-	1/5/5/5	-
58	MPD	AA	1676	-	-	2/5/5/5	-
59	PUT	DA	3222	-	-	2/3/3/3	-
61	PEG	DP	201	-	-	4/4/4/4	-
57	PG4	BA	1642	-	-	2/10/10/10	-
59	PUT	DM	201	-	-	3/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	1PE	DA	3203	-	-	6/13/13/13	-
59	PUT	DA	3220	-	-	0/3/3/3	-
58	MPD	DA	3192	-	-	5/5/5/5	-
64	PGE	DA	3186	-	-	2/7/7/7	-
59	PUT	AA	1674	-	-	1/3/3/3	-
57	PG4	DA	3193	-	-	7/10/10/10	-
61	PEG	D3	102	-	-	3/4/4/4	-
58	MPD	DA	3211	-	-	4/5/5/5	-
58	MPD	DE	301	-	-	3/5/5/5	-
66	EDO	DB	211	-	-	1/1/1/1	-
61	PEG	DL	201	-	-	3/4/4/4	-
59	PUT	AA	1675	-	-	2/3/3/3	-
66	EDO	DA	3197	-	-	1/1/1/1	-
66	EDO	DA	3216	-	-	1/1/1/1	-
66	EDO	DB	212	-	-	0/1/1/1	-
62	SPD	DA	3225	-	-	2/7/7/7	-
63	1PE	DA	3185	-	-	7/13/13/13	-
61	PEG	DA	3199	-	-	2/4/4/4	-
59	PUT	DA	3195	-	-	2/3/3/3	-
57	PG4	DS	202	-	-	3/10/10/10	-
58	MPD	DT	202	-	-	3/5/5/5	-
61	PEG	DQ	201	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3212	GUN	C5-C4	3.07	1.48	1.39
58	DS	203	MPD	O2-C2	-2.19	1.39	1.44
58	DT	201	MPD	O2-C2	-2.03	1.39	1.44
67	DA	3212	GUN	C2-N3	2.00	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3212	GUN	N9-C4-N3	8.02	135.75	125.99
67	DA	3212	GUN	C2-N3-C4	4.99	122.17	113.36
67	DA	3212	GUN	C6-C5-N7	3.92	137.42	130.29
67	DA	3212	GUN	C8-N7-C5	3.65	109.31	104.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DA	3192	MPD	CM-C2-C1	-3.31	103.22	110.63

There are no chirality outliers.

5 of 160 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1671	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-C5
58	DA	3192	MPD	O2-C2-C3-C4
58	DA	3192	MPD	CM-C2-C3-C4

There are no ring outliers.

42 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	DA	3210	EDO	3	0
62	DA	3187	SPD	1	0
59	AA	1673	PUT	1	0
61	DA	3201	PEG	1	0
59	DA	3213	PUT	1	0
62	DA	3183	SPD	1	0
57	DA	3217	PG4	1	0
66	DA	3198	EDO	3	0
59	DA	3214	PUT	2	0
61	DA	3227	PEG	1	0
64	DA	3218	PGE	1	0
57	DQ	202	PG4	3	0
58	DA	3205	MPD	3	0
67	DA	3212	GUN	1	0
58	DA	3190	MPD	1	0
66	DA	3209	EDO	1	0
59	DA	3224	PUT	2	0
59	DA	3189	PUT	1	0
64	DA	3204	PGE	2	0
66	DA	3194	EDO	3	0
64	DU	101	PGE	1	0
58	DN	201	MPD	6	0
61	DA	3200	PEG	1	0
57	DR	202	PG4	10	0
57	AA	1670	PG4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	DA	3223	PUT	4	0
59	DA	3222	PUT	2	0
61	DP	201	PEG	4	0
57	BA	1642	PG4	2	0
63	DA	3203	1PE	3	0
59	DA	3220	PUT	1	0
57	DA	3193	PG4	7	0
61	D3	102	PEG	5	0
58	DA	3211	MPD	1	0
66	DA	3197	EDO	1	0
66	DB	212	EDO	1	0
62	DA	3225	SPD	5	0
63	DA	3185	1PE	1	0
59	DA	3195	PUT	3	0
57	DS	202	PG4	2	0
65	DA	3202	ACY	1	0
61	DQ	201	PEG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	1523/1534 (99%)	0.00	19 (1%) 76 78	50, 82, 132, 172	0
1	BA	1522/1534 (99%)	0.94	85 (5%) 30 32	64, 105, 192, 222	0
2	AB	224/224 (100%)	1.88	96 (42%) 0 1	74, 117, 124, 132	0
2	BB	224/224 (100%)	2.43	136 (60%) 0 0	74, 114, 123, 130	0
3	AC	206/206 (100%)	1.16	16 (7%) 19 20	77, 88, 100, 105	0
3	BC	206/206 (100%)	2.40	115 (55%) 0 0	100, 117, 150, 166	0
4	AD	205/205 (100%)	1.28	32 (15%) 5 5	70, 91, 116, 125	0
4	BD	205/205 (100%)	1.80	77 (37%) 1 1	64, 76, 86, 91	0
5	AE	155/155 (100%)	1.35	32 (20%) 2 3	68, 79, 89, 95	0
5	BE	150/155 (96%)	2.71	106 (70%) 0 0	77, 91, 103, 114	0
6	AF	106/106 (100%)	1.47	25 (23%) 2 2	65, 92, 100, 102	0
6	BF	100/106 (94%)	2.35	55 (55%) 0 0	92, 104, 113, 117	0
7	AG	151/151 (100%)	2.13	68 (45%) 0 1	90, 117, 127, 132	0
7	BG	151/151 (100%)	2.99	113 (74%) 0 0	111, 153, 177, 185	0
8	AH	129/129 (100%)	1.05	9 (6%) 22 24	69, 82, 95, 103	0
8	BH	129/129 (100%)	2.54	84 (65%) 0 0	72, 111, 132, 139	0
9	AI	127/127 (100%)	2.24	74 (58%) 0 0	81, 111, 124, 130	0
9	BI	127/127 (100%)	3.28	104 (81%) 0 0	130, 152, 171, 177	0
10	AJ	99/99 (100%)	2.22	57 (57%) 0 0	60, 70, 76, 77	0
10	BJ	98/99 (98%)	3.58	90 (91%) 0 0	69, 76, 80, 81	0
11	AK	117/117 (100%)	1.41	25 (21%) 2 2	60, 90, 104, 108	0
11	BK	117/117 (100%)	1.93	55 (47%) 0 0	75, 102, 115, 118	0
12	AL	122/123 (99%)	1.08	16 (13%) 7 7	55, 67, 77, 88	0
12	BL	122/123 (99%)	2.54	79 (64%) 0 0	72, 84, 92, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	2.12	58 (50%)	0	0	84, 112, 124, 128	0
13	BM	114/114 (100%)	3.48	91 (79%)	0	0	190, 219, 233, 235	0
14	AN	100/100 (100%)	2.21	46 (46%)	0	0	80, 100, 134, 140	0
14	BN	100/100 (100%)	3.17	86 (86%)	0	0	126, 174, 220, 227	0
15	AO	88/88 (100%)	1.33	14 (15%)	5	5	69, 82, 93, 98	0
15	BO	88/88 (100%)	2.23	53 (60%)	0	0	80, 105, 118, 125	0
16	AP	82/82 (100%)	1.42	14 (17%)	4	4	70, 85, 104, 113	0
16	BP	82/82 (100%)	3.67	75 (91%)	0	0	84, 106, 122, 126	0
17	AQ	80/80 (100%)	1.29	16 (20%)	3	3	69, 83, 96, 101	0
17	BQ	80/80 (100%)	3.18	62 (77%)	0	0	89, 120, 129, 133	0
18	AR	55/55 (100%)	1.58	12 (21%)	2	2	79, 86, 96, 98	0
18	BR	55/55 (100%)	2.17	27 (49%)	0	0	83, 90, 98, 100	0
19	AS	79/79 (100%)	2.04	36 (45%)	0	1	91, 110, 123, 127	0
19	BS	79/79 (100%)	2.96	60 (75%)	0	0	199, 217, 228, 231	0
20	AT	86/86 (100%)	1.59	21 (24%)	2	2	58, 84, 101, 107	0
20	BT	85/86 (98%)	3.62	69 (81%)	0	0	107, 131, 142, 144	0
21	AU	56/56 (100%)	1.79	21 (37%)	1	1	67, 80, 103, 113	0
21	BU	56/56 (100%)	2.13	27 (48%)	0	0	65, 85, 106, 113	0
22	CA	2876/2904 (99%)	1.31	429 (14%)	5	5	77, 118, 180, 217	0
23	CB	118/120 (98%)	0.73	0	100	100	108, 157, 167, 168	0
23	DB	120/120 (100%)	-0.13	0	100	100	37, 58, 73, 81	0
24	CC	271/271 (100%)	3.70	243 (89%)	0	0	83, 107, 126, 131	0
24	DC	271/271 (100%)	1.26	49 (18%)	3	3	35, 59, 71, 78	0
25	CD	209/209 (100%)	3.28	178 (85%)	0	0	87, 108, 121, 126	0
26	CE	201/201 (100%)	3.73	171 (85%)	0	0	90, 157, 187, 196	0
26	DE	201/201 (100%)	0.55	5 (2%)	58	61	33, 57, 72, 78	0
27	CF	177/177 (100%)	2.40	110 (62%)	0	0	167, 172, 174, 176	0
27	DF	177/177 (100%)	1.53	45 (25%)	1	2	58, 75, 91, 94	0
28	CG	176/176 (100%)	2.61	114 (64%)	0	0	108, 120, 130, 134	0
28	DG	176/176 (100%)	1.00	16 (9%)	15	15	49, 62, 71, 75	0
29	CH	149/149 (100%)	2.75	100 (67%)	0	0	96, 121, 141, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	DH	149/149 (100%)	2.25	83 (55%) 0 0	65, 128, 133, 154	0
30	CJ	134/134 (100%)	3.05	97 (72%) 0 0	202, 219, 225, 228	0
30	DJ	134/134 (100%)	3.52	106 (79%) 0 0	155, 183, 202, 208	0
31	CK	142/142 (100%)	2.92	103 (72%) 0 0	98, 110, 115, 120	0
31	DK	142/142 (100%)	0.19	5 (3%) 47 49	33, 41, 51, 60	0
32	CL	122/123 (99%)	2.78	89 (72%) 0 0	94, 107, 113, 114	0
32	DL	123/123 (100%)	0.42	2 (1%) 70 73	37, 48, 59, 68	0
33	CM	144/144 (100%)	4.02	126 (87%) 0 0	100, 137, 162, 166	0
33	DM	144/144 (100%)	0.63	4 (2%) 55 57	28, 53, 69, 73	0
34	CN	135/136 (99%)	3.01	110 (81%) 0 0	95, 122, 142, 150	0
34	DN	135/136 (99%)	0.33	2 (1%) 72 74	23, 44, 57, 63	1 (0%)
35	CO	120/125 (96%)	3.64	110 (91%) 0 0	103, 120, 137, 142	0
35	DO	125/125 (100%)	0.47	8 (6%) 25 27	35, 44, 60, 69	0
36	CP	116/117 (99%)	2.61	65 (56%) 0 0	146, 155, 162, 164	0
36	DP	117/117 (100%)	1.02	5 (4%) 40 41	49, 59, 69, 73	0
37	CQ	114/114 (100%)	3.13	90 (78%) 0 0	110, 116, 124, 131	0
37	DQ	114/114 (100%)	0.75	9 (7%) 18 20	40, 52, 63, 73	0
38	CR	117/117 (100%)	3.51	91 (77%) 0 0	100, 115, 126, 128	0
38	DR	117/117 (100%)	0.10	3 (2%) 57 60	30, 40, 49, 64	0
39	CS	103/103 (100%)	3.31	85 (82%) 0 0	103, 125, 133, 137	0
39	DS	103/103 (100%)	0.46	2 (1%) 66 69	29, 48, 59, 73	0
40	CT	110/110 (100%)	3.81	99 (90%) 0 0	91, 121, 146, 150	0
40	DT	110/110 (100%)	0.14	1 (0%) 81 83	33, 39, 52, 68	0
41	CU	93/93 (100%)	4.19	83 (89%) 0 0	117, 149, 169, 176	0
41	DU	93/93 (100%)	1.18	15 (16%) 4 5	41, 57, 76, 83	0
42	CV	102/102 (100%)	5.01	98 (96%) 0 0	151, 176, 205, 210	0
42	DV	102/102 (100%)	1.08	13 (12%) 8 8	48, 60, 69, 80	0
43	CW	94/94 (100%)	2.21	50 (53%) 0 0	129, 148, 161, 165	0
43	DW	94/94 (100%)	0.70	2 (2%) 63 66	40, 54, 65, 71	0
44	CX	75/76 (98%)	2.99	63 (84%) 0 0	109, 118, 122, 126	0
44	DX	76/76 (100%)	0.62	5 (6%) 24 26	22, 46, 59, 65	1 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	CY	77/77 (100%)	4.00	72 (93%) 0 0	99, 116, 133, 135	0
45	DY	77/77 (100%)	1.10	12 (15%) 5 5	42, 59, 73, 78	0
46	CZ	62/62 (100%)	3.72	55 (88%) 0 0	158, 174, 193, 199	0
46	DZ	62/62 (100%)	1.47	15 (24%) 2 2	56, 66, 81, 82	0
47	C0	58/58 (100%)	2.99	41 (70%) 0 0	119, 130, 142, 143	0
47	D0	58/58 (100%)	0.50	5 (8%) 16 17	24, 42, 50, 56	2 (3%)
48	C1	56/56 (100%)	3.68	49 (87%) 0 0	92, 123, 140, 144	0
48	D1	56/56 (100%)	0.34	4 (7%) 22 23	27, 44, 58, 64	0
49	C2	50/51 (98%)	2.83	29 (58%) 0 0	113, 122, 128, 132	0
49	D2	51/51 (100%)	1.00	8 (15%) 5 5	50, 59, 66, 67	0
50	C3	46/46 (100%)	4.45	45 (97%) 0 0	95, 108, 115, 117	0
50	D3	46/46 (100%)	0.66	1 (2%) 62 65	35, 44, 53, 62	0
51	C4	64/64 (100%)	4.50	63 (98%) 0 0	109, 119, 126, 127	0
51	D4	64/64 (100%)	0.39	2 (3%) 51 54	39, 45, 51, 57	0
52	C5	38/38 (100%)	4.15	36 (94%) 0 0	106, 114, 120, 125	0
52	D5	38/38 (100%)	0.45	2 (5%) 32 34	42, 48, 58, 63	0
53	DA	2873/2903 (98%)	-0.30	67 (2%) 61 64	22, 49, 130, 199	8 (0%)
54	DD	208/209 (99%)	0.23	3 (1%) 73 75	29, 44, 58, 63	0
55	DI	135/135 (100%)	3.63	114 (84%) 0 0	76, 123, 152, 159	1 (0%)
All	All	20634/20744 (99%)	1.42	6063 (29%) 1 1	22, 96, 176, 235	13 (0%)

The worst 5 of 6063 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BT	4	ILE	11.7
7	AG	5	ARG	11.4
42	CV	78	GLY	10.8
26	CE	73	ILE	10.6
38	CR	8	VAL	10.2

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

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

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	2MG	BA	1207	24/25	0.73	0.15	122,126,131,131	0
22	3TD	CA	1915	21/22	0.75	0.12	109,112,115,116	0
22	PSU	CA	1917	20/21	0.75	0.11	102,107,110,112	0
1	2MG	BA	966	24/25	0.76	0.15	128,136,145,147	0
22	2MA	CA	2503	23/24	0.77	0.21	87,90,92,94	0
22	PSU	CA	1911	20/21	0.79	0.10	103,108,113,116	0
22	PSU	CA	746	20/21	0.82	0.17	88,91,95,95	0
22	6MZ	CA	2030	23/24	0.83	0.20	93,99,101,102	0
22	6MZ	CA	1618	23/24	0.84	0.15	91,97,99,100	0
22	PSU	CA	955	20/21	0.85	0.17	100,105,109,110	0
1	5MC	BA	967	21/22	0.86	0.12	127,132,143,145	0
1	5MC	BA	1407	21/22	0.86	0.15	86,91,95,96	0
22	PSU	CA	2457	20/21	0.87	0.14	91,97,101,102	0
1	G7M	BA	527	24/25	0.87	0.15	63,71,78,84	0
22	1MG	CA	745	24/25	0.88	0.16	85,88,93,95	0
22	PSU	CA	2580	20/21	0.89	0.12	83,88,90,92	0
34	4D4	CN	81	12/13	0.89	0.18	94,97,99,100	0
53	3TD	DA	1915	21/22	0.89	0.09	76,81,87,94	0
1	2MG	BA	1516	24/25	0.90	0.14	67,74,79,83	0
1	MA6	BA	1518	24/25	0.90	0.14	68,73,78,85	0
22	PSU	CA	2504	20/21	0.90	0.14	83,87,90,91	0
1	PSU	BA	516	20/21	0.90	0.11	73,79,89,91	0
22	PSU	CA	2605	20/21	0.90	0.14	71,79,82,83	0
22	2MG	CA	1835	24/25	0.90	0.15	74,82,84,86	0
22	G7M	CA	2069	24/25	0.90	0.17	88,94,96,100	0
53	PSU	DA	1917	20/21	0.90	0.09	63,72,79,84	0
1	2MG	AA	1207	24/25	0.91	0.12	89,94,98,100	0
22	5MC	CA	1962	21/22	0.91	0.13	73,78,80,83	0
1	UR3	BA	1498	21/22	0.91	0.13	69,76,83,83	0
22	5MU	CA	747	21/22	0.91	0.14	82,91,96,97	0
22	OMG	CA	2251	24/25	0.91	0.17	85,92,95,98	0
1	MA6	BA	1519	24/25	0.91	0.15	67,73,79,81	0
22	OMC	CA	2498	21/22	0.91	0.18	90,97,99,102	0
22	OMU	CA	2552	21/22	0.92	0.15	80,85,87,87	0
22	2MG	CA	2445	24/25	0.92	0.14	88,92,96,99	0
1	4OC	BA	1402	22/23	0.92	0.14	82,86,90,90	0
1	2MG	AA	966	24/25	0.92	0.13	69,75,80,83	0
12	D2T	BL	89	10/11	0.92	0.13	64,74,78,93	0
22	5MU	CA	1939	21/22	0.92	0.13	70,78,83,83	0
1	PSU	AA	516	20/21	0.93	0.09	68,75,81,81	0
53	PSU	DA	1911	20/21	0.93	0.08	69,74,80,80	0
1	G7M	AA	527	24/25	0.94	0.11	64,66,70,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MEQ	DD	150[A]	10/11	0.94	0.10	23,32,39,40	10
54	MEQ	DD	150[B]	10/11	0.94	0.10	28,32,38,39	10
1	5MC	AA	967	21/22	0.95	0.10	70,76,83,84	0
12	D2T	AL	89	10/11	0.95	0.10	59,65,70,77	0
53	2MG	DA	1835	24/25	0.96	0.09	45,50,57,57	0
53	5MC	DA	1962	21/22	0.96	0.10	38,48,55,59	0
53	PSU	DA	2604	20/21	0.96	0.08	33,44,54,57	0
1	UR3	AA	1498	21/22	0.96	0.09	50,58,65,69	0
1	MA6	AA	1519	24/25	0.96	0.10	51,56,63,67	0
34	4D4	DN	81[A]	12/13	0.96	0.09	33,38,42,43	9
34	4D4	DN	81[B]	12/13	0.96	0.09	33,36,40,41	9
1	MA6	AA	1518	24/25	0.97	0.08	45,54,59,64	0
1	5MC	AA	1407	21/22	0.97	0.07	51,59,62,63	0
53	1MG	DA	745	24/25	0.97	0.07	25,34,41,44	0
53	6MZ	DA	2030	23/24	0.97	0.07	22,30,36,42	0
53	2MA	DA	2503	23/24	0.97	0.07	21,37,44,48	0
53	OMU	DA	2552	21/22	0.97	0.09	35,42,46,49	0
53	PSU	DA	2580	20/21	0.97	0.07	27,32,38,42	0
53	PSU	DA	746	20/21	0.97	0.07	28,37,43,44	0
53	5MU	DA	747	21/22	0.97	0.07	27,36,43,46	0
53	6MZ	DA	1618	23/24	0.97	0.07	29,36,44,47	0
1	4OC	AA	1402	22/23	0.97	0.08	59,62,68,70	0
1	2MG	AA	1516	24/25	0.97	0.07	47,53,60,67	0
53	PSU	DA	955	20/21	0.98	0.05	28,33,40,40	0
53	PSU	DA	2504	20/21	0.98	0.05	28,36,44,45	0
53	5MU	DA	1939	21/22	0.98	0.07	36,42,45,50	0
53	G7M	DA	2069	24/25	0.98	0.06	34,38,43,43	0
53	OMG	DA	2251	24/25	0.98	0.06	23,34,41,43	0
53	PSU	DA	2605	20/21	0.98	0.06	38,45,49,50	0
53	2MG	DA	2445	24/25	0.98	0.06	23,32,38,40	0
53	H2U	DA	2449	20/21	0.98	0.06	26,32,38,42	0
53	PSU	DA	2457	20/21	0.98	0.05	31,36,43,45	0
53	OMC	DA	2498	21/22	0.98	0.06	28,33,38,40	0

### 6.3 Carbohydrates i

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3036	1/1	0.45	0.24	94,94,94,94	0
56	MG	CA	3073	1/1	0.54	0.19	93,93,93,93	0
56	MG	CA	3074	1/1	0.54	0.24	91,91,91,91	0
56	MG	CA	3145	1/1	0.54	0.15	90,90,90,90	0
56	MG	CA	3093	1/1	0.58	0.20	91,91,91,91	0
58	MPD	DE	301	8/8	0.59	0.25	57,67,76,80	0
56	MG	CA	3059	1/1	0.62	0.24	91,91,91,91	0
66	EDO	DB	211	4/4	0.62	0.24	68,70,71,73	0
56	MG	CA	3006	1/1	0.63	0.26	100,100,100,100	0
56	MG	CA	3155	1/1	0.63	0.21	93,93,93,93	0
56	MG	CA	3079	1/1	0.66	0.22	94,94,94,94	0
56	MG	CA	3146	1/1	0.67	0.29	60,60,60,60	1
56	MG	CA	3062	1/1	0.67	0.20	90,90,90,90	0
56	MG	CA	3122	1/1	0.68	0.17	85,85,85,85	0
56	MG	AA	1628	1/1	0.69	0.17	80,80,80,80	0
56	MG	CA	3083	1/1	0.69	0.16	93,93,93,93	0
56	MG	CA	3153	1/1	0.69	0.17	86,86,86,86	0
56	MG	CA	3121	1/1	0.70	0.18	86,86,86,86	0
56	MG	DA	3109	1/1	0.70	0.26	88,88,88,88	0
56	MG	CA	3035	1/1	0.71	0.20	81,81,81,81	0
59	PUT	AA	1675	6/6	0.71	0.22	65,66,71,72	0
56	MG	CA	3075	1/1	0.71	0.15	92,92,92,92	0
56	MG	AA	1610	1/1	0.72	0.28	85,85,85,85	0
56	MG	CA	3030	1/1	0.72	0.14	74,74,74,74	0
56	MG	CA	3131	1/1	0.73	0.25	79,79,79,79	0
56	MG	CA	3086	1/1	0.73	0.18	78,78,78,78	0
56	MG	CA	3031	1/1	0.73	0.22	90,90,90,90	0
56	MG	CA	3096	1/1	0.74	0.16	92,92,92,92	0
56	MG	CA	3070	1/1	0.74	0.14	90,90,90,90	0
56	MG	BA	1609	1/1	0.74	0.25	89,89,89,89	0
58	MPD	DA	3205	8/8	0.75	0.19	58,63,68,70	0
56	MG	CA	3089	1/1	0.75	0.17	80,80,80,80	0
56	MG	CA	3112	1/1	0.75	0.30	81,81,81,81	0
56	MG	DA	3137	1/1	0.75	0.43	56,56,56,56	1
56	MG	CA	3154	1/1	0.76	0.16	90,90,90,90	0
56	MG	CA	3080	1/1	0.77	0.17	88,88,88,88	0
58	MPD	DT	201	8/8	0.77	0.30	55,63,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	1639	1/1	0.77	0.18	78,78,78,78	0
65	ACY	DA	3196	4/4	0.77	0.25	59,65,67,71	0
56	MG	BA	1640	1/1	0.77	0.19	79,79,79,79	0
58	MPD	DK	201	8/8	0.78	0.21	60,66,71,73	0
56	MG	DA	3128	1/1	0.78	0.29	74,74,74,74	0
56	MG	CA	3037	1/1	0.78	0.17	102,102,102,102	0
61	PEG	DQ	201	7/7	0.78	0.17	63,70,74,76	0
56	MG	AA	1617	1/1	0.78	0.15	82,82,82,82	0
56	MG	BA	1601	1/1	0.78	0.18	78,78,78,78	0
68	TRS	DA	3221	8/8	0.78	0.20	65,69,75,77	0
56	MG	BA	1627	1/1	0.79	0.20	83,83,83,83	0
56	MG	CA	3140	1/1	0.79	0.19	76,76,76,76	0
67	GUN	DA	3212	11/11	0.79	0.16	52,58,63,69	0
56	MG	DA	3182	1/1	0.79	0.29	86,86,86,86	0
56	MG	DA	3181	1/1	0.80	0.18	79,79,79,79	0
56	MG	AA	1654	1/1	0.80	0.27	91,91,91,91	0
59	PUT	DA	3195	6/6	0.80	0.20	39,46,50,57	0
56	MG	DB	206	1/1	0.80	0.20	82,82,82,82	0
62	SPD	DA	3207	10/10	0.80	0.28	57,63,68,70	0
56	MG	BA	1637	1/1	0.80	0.20	80,80,80,80	0
56	MG	AA	1664	1/1	0.80	0.13	78,78,78,78	0
58	MPD	DE	302	8/8	0.80	0.27	60,65,67,67	0
56	MG	DA	3177	1/1	0.80	0.24	75,75,75,75	0
56	MG	C3	101	1/1	0.81	0.14	97,97,97,97	0
56	MG	DA	3041	1/1	0.81	0.16	50,50,50,50	0
56	MG	CA	3123	1/1	0.81	0.11	75,75,75,75	0
58	MPD	DA	3208	8/8	0.81	0.19	56,62,70,74	0
56	MG	CA	3018	1/1	0.81	0.15	79,79,79,79	0
56	MG	CA	3084	1/1	0.81	0.15	80,80,80,80	0
56	MG	AA	1623	1/1	0.81	0.18	71,71,71,71	0
56	MG	CB	202	1/1	0.81	0.12	86,86,86,86	0
56	MG	BA	1631	1/1	0.82	0.16	76,76,76,76	0
59	PUT	AA	1674	6/6	0.82	0.18	61,62,67,69	0
56	MG	DA	3118	1/1	0.82	0.27	79,79,79,79	0
56	MG	DA	3119	1/1	0.82	0.25	66,66,66,66	0
60	ZN	AB	301	1/1	0.82	0.23	140,140,140,140	0
56	MG	CA	3090	1/1	0.82	0.14	80,80,80,80	0
56	MG	DA	3129	1/1	0.82	0.14	70,70,70,70	0
64	PGE	D1	102	10/10	0.82	0.21	61,66,71,74	0
56	MG	DA	3132	1/1	0.82	0.18	71,71,71,71	0
56	MG	CA	3116	1/1	0.82	0.32	75,75,75,75	0
56	MG	CA	3025	1/1	0.82	0.23	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
58	MPD	DN	201	8/8	0.82	0.17	57,63,66,71	0
56	MG	AA	1603	1/1	0.83	0.18	82,82,82,82	0
56	MG	CA	3124	1/1	0.83	0.17	87,87,87,87	0
56	MG	DA	3141	1/1	0.83	0.22	73,73,73,73	0
56	MG	DA	3168	1/1	0.83	0.14	77,77,77,77	0
56	MG	DA	3171	1/1	0.83	0.21	76,76,76,76	0
56	MG	CA	3019	1/1	0.83	0.14	81,81,81,81	0
59	PUT	DA	3223	6/6	0.83	0.21	46,49,51,53	0
56	MG	CA	3133	1/1	0.83	0.16	75,75,75,75	0
56	MG	CA	3020	1/1	0.83	0.29	83,83,83,83	0
56	MG	AA	1658	1/1	0.83	0.13	70,70,70,70	0
58	MPD	DA	3192	8/8	0.83	0.23	56,60,64,66	0
56	MG	BA	1641	1/1	0.83	0.17	86,86,86,86	0
56	MG	CA	3002	1/1	0.83	0.30	91,91,91,91	0
56	MG	AA	1661	1/1	0.83	0.14	79,79,79,79	0
56	MG	DA	3130	1/1	0.83	0.26	77,77,77,77	0
56	MG	BA	1632	1/1	0.84	0.20	68,68,68,68	0
56	MG	CA	3021	1/1	0.84	0.24	93,93,93,93	0
56	MG	CA	3129	1/1	0.84	0.25	84,84,84,84	0
56	MG	CA	3066	1/1	0.84	0.23	85,85,85,85	0
58	MPD	DT	202	8/8	0.84	0.29	65,66,75,75	0
56	MG	DA	3003	1/1	0.84	0.12	75,75,75,75	0
56	MG	CA	3109	1/1	0.84	0.21	72,72,72,72	0
56	MG	DA	3179	1/1	0.84	0.12	76,76,76,76	0
56	MG	CA	3137	1/1	0.84	0.16	78,78,78,78	0
56	MG	AA	1613	1/1	0.84	0.27	80,80,80,80	0
56	MG	DB	205	1/1	0.84	0.16	74,74,74,74	0
56	MG	CA	3072	1/1	0.84	0.16	92,92,92,92	0
58	MPD	DA	3190	8/8	0.84	0.18	55,64,69,72	0
56	MG	DA	3122	1/1	0.84	0.27	77,77,77,77	0
56	MG	AA	1609	1/1	0.84	0.30	79,79,79,79	0
56	MG	CA	3147	1/1	0.84	0.21	55,55,55,55	1
56	MG	CA	3058	1/1	0.84	0.16	76,76,76,76	0
56	MG	BA	1605	1/1	0.85	0.14	81,81,81,81	0
56	MG	CA	3135	1/1	0.85	0.20	83,83,83,83	0
56	MG	AA	1606	1/1	0.85	0.27	83,83,83,83	0
56	MG	DA	3138	1/1	0.85	0.16	60,60,60,60	0
56	MG	CA	3138	1/1	0.85	0.13	80,80,80,80	0
56	MG	DA	3163	1/1	0.85	0.14	73,73,73,73	0
56	MG	AA	1627	1/1	0.85	0.24	80,80,80,80	0
56	MG	CA	3144	1/1	0.85	0.26	73,73,73,73	0
56	MG	DA	3175	1/1	0.85	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3034	1/1	0.85	0.11	82,82,82,82	0
56	MG	CA	3063	1/1	0.85	0.23	93,93,93,93	0
59	PUT	DA	3206	6/6	0.85	0.21	58,61,62,63	0
59	PUT	DA	3222	6/6	0.85	0.20	62,64,65,68	0
56	MG	DA	3121	1/1	0.85	0.27	85,85,85,85	0
56	MG	AA	1608	1/1	0.85	0.26	76,76,76,76	0
61	PEG	DA	3200	7/7	0.85	0.19	52,54,67,67	0
56	MG	DA	3125	1/1	0.85	0.29	69,69,69,69	0
56	MG	DA	3126	1/1	0.85	0.25	75,75,75,75	0
56	MG	DB	207	1/1	0.85	0.19	75,75,75,75	0
57	PG4	BA	1642	13/13	0.85	0.15	52,61,66,69	0
57	PG4	DR	202	13/13	0.85	0.17	47,56,62,65	0
56	MG	CA	3098	1/1	0.85	0.11	89,89,89,89	0
56	MG	AA	1619	1/1	0.85	0.14	81,81,81,81	0
56	MG	DA	3169	1/1	0.86	0.23	77,77,77,77	0
58	MPD	AA	1671	8/8	0.86	0.18	63,65,70,73	0
56	MG	CA	3060	1/1	0.86	0.21	93,93,93,93	0
56	MG	CA	3118	1/1	0.86	0.17	87,87,87,87	0
56	MG	DA	3115	1/1	0.86	0.13	56,56,56,56	0
56	MG	AA	1602	1/1	0.86	0.15	79,79,79,79	0
61	PEG	DA	3199	7/7	0.86	0.18	49,56,67,67	0
56	MG	AA	1663	1/1	0.86	0.13	79,79,79,79	0
61	PEG	DA	3219	7/7	0.86	0.24	61,66,70,73	0
61	PEG	DA	3227	7/7	0.86	0.22	57,59,71,73	0
61	PEG	DP	201	7/7	0.86	0.14	61,65,67,67	0
56	MG	AA	1615	1/1	0.86	0.18	74,74,74,74	0
56	MG	CA	3087	1/1	0.86	0.13	83,83,83,83	0
56	MG	DA	3146	1/1	0.86	0.13	77,77,77,77	0
56	MG	CA	3125	1/1	0.86	0.15	84,84,84,84	0
56	MG	DB	208	1/1	0.86	0.24	79,79,79,79	0
66	EDO	D0	101	4/4	0.86	0.23	61,63,66,68	0
59	PUT	AA	1672	6/6	0.86	0.20	63,63,66,70	0
56	MG	AA	1601	1/1	0.86	0.25	66,66,66,66	0
56	MG	DA	3133	1/1	0.87	0.17	67,67,67,67	0
56	MG	CA	3141	1/1	0.87	0.21	77,77,77,77	0
56	MG	DA	3042	1/1	0.87	0.09	75,75,75,75	0
56	MG	CA	3014	1/1	0.87	0.11	78,78,78,78	0
56	MG	DA	3144	1/1	0.87	0.11	69,69,69,69	0
56	MG	CA	3071	1/1	0.87	0.22	95,95,95,95	0
56	MG	DA	3161	1/1	0.87	0.16	71,71,71,71	0
56	MG	CA	3111	1/1	0.87	0.18	77,77,77,77	0
56	MG	CA	3130	1/1	0.87	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3150	1/1	0.87	0.23	85,85,85,85	0
56	MG	BA	1617	1/1	0.87	0.11	82,82,82,82	0
56	MG	DA	3173	1/1	0.87	0.22	77,77,77,77	0
56	MG	AA	1644	1/1	0.87	0.11	76,76,76,76	0
56	MG	CA	3061	1/1	0.87	0.14	86,86,86,86	0
64	PGE	D3	101	10/10	0.87	0.18	58,65,67,68	0
56	MG	BA	1633	1/1	0.87	0.25	85,85,85,85	0
66	EDO	DB	210	4/4	0.87	0.22	65,67,68,69	0
56	MG	BA	1636	1/1	0.87	0.25	83,83,83,83	0
56	MG	BA	1630	1/1	0.87	0.10	98,98,98,98	0
59	PUT	AA	1673	6/6	0.87	0.16	63,64,68,69	0
56	MG	DA	3008	1/1	0.87	0.14	55,55,55,55	0
56	MG	CA	3047	1/1	0.88	0.10	77,77,77,77	0
56	MG	DA	3035	1/1	0.88	0.17	38,38,38,38	0
56	MG	CA	3119	1/1	0.88	0.08	83,83,83,83	0
56	MG	CA	3120	1/1	0.88	0.21	74,74,74,74	0
59	PUT	DA	3213	6/6	0.88	0.18	49,55,55,58	0
56	MG	DA	3140	1/1	0.88	0.16	65,65,65,65	0
56	MG	BA	1620	1/1	0.88	0.11	78,78,78,78	0
56	MG	BA	1625	1/1	0.88	0.17	89,89,89,89	0
56	MG	AA	1616	1/1	0.88	0.42	83,83,83,83	0
56	MG	DA	3152	1/1	0.88	0.33	65,65,65,65	0
61	PEG	DA	3201	7/7	0.88	0.19	53,56,63,66	0
58	MPD	AA	1676	8/8	0.88	0.20	60,66,72,76	0
56	MG	BA	1638	1/1	0.88	0.17	75,75,75,75	0
56	MG	DA	3162	1/1	0.88	0.13	69,69,69,69	0
56	MG	CA	3076	1/1	0.88	0.18	83,83,83,83	0
56	MG	AA	1625	1/1	0.88	0.18	70,70,70,70	0
56	MG	AA	1651	1/1	0.88	0.11	69,69,69,69	0
56	MG	DA	3170	1/1	0.88	0.15	66,66,66,66	0
56	MG	AA	1621	1/1	0.88	0.28	79,79,79,79	0
66	EDO	DA	3209	4/4	0.88	0.28	55,59,62,67	0
56	MG	DA	3172	1/1	0.88	0.19	73,73,73,73	0
56	MG	CA	3045	1/1	0.88	0.10	80,80,80,80	0
56	MG	CA	3115	1/1	0.88	0.28	73,73,73,73	0
56	MG	CA	3085	1/1	0.88	0.12	78,78,78,78	0
56	MG	DA	3131	1/1	0.88	0.19	70,70,70,70	0
56	MG	CA	3055	1/1	0.89	0.20	78,78,78,78	0
59	PUT	DA	3189	6/6	0.89	0.16	44,48,51,54	0
56	MG	DA	3147	1/1	0.89	0.29	73,73,73,73	0
56	MG	DA	3149	1/1	0.89	0.10	62,62,62,62	0
56	MG	AA	1612	1/1	0.89	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3153	1/1	0.89	0.19	67,67,67,67	0
57	PG4	DA	3193	13/13	0.89	0.18	52,56,66,66	0
57	PG4	DA	3217	13/13	0.89	0.15	57,66,72,75	0
61	PEG	AL	201	7/7	0.89	0.12	57,64,71,73	0
57	PG4	DQ	202	13/13	0.89	0.13	50,58,66,66	0
56	MG	DA	3160	1/1	0.89	0.23	71,71,71,71	0
56	MG	CA	3097	1/1	0.89	0.10	83,83,83,83	0
56	MG	CA	3126	1/1	0.89	0.23	74,74,74,74	0
56	MG	CA	3127	1/1	0.89	0.14	84,84,84,84	0
56	MG	CA	3128	1/1	0.89	0.27	82,82,82,82	0
56	MG	DA	3016	1/1	0.89	0.14	63,63,63,63	0
61	PEG	D3	102	7/7	0.89	0.19	50,54,70,71	0
56	MG	BA	1611	1/1	0.89	0.12	64,64,64,64	0
56	MG	CA	3024	1/1	0.89	0.17	75,75,75,75	0
56	MG	AA	1620	1/1	0.89	0.19	72,72,72,72	0
56	MG	DA	3065	1/1	0.89	0.11	70,70,70,70	0
56	MG	CA	3148	1/1	0.89	0.19	73,73,73,73	0
56	MG	CA	3051	1/1	0.89	0.10	71,71,71,71	0
56	MG	CA	3151	1/1	0.89	0.10	82,82,82,82	0
66	EDO	DB	212	4/4	0.89	0.23	59,60,64,64	0
66	EDO	DR	203	4/4	0.89	0.26	53,54,57,60	0
56	MG	DA	3180	1/1	0.89	0.22	78,78,78,78	0
56	MG	DA	3143	1/1	0.89	0.14	77,77,77,77	0
56	MG	CA	3134	1/1	0.89	0.15	79,79,79,79	0
56	MG	AA	1626	1/1	0.90	0.15	84,84,84,84	0
56	MG	CA	3007	1/1	0.90	0.16	82,82,82,82	0
56	MG	DA	3145	1/1	0.90	0.11	69,69,69,69	0
56	MG	DA	3174	1/1	0.90	0.13	77,77,77,77	0
56	MG	DA	3021	1/1	0.90	0.09	36,36,36,36	0
56	MG	DA	3127	1/1	0.90	0.34	65,65,65,65	0
56	MG	DA	3178	1/1	0.90	0.12	79,79,79,79	0
58	MPD	DA	3211	8/8	0.90	0.17	54,57,64,66	0
56	MG	CA	3038	1/1	0.90	0.18	78,78,78,78	0
56	MG	CA	3039	1/1	0.90	0.10	81,81,81,81	0
56	MG	CA	3081	1/1	0.90	0.09	83,83,83,83	0
56	MG	DA	3156	1/1	0.90	0.30	74,74,74,74	0
56	MG	DA	3158	1/1	0.90	0.11	63,63,63,63	0
64	PGE	DA	3226	10/10	0.90	0.18	59,63,67,69	0
64	PGE	DU	101	10/10	0.90	0.14	44,60,69,71	0
56	MG	CA	3010	1/1	0.90	0.10	77,77,77,77	0
56	MG	DA	3103	1/1	0.90	0.12	44,44,44,44	0
56	MG	BA	1623	1/1	0.90	0.25	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	209	1/1	0.90	0.17	69,69,69,69	0
57	PG4	AA	1670	13/13	0.90	0.14	52,62,68,68	0
59	PUT	DA	3188	6/6	0.90	0.12	32,39,44,48	0
56	MG	AA	1624	1/1	0.90	0.18	80,80,80,80	0
56	MG	CA	3033	1/1	0.90	0.19	90,90,90,90	0
56	MG	AA	1605	1/1	0.90	0.35	76,76,76,76	0
56	MG	AA	1630	1/1	0.90	0.16	86,86,86,86	0
59	PUT	DA	3214	6/6	0.90	0.21	49,52,56,57	0
56	MG	CA	3026	1/1	0.91	0.08	75,75,75,75	0
56	MG	CA	3041	1/1	0.91	0.09	72,72,72,72	0
56	MG	CA	3149	1/1	0.91	0.12	69,69,69,69	0
59	PUT	DA	3184	6/6	0.91	0.17	45,52,53,56	0
56	MG	CA	3068	1/1	0.91	0.10	85,85,85,85	0
56	MG	CA	3029	1/1	0.91	0.08	79,79,79,79	0
56	MG	CA	3046	1/1	0.91	0.20	85,85,85,85	0
56	MG	CA	3091	1/1	0.91	0.20	77,77,77,77	0
56	MG	CA	3092	1/1	0.91	0.10	83,83,83,83	0
56	MG	AA	1669	1/1	0.91	0.18	76,76,76,76	0
59	PUT	DA	3220	6/6	0.91	0.19	56,58,62,67	0
56	MG	CA	3048	1/1	0.91	0.09	74,74,74,74	0
56	MG	AA	1642	1/1	0.91	0.17	88,88,88,88	0
56	MG	DA	3005	1/1	0.91	0.10	72,72,72,72	0
56	MG	CA	3052	1/1	0.91	0.10	79,79,79,79	0
56	MG	CA	3103	1/1	0.91	0.14	86,86,86,86	0
56	MG	CA	3104	1/1	0.91	0.24	83,83,83,83	0
56	MG	DA	3028	1/1	0.91	0.08	49,49,49,49	0
56	MG	AA	1614	1/1	0.91	0.20	75,75,75,75	0
56	MG	CA	3001	1/1	0.91	0.10	80,80,80,80	0
61	PEG	DL	201	7/7	0.91	0.12	55,58,62,66	0
56	MG	AA	1632	1/1	0.91	0.10	79,79,79,79	0
56	MG	CA	3113	1/1	0.91	0.16	63,63,63,63	0
56	MG	DA	3151	1/1	0.91	0.26	80,80,80,80	0
62	SPD	DA	3183	10/10	0.91	0.12	42,51,57,57	0
56	MG	DA	3070	1/1	0.91	0.10	52,52,52,52	0
63	1PE	DA	3185	16/16	0.91	0.15	39,51,68,74	0
64	PGE	DA	3204	10/10	0.91	0.16	53,61,69,70	0
64	PGE	DA	3215	10/10	0.91	0.15	56,62,66,70	0
64	PGE	DA	3218	10/10	0.91	0.13	50,55,64,68	0
56	MG	DA	3072	1/1	0.91	0.10	53,53,53,53	0
64	PGE	DS	201	10/10	0.91	0.13	50,56,66,68	0
56	MG	DA	3085	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3087	1/1	0.91	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3092	1/1	0.91	0.11	39,39,39,39	0
56	MG	DA	3097	1/1	0.91	0.10	37,37,37,37	0
65	ACY	DA	3202	4/4	0.91	0.20	53,59,61,64	0
56	MG	CA	3139	1/1	0.91	0.15	71,71,71,71	0
66	EDO	DA	3216	4/4	0.91	0.17	60,61,62,67	0
56	MG	CA	3005	1/1	0.91	0.10	96,96,96,96	0
56	MG	DA	3165	1/1	0.91	0.28	70,70,70,70	0
56	MG	DA	3167	1/1	0.91	0.17	64,64,64,64	0
56	MG	CA	3082	1/1	0.91	0.12	79,79,79,79	0
56	MG	CA	3117	1/1	0.91	0.27	79,79,79,79	0
56	MG	AA	1641	1/1	0.91	0.10	71,71,71,71	0
56	MG	BA	1613	1/1	0.91	0.08	65,65,65,65	0
56	MG	CA	3078	1/1	0.92	0.16	85,85,85,85	0
56	MG	CA	3132	1/1	0.92	0.11	80,80,80,80	0
56	MG	BA	1626	1/1	0.92	0.15	80,80,80,80	0
56	MG	DA	3040	1/1	0.92	0.10	48,48,48,48	0
56	MG	DA	3154	1/1	0.92	0.17	68,68,68,68	0
56	MG	CA	3107	1/1	0.92	0.16	70,70,70,70	0
62	SPD	DA	3225	10/10	0.92	0.13	34,45,52,63	0
56	MG	AA	1655	1/1	0.92	0.11	77,77,77,77	0
56	MG	DA	3055	1/1	0.92	0.07	36,36,36,36	0
56	MG	DA	3060	1/1	0.92	0.10	77,77,77,77	0
56	MG	CA	3152	1/1	0.92	0.14	77,77,77,77	0
56	MG	DA	3066	1/1	0.92	0.09	44,44,44,44	0
56	MG	CA	3110	1/1	0.92	0.15	70,70,70,70	0
56	MG	CA	3003	1/1	0.92	0.07	80,80,80,80	0
56	MG	DA	3079	1/1	0.92	0.08	55,55,55,55	0
56	MG	CA	3008	1/1	0.92	0.08	79,79,79,79	0
57	PG4	DS	202	13/13	0.92	0.10	42,48,56,56	0
56	MG	CA	3042	1/1	0.92	0.07	70,70,70,70	0
66	EDO	DA	3198	4/4	0.92	0.32	49,53,54,55	0
56	MG	CA	3004	1/1	0.92	0.18	95,95,95,95	0
66	EDO	DA	3210	4/4	0.92	0.21	62,65,69,73	0
56	MG	DA	3093	1/1	0.92	0.11	57,57,57,57	0
56	MG	CA	3142	1/1	0.92	0.10	69,69,69,69	0
56	MG	DA	3100	1/1	0.92	0.09	46,46,46,46	0
56	MG	CA	3065	1/1	0.92	0.10	73,73,73,73	0
56	MG	DA	3176	1/1	0.92	0.14	70,70,70,70	0
56	MG	CA	3057	1/1	0.92	0.09	82,82,82,82	0
56	MG	CA	3102	1/1	0.92	0.11	78,78,78,78	0
61	PEG	DA	3228	7/7	0.92	0.15	55,58,61,64	0
56	MG	BA	1602	1/1	0.93	0.09	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3004	1/1	0.93	0.10	66,66,66,66	0
56	MG	BA	1621	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3104	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3106	1/1	0.93	0.10	44,44,44,44	0
56	MG	CA	3101	1/1	0.93	0.12	82,82,82,82	0
56	MG	DA	3012	1/1	0.93	0.08	56,56,56,56	0
56	MG	BA	1603	1/1	0.93	0.14	83,83,83,83	0
56	MG	CA	3028	1/1	0.93	0.08	69,69,69,69	0
56	MG	DA	3120	1/1	0.93	0.23	75,75,75,75	0
56	MG	DA	3022	1/1	0.93	0.09	40,40,40,40	0
56	MG	AA	1645	1/1	0.93	0.13	67,67,67,67	0
56	MG	DA	3029	1/1	0.93	0.08	41,41,41,41	0
56	MG	DA	3033	1/1	0.93	0.10	47,47,47,47	0
63	1PE	DA	3203	16/16	0.93	0.14	50,55,64,65	0
56	MG	BA	1606	1/1	0.93	0.11	85,85,85,85	0
56	MG	CA	3108	1/1	0.93	0.16	65,65,65,65	0
56	MG	CA	3011	1/1	0.93	0.12	78,78,78,78	0
56	MG	AA	1646	1/1	0.93	0.08	59,59,59,59	0
56	MG	CA	3016	1/1	0.93	0.08	71,71,71,71	0
56	MG	DA	3058	1/1	0.93	0.12	38,38,38,38	0
56	MG	AA	1640	1/1	0.93	0.12	65,65,65,65	0
56	MG	DA	3136	1/1	0.93	0.22	74,74,74,74	0
56	MG	AA	1659	1/1	0.93	0.08	68,68,68,68	0
56	MG	CA	3114	1/1	0.93	0.22	68,68,68,68	0
66	EDO	DA	3194	4/4	0.93	0.25	52,52,52,58	0
56	MG	DA	3069	1/1	0.93	0.14	53,53,53,53	0
56	MG	BA	1614	1/1	0.93	0.11	77,77,77,77	0
56	MG	DA	3142	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3229	1/1	0.93	0.09	42,42,42,42	0
56	MG	DB	201	1/1	0.93	0.07	62,62,62,62	0
56	MG	AA	1660	1/1	0.93	0.21	86,86,86,86	0
56	MG	CA	3094	1/1	0.93	0.12	68,68,68,68	0
56	MG	CB	201	1/1	0.93	0.10	91,91,91,91	0
56	MG	CA	3136	1/1	0.93	0.09	87,87,87,87	0
66	EDO	D1	101	4/4	0.93	0.15	47,52,57,63	0
56	MG	CA	3022	1/1	0.93	0.19	78,78,78,78	0
56	MG	DA	3002	1/1	0.93	0.10	66,66,66,66	0
56	MG	CB	203	1/1	0.94	0.08	90,90,90,90	0
56	MG	DA	3094	1/1	0.94	0.08	38,38,38,38	0
56	MG	DA	3095	1/1	0.94	0.07	49,49,49,49	0
59	PUT	DA	3224	6/6	0.94	0.12	43,45,54,60	0
56	MG	CA	3100	1/1	0.94	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1647	1/1	0.94	0.12	82,82,82,82	0
56	MG	DA	3047	1/1	0.94	0.07	54,54,54,54	0
56	MG	DA	3053	1/1	0.94	0.07	38,38,38,38	0
56	MG	AA	1607	1/1	0.94	0.21	76,76,76,76	0
56	MG	DA	3139	1/1	0.94	0.08	57,57,57,57	0
56	MG	CA	3064	1/1	0.94	0.13	75,75,75,75	0
56	MG	AA	1604	1/1	0.94	0.21	73,73,73,73	0
56	MG	CA	3106	1/1	0.94	0.20	67,67,67,67	0
56	MG	AA	1611	1/1	0.94	0.10	63,63,63,63	0
56	MG	BA	1607	1/1	0.94	0.11	84,84,84,84	0
56	MG	CA	3069	1/1	0.94	0.07	80,80,80,80	0
56	MG	CA	3043	1/1	0.94	0.14	67,67,67,67	0
56	MG	CA	3095	1/1	0.94	0.09	71,71,71,71	0
56	MG	DA	3148	1/1	0.94	0.07	66,66,66,66	0
56	MG	AA	1636	1/1	0.94	0.10	81,81,81,81	0
56	MG	BA	1624	1/1	0.94	0.23	86,86,86,86	0
56	MG	AA	1618	1/1	0.94	0.28	78,78,78,78	0
56	MG	DA	3090	1/1	0.95	0.11	42,42,42,42	0
56	MG	CA	3013	1/1	0.95	0.21	89,89,89,89	0
56	MG	DA	3038	1/1	0.95	0.07	44,44,44,44	0
56	MG	AA	1653	1/1	0.95	0.06	63,63,63,63	0
56	MG	DA	3164	1/1	0.95	0.13	70,70,70,70	0
56	MG	CA	3044	1/1	0.95	0.14	73,73,73,73	0
56	MG	DA	3166	1/1	0.95	0.18	73,73,73,73	0
56	MG	CA	3077	1/1	0.95	0.07	83,83,83,83	0
56	MG	DA	3099	1/1	0.95	0.08	60,60,60,60	0
56	MG	AA	1657	1/1	0.95	0.14	77,77,77,77	0
56	MG	BA	1604	1/1	0.95	0.17	75,75,75,75	0
56	MG	AA	1667	1/1	0.95	0.09	57,57,57,57	0
56	MG	DA	3057	1/1	0.95	0.09	40,40,40,40	0
59	PUT	DM	201	6/6	0.95	0.10	46,49,53,54	0
56	MG	BA	1616	1/1	0.95	0.07	86,86,86,86	0
56	MG	CA	3067	1/1	0.95	0.16	84,84,84,84	0
56	MG	AA	1622	1/1	0.95	0.20	74,74,74,74	0
56	MG	BA	1628	1/1	0.95	0.06	74,74,74,74	0
56	MG	CA	3009	1/1	0.95	0.19	78,78,78,78	0
56	MG	BA	1619	1/1	0.95	0.11	66,66,66,66	0
56	MG	DA	3025	1/1	0.95	0.06	41,41,41,41	0
56	MG	DA	3124	1/1	0.95	0.23	72,72,72,72	0
56	MG	DA	3076	1/1	0.95	0.07	67,67,67,67	0
56	MG	AA	1662	1/1	0.95	0.08	74,74,74,74	0
56	MG	CA	3105	1/1	0.95	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3027	1/1	0.95	0.12	97,97,97,97	0
56	MG	DA	3088	1/1	0.95	0.08	32,32,32,32	0
56	MG	CA	3054	1/1	0.96	0.09	83,83,83,83	0
56	MG	DA	3043	1/1	0.96	0.06	49,49,49,49	0
56	MG	DA	3135	1/1	0.96	0.09	56,56,56,56	0
56	MG	AA	1635	1/1	0.96	0.07	74,74,74,74	0
56	MG	DA	3096	1/1	0.96	0.16	69,69,69,69	0
56	MG	DA	3049	1/1	0.96	0.05	45,45,45,45	0
56	MG	DA	3051	1/1	0.96	0.07	53,53,53,53	0
62	SPD	DA	3187	10/10	0.96	0.09	36,43,46,47	0
56	MG	CA	3056	1/1	0.96	0.14	75,75,75,75	0
56	MG	DA	3054	1/1	0.96	0.06	35,35,35,35	0
58	MPD	DS	203	8/8	0.96	0.10	41,45,50,53	0
56	MG	DA	3010	1/1	0.96	0.08	37,37,37,37	0
64	PGE	DA	3186	10/10	0.96	0.09	37,42,58,59	0
56	MG	BA	1622	1/1	0.96	0.09	70,70,70,70	0
56	MG	AA	1631	1/1	0.96	0.08	54,54,54,54	0
56	MG	DA	3110	1/1	0.96	0.04	33,33,33,33	0
56	MG	DA	3111	1/1	0.96	0.09	61,61,61,61	0
56	MG	DA	3017	1/1	0.96	0.12	36,36,36,36	0
56	MG	DA	3116	1/1	0.96	0.05	57,57,57,57	0
56	MG	DA	3117	1/1	0.96	0.07	54,54,54,54	0
56	MG	AA	1656	1/1	0.96	0.11	67,67,67,67	0
65	ACY	DA	3191	4/4	0.96	0.10	48,50,52,53	0
56	MG	DB	203	1/1	0.96	0.05	51,51,51,51	0
56	MG	BA	1634	1/1	0.96	0.06	76,76,76,76	0
56	MG	CA	3017	1/1	0.96	0.10	82,82,82,82	0
56	MG	DA	3027	1/1	0.96	0.14	42,42,42,42	0
56	MG	DA	3155	1/1	0.96	0.10	66,66,66,66	0
56	MG	BA	1608	1/1	0.96	0.06	78,78,78,78	0
56	MG	DA	3157	1/1	0.96	0.16	65,65,65,65	0
56	MG	DA	3074	1/1	0.96	0.12	42,42,42,42	0
56	MG	BA	1618	1/1	0.96	0.15	74,74,74,74	0
56	MG	CA	3032	1/1	0.96	0.06	71,71,71,71	0
56	MG	AA	1666	1/1	0.96	0.06	73,73,73,73	0
56	MG	DA	3036	1/1	0.96	0.07	43,43,43,43	0
56	MG	AA	1638	1/1	0.96	0.09	86,86,86,86	0
56	MG	BA	1629	1/1	0.96	0.14	77,77,77,77	0
56	MG	CA	3023	1/1	0.96	0.09	75,75,75,75	0
56	MG	AA	1677	1/1	0.97	0.07	79,79,79,79	0
56	MG	DA	3082	1/1	0.97	0.08	49,49,49,49	0
56	MG	DA	3083	1/1	0.97	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3053	1/1	0.97	0.14	80,80,80,80	0
56	MG	AA	1643	1/1	0.97	0.06	66,66,66,66	0
56	MG	DA	3006	1/1	0.97	0.08	43,43,43,43	0
56	MG	DA	3007	1/1	0.97	0.05	40,40,40,40	0
56	MG	AA	1639	1/1	0.97	0.07	79,79,79,79	0
56	MG	DA	3044	1/1	0.97	0.06	41,41,41,41	0
56	MG	DA	3046	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3009	1/1	0.97	0.07	59,59,59,59	0
56	MG	CA	3012	1/1	0.97	0.05	69,69,69,69	0
56	MG	DA	3050	1/1	0.97	0.11	55,55,55,55	0
56	MG	DA	3098	1/1	0.97	0.04	37,37,37,37	0
56	MG	AA	1648	1/1	0.97	0.06	56,56,56,56	0
56	MG	BA	1612	1/1	0.97	0.06	77,77,77,77	0
56	MG	DA	3101	1/1	0.97	0.06	51,51,51,51	0
56	MG	CA	3015	1/1	0.97	0.14	76,76,76,76	0
56	MG	AA	1629	1/1	0.97	0.07	67,67,67,67	0
56	MG	AA	1668	1/1	0.97	0.14	60,60,60,60	0
56	MG	CA	3099	1/1	0.97	0.06	69,69,69,69	0
56	MG	CA	3049	1/1	0.97	0.06	64,64,64,64	0
56	MG	DA	3062	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3150	1/1	0.97	0.11	49,49,49,49	0
66	EDO	DA	3197	4/4	0.97	0.12	56,58,62,65	0
56	MG	DA	3113	1/1	0.97	0.04	38,38,38,38	0
56	MG	DA	3063	1/1	0.97	0.07	42,42,42,42	0
56	MG	CA	3143	1/1	0.97	0.05	74,74,74,74	0
56	MG	AA	1652	1/1	0.97	0.10	49,49,49,49	0
56	MG	DA	3030	1/1	0.97	0.11	34,34,34,34	0
56	MG	DA	3031	1/1	0.97	0.04	34,34,34,34	0
56	MG	DA	3001	1/1	0.97	0.06	62,62,62,62	0
56	MG	DA	3073	1/1	0.97	0.05	38,38,38,38	0
56	MG	DA	3159	1/1	0.97	0.10	62,62,62,62	0
56	MG	DA	3034	1/1	0.97	0.04	33,33,33,33	0
56	MG	CA	3088	1/1	0.97	0.13	68,68,68,68	0
56	MG	DA	3077	1/1	0.97	0.05	70,70,70,70	0
56	MG	DA	3105	1/1	0.98	0.04	41,41,41,41	0
56	MG	DA	3080	1/1	0.98	0.04	61,61,61,61	0
56	MG	CA	3040	1/1	0.98	0.06	59,59,59,59	0
56	MG	DA	3061	1/1	0.98	0.05	60,60,60,60	0
56	MG	DA	3024	1/1	0.98	0.05	64,64,64,64	0
56	MG	DA	3048	1/1	0.98	0.06	35,35,35,35	0
60	ZN	C5	101	1/1	0.98	0.07	117,117,117,117	0
56	MG	DA	3064	1/1	0.98	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1634	1/1	0.98	0.10	78,78,78,78	0
56	MG	DB	202	1/1	0.98	0.04	40,40,40,40	0
56	MG	DA	3091	1/1	0.98	0.12	36,36,36,36	0
56	MG	AA	1637	1/1	0.98	0.08	57,57,57,57	0
56	MG	DA	3068	1/1	0.98	0.05	70,70,70,70	0
56	MG	DA	3039	1/1	0.98	0.04	39,39,39,39	0
56	MG	DA	3052	1/1	0.98	0.11	41,41,41,41	0
56	MG	BA	1635	1/1	0.98	0.09	72,72,72,72	0
56	MG	DR	201	1/1	0.98	0.27	66,66,66,66	0
56	MG	BA	1615	1/1	0.98	0.06	62,62,62,62	0
56	MG	AA	1633	1/1	0.98	0.10	72,72,72,72	0
56	MG	DA	3075	1/1	0.98	0.04	48,48,48,48	0
56	MG	DA	3019	1/1	0.98	0.04	34,34,34,34	0
56	MG	AA	1665	1/1	0.98	0.10	78,78,78,78	0
56	MG	DA	3102	1/1	0.98	0.07	35,35,35,35	0
56	MG	DA	3078	1/1	0.98	0.09	72,72,72,72	0
56	MG	DA	3059	1/1	0.98	0.05	42,42,42,42	0
56	MG	DA	3023	1/1	0.99	0.03	41,41,41,41	0
56	MG	DA	3037	1/1	0.99	0.07	37,37,37,37	0
56	MG	DA	3013	1/1	0.99	0.04	52,52,52,52	0
56	MG	DA	3071	1/1	0.99	0.08	37,37,37,37	0
56	MG	DA	3014	1/1	0.99	0.07	36,36,36,36	0
56	MG	DA	3026	1/1	0.99	0.04	50,50,50,50	0
56	MG	DA	3056	1/1	0.99	0.08	44,44,44,44	0
56	MG	DA	3015	1/1	0.99	0.07	54,54,54,54	0
56	MG	DA	3123	1/1	0.99	0.05	43,43,43,43	0
56	MG	BA	1610	1/1	0.99	0.05	69,69,69,69	0
56	MG	AA	1650	1/1	0.99	0.04	63,63,63,63	0
56	MG	DA	3018	1/1	0.99	0.04	54,54,54,54	0
60	ZN	D5	101	1/1	0.99	0.03	63,63,63,63	0
56	MG	DA	3045	1/1	0.99	0.06	44,44,44,44	0
56	MG	AA	1649	1/1	0.99	0.04	64,64,64,64	0
56	MG	DA	3081	1/1	0.99	0.03	52,52,52,52	0
56	MG	DA	3032	1/1	0.99	0.05	31,31,31,31	0
56	MG	DA	3020	1/1	0.99	0.03	30,30,30,30	0
56	MG	DA	3084	1/1	0.99	0.06	48,48,48,48	0
56	MG	DA	3107	1/1	0.99	0.03	33,33,33,33	0
56	MG	DA	3134	1/1	0.99	0.08	65,65,65,65	0
56	MG	DB	204	1/1	0.99	0.07	57,57,57,57	0
56	MG	DA	3108	1/1	0.99	0.08	38,38,38,38	0
56	MG	DA	3011	1/1	0.99	0.10	33,33,33,33	0
56	MG	CA	3050	1/1	0.99	0.04	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3067	1/1	0.99	0.05	50,50,50,50	0
56	MG	DA	3112	1/1	0.99	0.10	44,44,44,44	0
56	MG	DA	3089	1/1	0.99	0.09	32,32,32,32	0
56	MG	DA	3086	1/1	1.00	0.05	40,40,40,40	0
56	MG	DA	3114	1/1	1.00	0.01	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.