



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:00 PM UTC

PDB ID : 4V50 / pdb_00004v50
Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA.
Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.
Deposited on : 2006-08-16
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

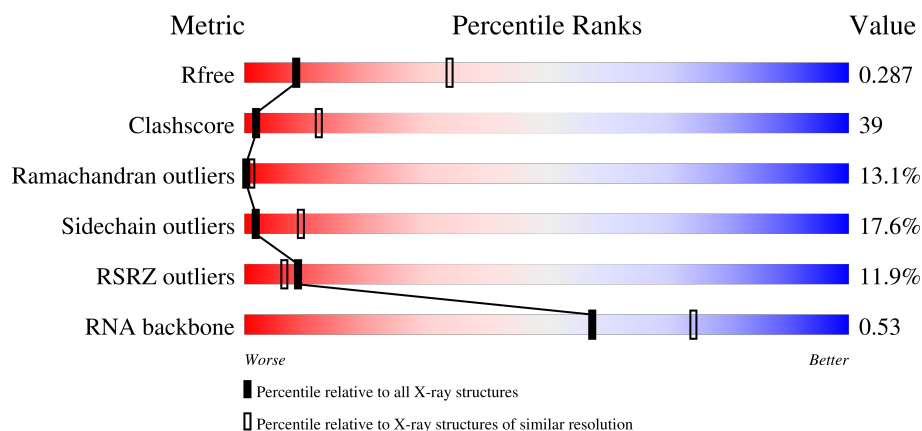
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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.



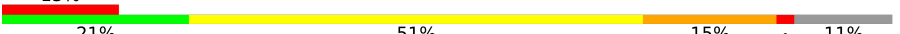
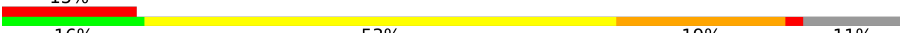
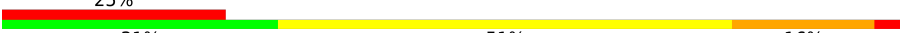
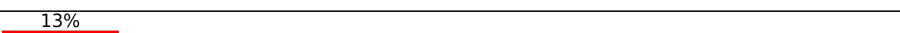
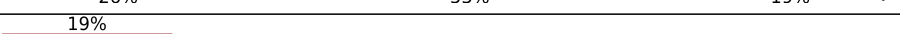
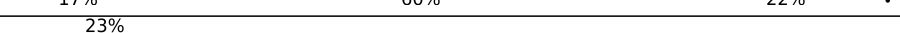
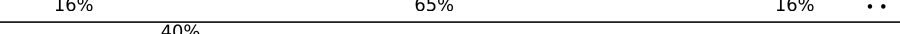
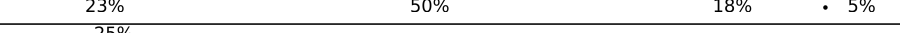
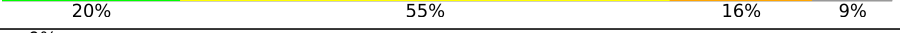
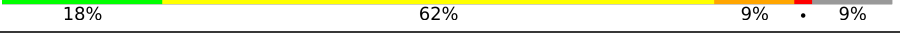
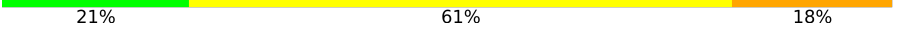
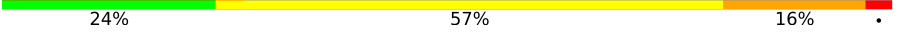
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	3% 19% 65% 14% ..
1	CA	1542	5% 20% 64% 14% ..
2	AW	17	47% 53%
2	CW	17	47% 53%

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Mol	Chain	Length	Quality of chain
3	AX	6	
3	CX	6	
4	AB	240	
4	CB	240	
5	AC	232	
5	CC	232	
6	AD	205	
6	CD	205	
7	AE	166	
7	CE	166	
8	AF	135	
8	CF	135	
9	AG	178	
9	CG	178	
10	AH	129	
10	CH	129	
11	AI	129	
11	CI	129	
12	AJ	103	
12	CJ	103	
13	AK	128	
13	CK	128	
14	AL	123	
14	CL	123	
15	AM	117	

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Mol	Chain	Length	Quality of chain
15	CM	117	
16	AN	100	
16	CN	100	
17	AO	88	
17	CO	88	
18	AP	82	
18	CP	82	
19	AQ	83	
19	CQ	83	
20	AR	74	
20	CR	74	
21	AS	91	
21	CS	91	
22	AT	86	
22	CT	86	
23	AU	70	
23	CU	70	
24	BA	120	
24	DA	120	
25	BB	2904	
25	DB	2904	
26	BC	272	
26	DC	272	
27	BD	209	
27	DD	209	

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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	178	
29	DF	178	
30	BG	176	
30	DG	176	
31	BH	149	
31	DH	149	
32	BI	141	
32	DI	141	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	114	
39	DP	114	
40	BQ	117	

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Mol	Chain	Length	Quality of chain
40	DQ	117	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	103	
44	DU	103	
45	BV	94	
45	DV	94	
46	BW	84	
46	DW	84	
47	BX	77	
47	DX	77	
48	BY	63	
48	DY	63	
49	BZ	58	
49	DZ	58	
50	B0	56	
50	D0	56	
51	B1	54	
51	D1	54	
52	B2	46	
52	D2	46	

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Mol	Chain	Length	Quality of chain
53	B3	64	
53	D3	64	
54	B4	38	
54	D4	38	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1637	-	-	-	X
55	MG	AA	1658	-	-	-	X
55	MG	CA	1655	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 285033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a RNA chain called PHE TRNA (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AW	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			
2	CW	17	Total	C	N	O	P	0	0	0
			360	161	64	118	17			

- Molecule 3 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AX	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			
3	CX	6	Total	C	N	O	P	0	0	0
			125	56	18	45	6			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
4	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
5	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
7	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
8	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
9	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
12	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

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

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
14	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
15	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
16	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
17	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
18	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
19	CQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
20	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
21	CS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
22	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 23 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
23	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
24	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
25	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
27	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
31	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
32	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
33	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
34	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
35	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
37	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BO	116	Total	C	N	O		0	0	0
			892	552	178	162				
38	DO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
39	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
40	DQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
41	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
43	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
44	DU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
45	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
46	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
47	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
48	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
49	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
50	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
51	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
52	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
53	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
54	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	60	Total	Mg	0	0
			60	60		
55	AX	2	Total	Mg	0	0
			2	2		
55	BB	118	Total	Mg	0	0
			118	118		
55	BJ	1	Total	Mg	0	0
			1	1		
55	CA	56	Total	Mg	0	0
			56	56		
55	CX	1	Total	Mg	0	0
			1	1		
55	CN	1	Total	Mg	0	0
			1	1		
55	DB	119	Total	Mg	0	0
			119	119		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Zn	0	0
			1	1		
56	D4	1	Total	Zn	0	0
			1	1		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	287	Total O 287 287	0	0
57	AX	9	Total O 9 9	0	0
57	AE	3	Total O 3 3	0	0
57	AI	1	Total O 1 1	0	0
57	AK	2	Total O 2 2	0	0
57	AL	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	BB	532	Total O 532 532	0	0
57	BC	7	Total O 7 7	0	0
57	BE	3	Total O 3 3	0	0
57	BH	3	Total O 3 3	0	0
57	BJ	3	Total O 3 3	0	0
57	BL	2	Total O 2 2	0	0
57	BN	3	Total O 3 3	0	0
57	B2	1	Total O 1 1	0	0
57	B4	5	Total O 5 5	0	0
57	CA	264	Total O 264 264	0	0
57	CX	6	Total O 6 6	0	0
57	CE	2	Total O 2 2	0	0
57	CI	3	Total O 3 3	0	0

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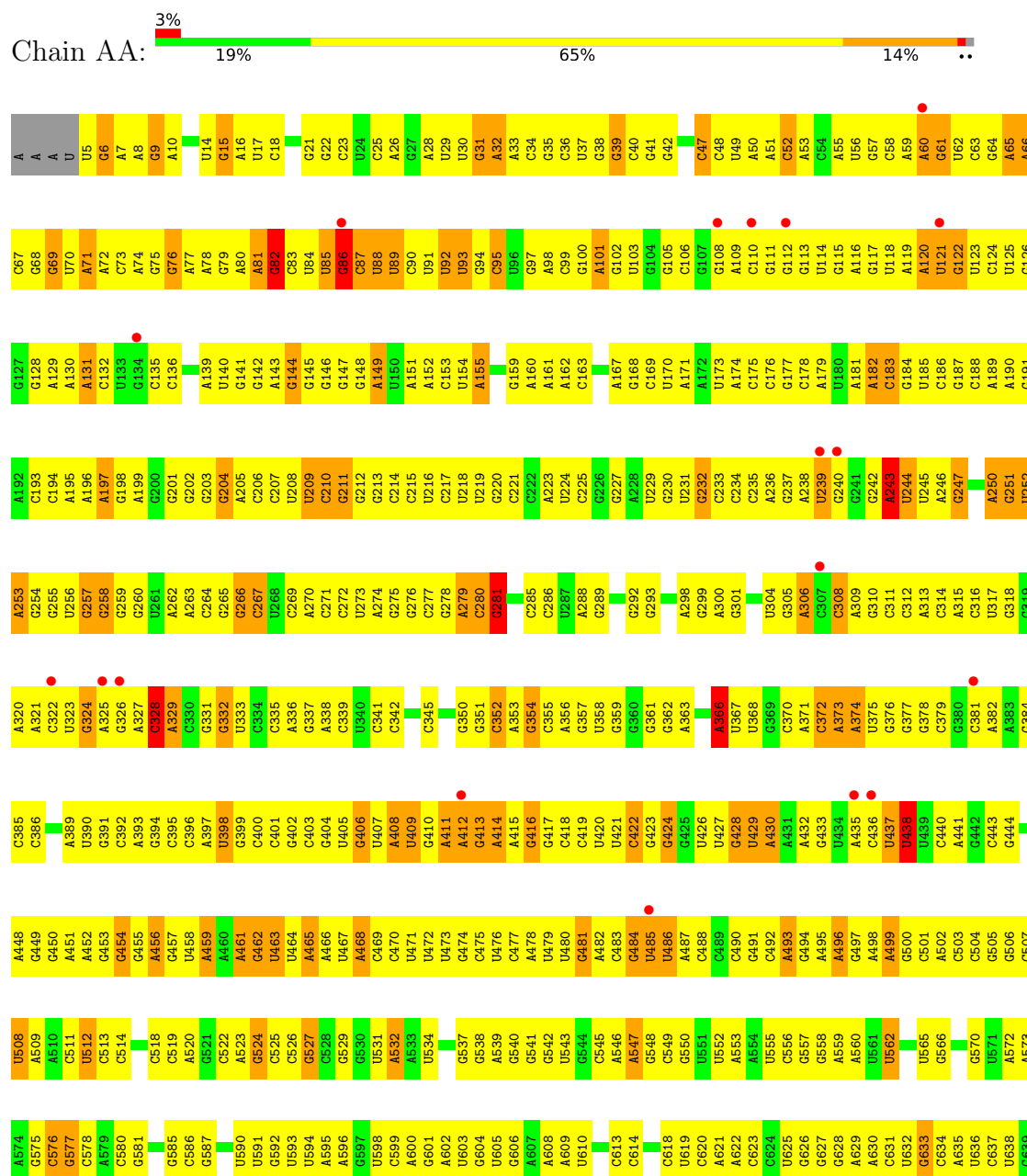
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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57	CN	1	Total 1	O 1	0	0
57	CP	1	Total 1	O 1	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	1	Total 1	O 1	0	0
57	DB	531	Total 531	O 531	0	0
57	DC	7	Total 7	O 7	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	2	Total 2	O 2	0	0
57	DL	3	Total 3	O 3	0	0
57	DN	3	Total 3	O 3	0	0
57	DT	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D4	4	Total 4	O 4	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.

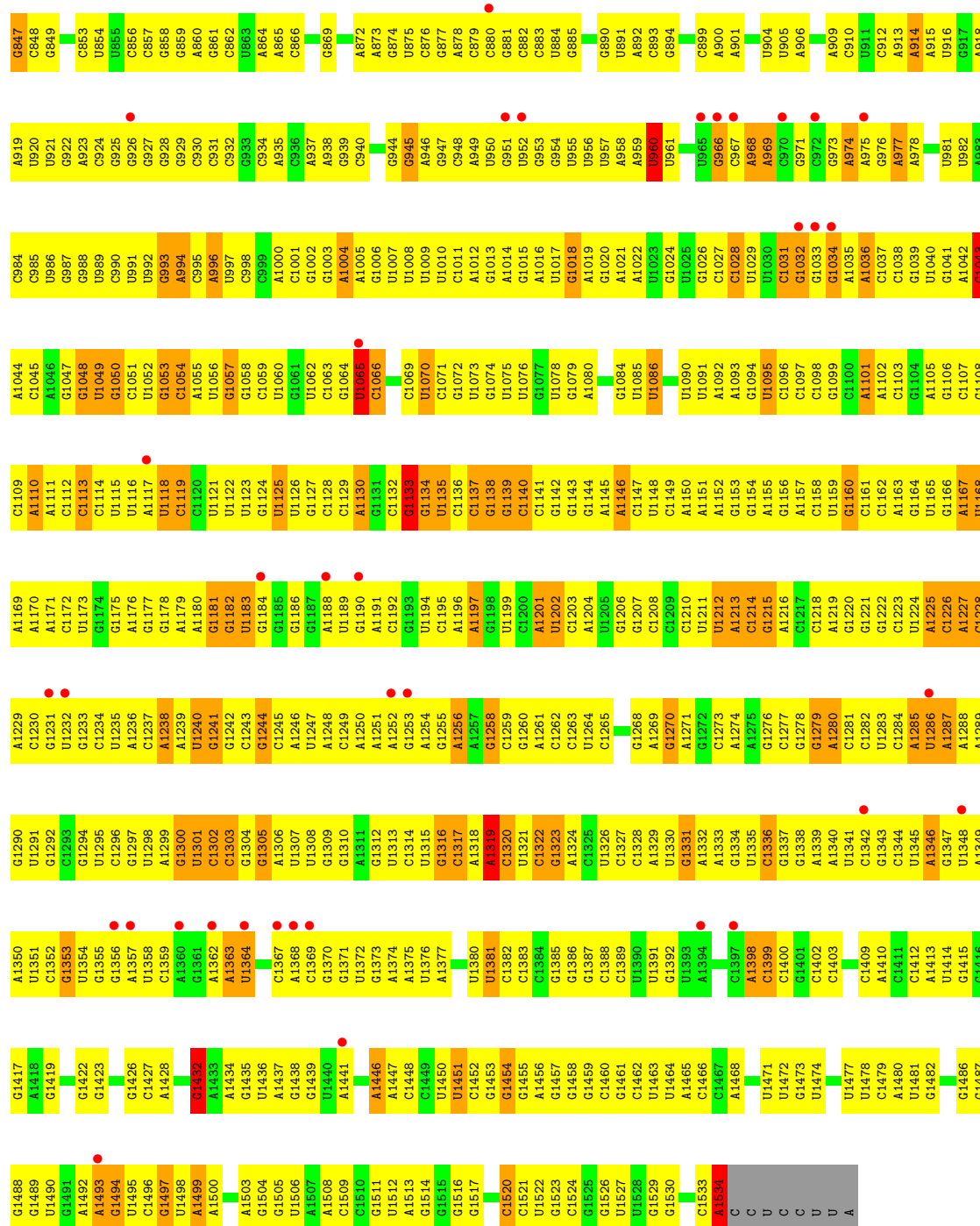
• Molecule 1: 16S ribosomal RNA

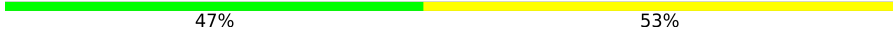


G1482	A1413	C1344	C1284	G1180	C1100	A1036	G976	C912	G836	G771	A640
G1483	U1414	U1345	A1285	C1161	A1101	C1037	A977	A913	U837	U707	U641
G1486	G1415	G1346	U1286	C1162	A1102	C1038	A978	A914	G838	C708	A642
G1487	G1416	A1287	C1226	A1163	C1103	G1039	C979	C910	C839	U709	C643
G1488	G1417	U1348	A1288	A1164	G1104	U1040	C980	U916	C940	U644	G645
G1489	A1418	A1349	A1289	U1165	A1105	G1041	U981	G917	C941	G711	G646
U1490	G1419	A1350	G1290	C1166	G1106	A1042	U982	A918	U942	A712	G646
G1491	C1351	U1352	U1291	A1167	C1107	G1043	A983	A919	U943	G713	C647
A1492	G1422	G1423	G1292	U1168	G1108	A1044	C984	U920	G844	G714	A648
A1493	G1423	C1353	C1293	A1169	C1109	C1045	C985	U921	A945	A715	A649
A1494	G1424	U1354	G1294	A1170	A1110	A1046	U986	G922	G846	A716	G650
U1495	G1426	G1355	U1295	C1171	C1111	A1047	C987	A923	G847	C783	C651
C1496	C1427	G1356	C1296	C1172	A1112	G1048	C988	C924	C948	U717	U652
G1497	A1428	A1357	G1297	U1173	C1113	U1049	U989	G925	G949	A718	U653
U1498	U1358	U1358	U1298	G1174	C1114	G1050	C990	G926	C853	A787	
A1499	A1432	C1359	A1299	G1175	U1115	C1051	U991	G927	G722	G722	U657
A1500	A1433	A1360	G1300	A1176	U1116	U1052	U992	G928	U854	G723	C658
	A1434	G1361	U1301	G1177	A1117	G1053	G993	G929	U855	U724	U659
A1503	U1435	A1362	C1302	G1178	U1118	C1054	A994	C930	C856	G725	C660
G1504	U1436	A1363	C1303	A1179	C1119	A1055	C995	C931	C857	C726	
G1505	A1437	U1364	G1304	A1180	C1120	U1056	A996	C932	G858	G727	A663
U1506	G1438	G1365	A1305	G1181	U1121	G1057	U997	G933	C859	C795	A664
A1507	G1439	C1366	C1245	G1182	U1122	G1058	C998	C934	A860	C796	A665
A1508	U1440	C1367	U1307	U1183	U1123	C1059	C999	A935	C797	C731	G666
C1509	A1441	U1368	U1247	G1184	G1124	U1060	A1000	C936	C936	C732	G667
G1510		C1369	A1248		U1125	G1361	C1001	A937	A864	G733	G668
U1511	A1446	G1370	C1249	A1188	U1126	U1062	G1002	A938	A865	G734	G669
U1512	A1447	G1371	A1250	U1189	G1127	C1063	G1003	G939	C866	C735	G670
A1513	C1448	U1372	G1312	G1190	C1128	A1004	U1010	C940	C867	G736	G671
G1514	G1373	A1374	A1251	A1191	C1129	U1065	C1011	C948	C877	C744	U672
U1515	C1449	C1374	A1252	A1192	A1130	U1066	A1012	U950	A878	C745	C679
U1516	U1450	A1375	G1253	G1193	G1131	C1069	A1014	G951	C879	A746	A673
U1451	U1451	A1376	A1254	G1194	C1132	U1070	U1015	U952	C880	A747	A675
G1452	G1376	U1376	G1255	C1195	G1133	C1071	C1016	G953	G881	G748	A676
A1518	G1453	C1377	A1256	C1196	U1134	G1072	A1017	G954	C882	C749	U677
U1519	G1454	A1378	A1257	A1197	C1135	U1073	A1018	U955	C883	U751	G683
C1520	U1380	C1320	G1258	G1198	U1136	U1074	G1019	U956	U984	C754	U684
C1521	U1381	A1320	C1259	G1199	C1137	U1075	A1020	U957	G885	G755	G685
U1522	C1382	U1321	G1260	U1199	C1138	U1076	A1021	A958	C890	A759	U686
G1523	C1383	C1322	A1261	C1200	G1139	U1077	U1022	U960	U891	C824	U687
G1524	C1384	G1323	C1262	A1201	C1140	G1078	U1023	U961	C892	G825	G688
G1525	G1386	A1324	G1263	C1202	C1141	U1079	U1024	C826	C893	G760	U689
G1526	G1387	C1325	U1264	U1203	G1142	U1080	U1025	C827	C894	U762	G690
U1527	C1388	U1326	C1265	U1204	G1143	A1081	G1026	C828	C895	G763	G691
U1528	C1389	C1327		U1205	G1144	U1086	C1027	C829	C896	C764	C692
G1529	U1390	C1328	G1268	G1206	A1145	U1090	U1028	C830	A901	G765	G700
U1463	U1391	A1329	A1269	G1207	A1146	U1091	C1029	C831	U904	A766	U701
U1464	C1466	U1330	G1270	C1208	C1147	U1092	U1030	C832	U905	A767	A702
A1465	G1392	A1331	A1271	U1211	C1148	A1093	U1031	C833	U906	A768	G703
C1467	G1397	A1332	G1272	U1212	A1150	U1094	U1032	C834	U907	U769	G704
A1468	A1398	C1333	A1273	U1213	A1151	U1095	G1032	C835	U908	C770	G705
U1471	C1399	G1334	A1274	A1214	U1152	U1096	G1033	C836	U909		
U1472	C1400	U1335	A1275	C1215	G1153	A1097	G1034	C837	U910		
U1473	G1401	C1336	G1276	G1216	U1154	A1098	G1035	C838	U911		
C1474	C1402	G1337	C1277	A1217	A1155	U1099	G1036	C839	U912		
C1475	C1403	G1338	G1278	C1218	U1156	U1099	G1037	C840	U913		
U1477	U1409	A1339	U1279	C1219	U1157	U1099	G1038	C841	U914		
U1478	U1478	U1341	A1280	C1218	U1158	U1099	G1039	C842	U915		
C1479	C1480	C1411	C1281	A1219	C1158	U1099	G1040	C843	U916		
U1481	U1481	C1412	U1283	G1222	U1159	U1099	G1041	C844	U917		

Chain CA:





Chain CW:  47% 53%



• Molecule 3: MRNA

Chain AX:  17% 33% 50%



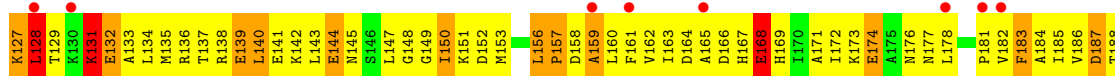
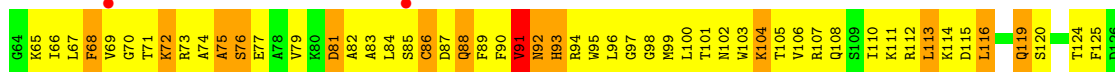
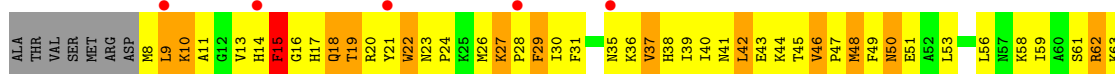
• Molecule 3: MRNA

Chain CX:  17% 33% 50%



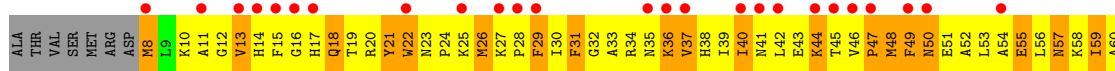
• Molecule 4: 30S ribosomal protein S2

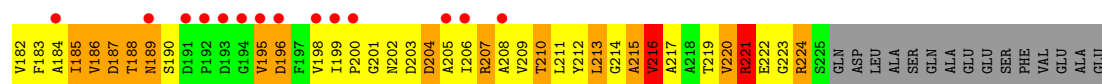
Chain AB:  8% 15% 55% 18% 9%



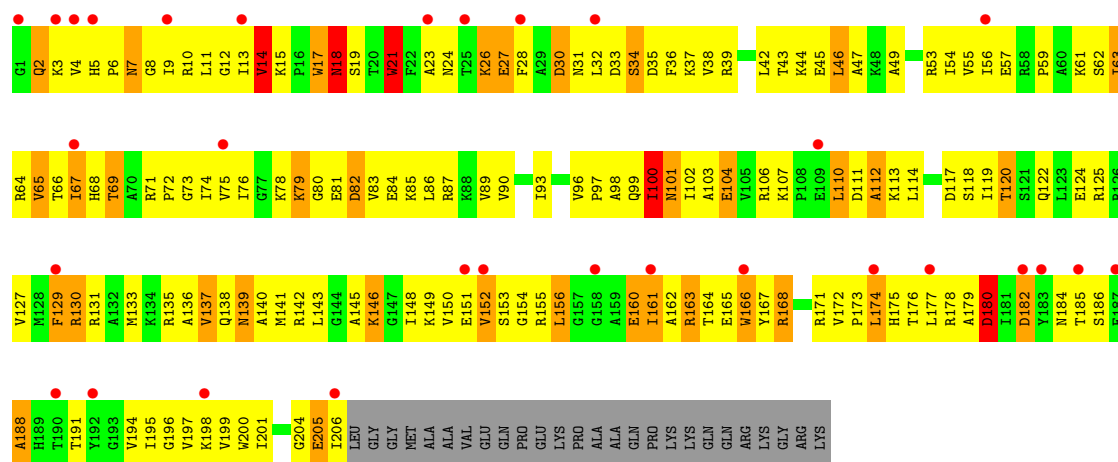
• Molecule 4: 30S ribosomal protein S2

Chain CB:  10% 26% 56% 23% 9%

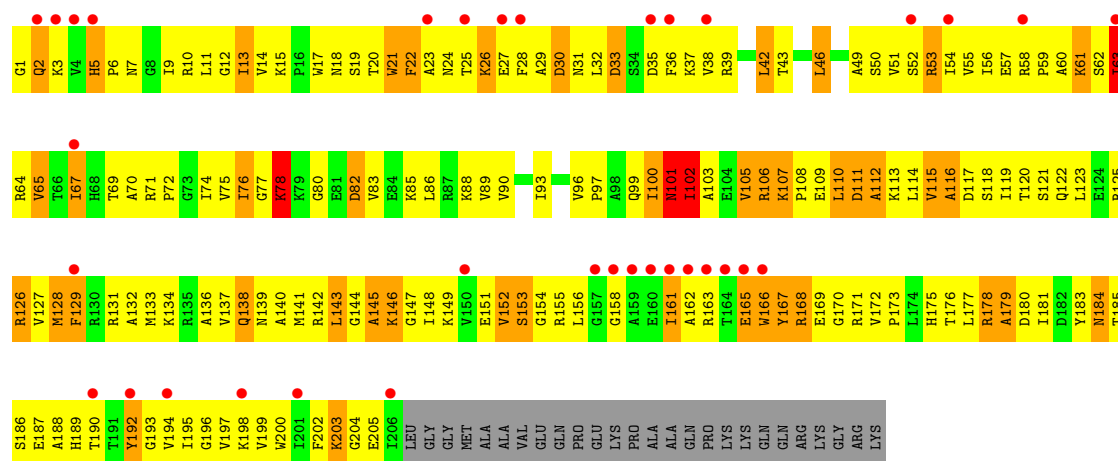
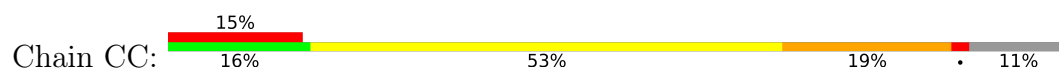




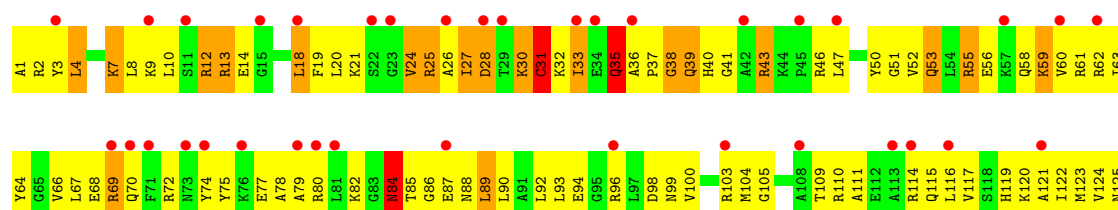
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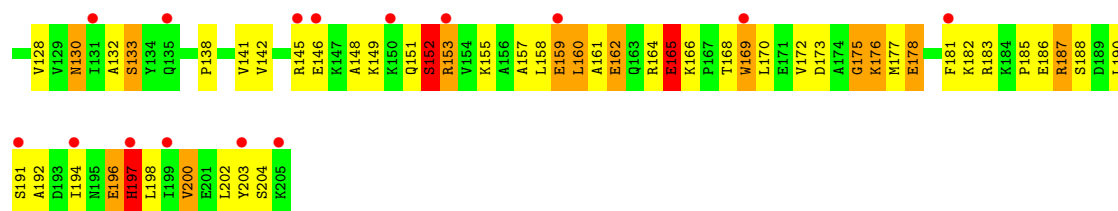


• Molecule 5: 30S ribosomal protein S3

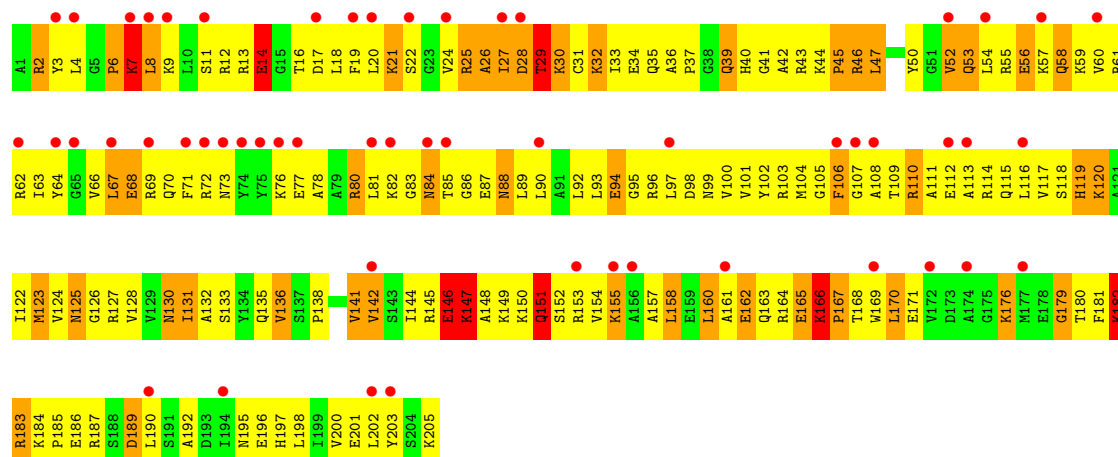
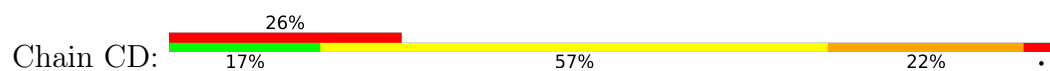


• Molecule 6: 30S ribosomal protein S4

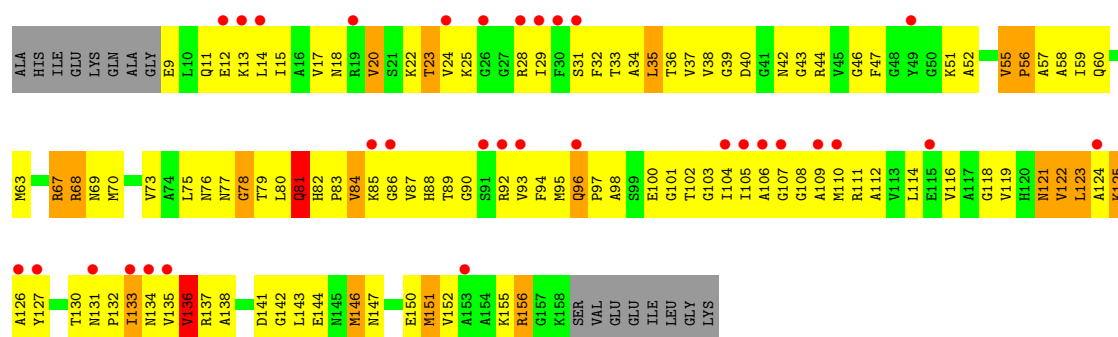




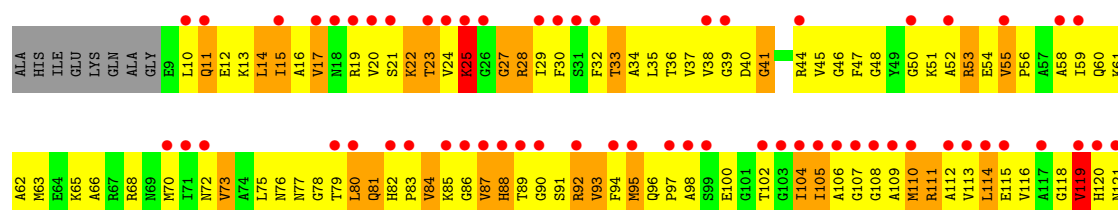
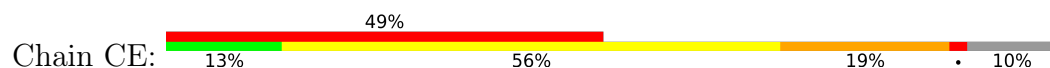
• Molecule 6: 30S ribosomal protein S4

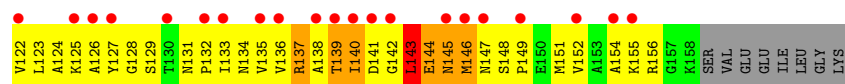


• Molecule 7: 30S ribosomal protein S5

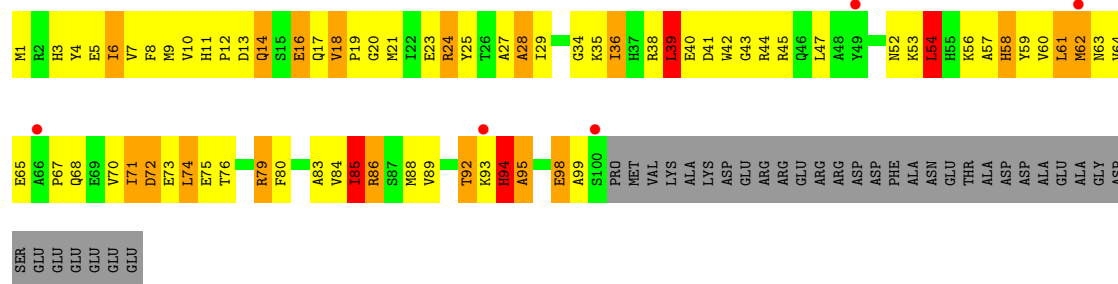
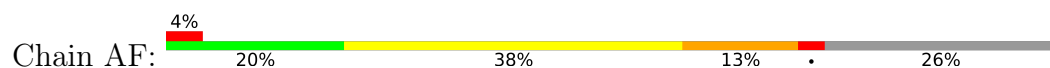


• Molecule 7: 30S ribosomal protein S5

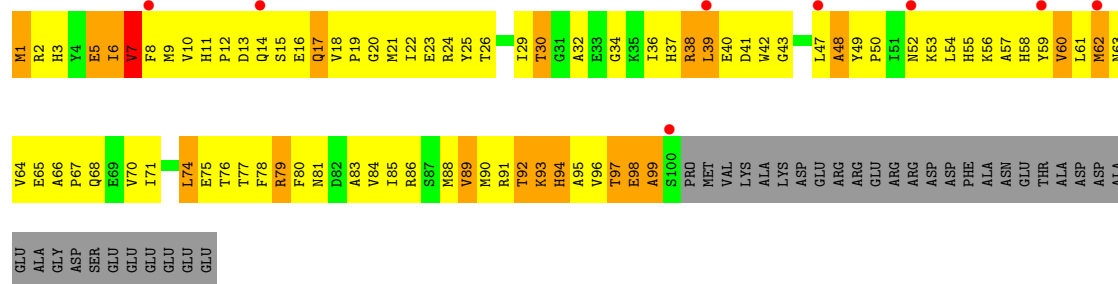
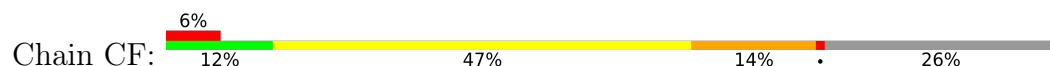




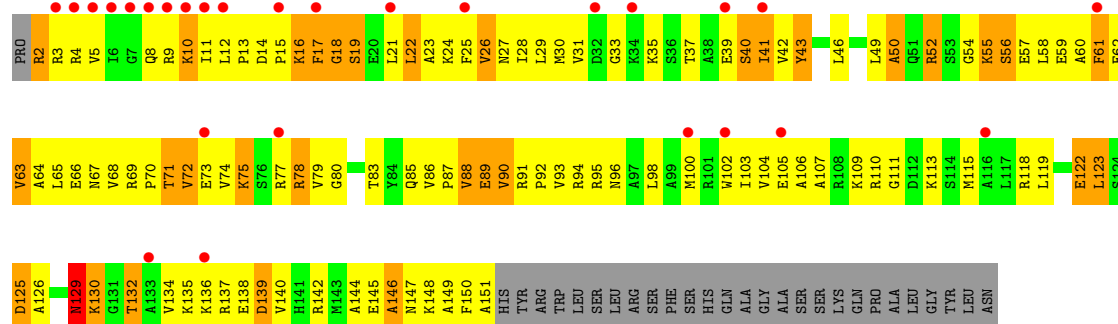
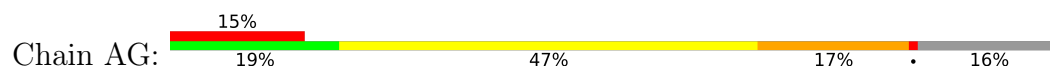
• Molecule 8: 30S ribosomal protein S6



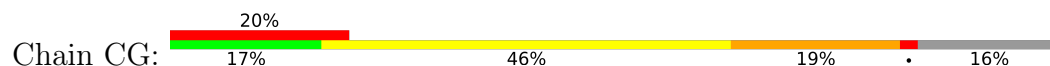
• Molecule 8: 30S ribosomal protein S6

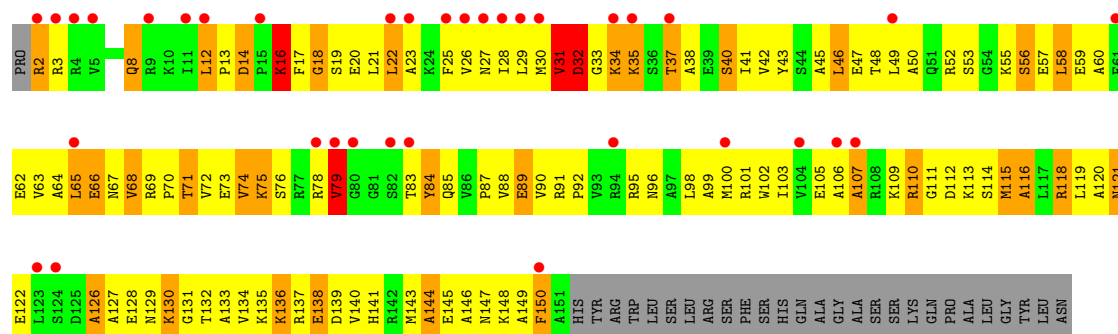


• Molecule 9: 30S ribosomal protein S7

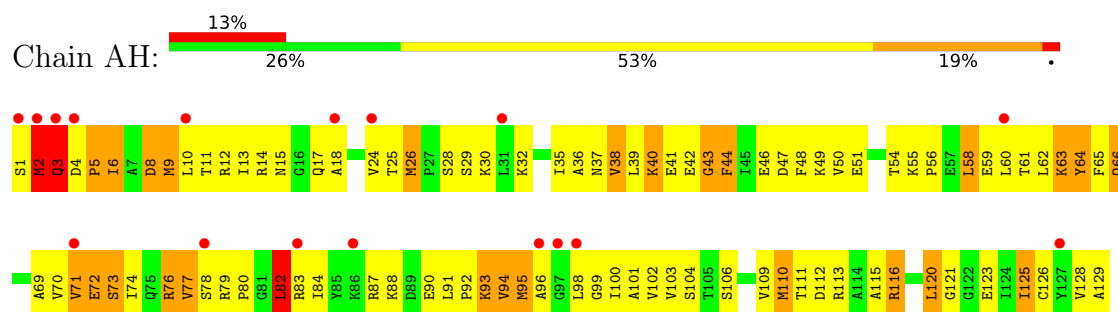


• Molecule 9: 30S ribosomal protein S7

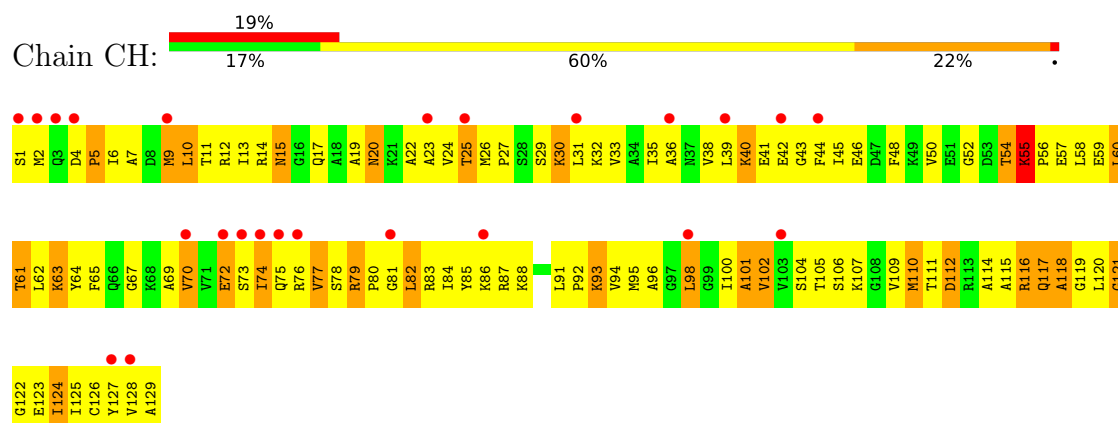




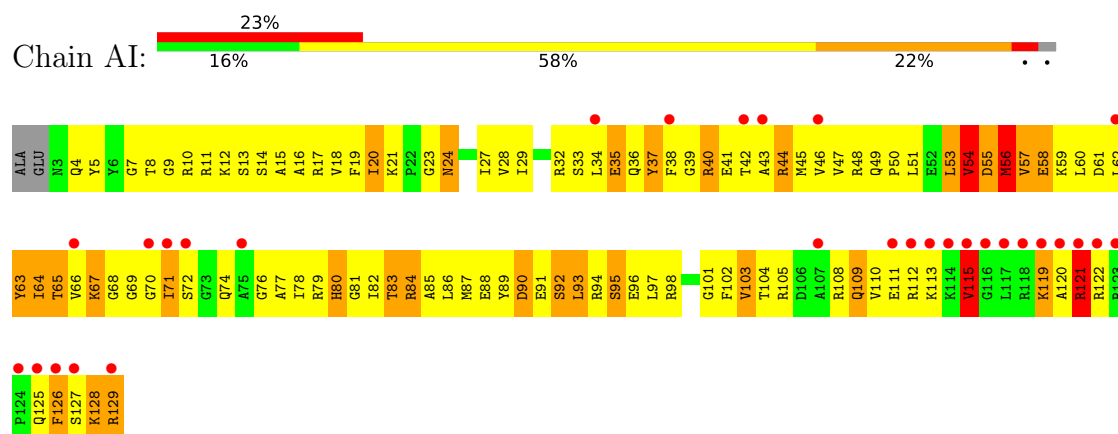
- Molecule 10: 30S ribosomal protein S8



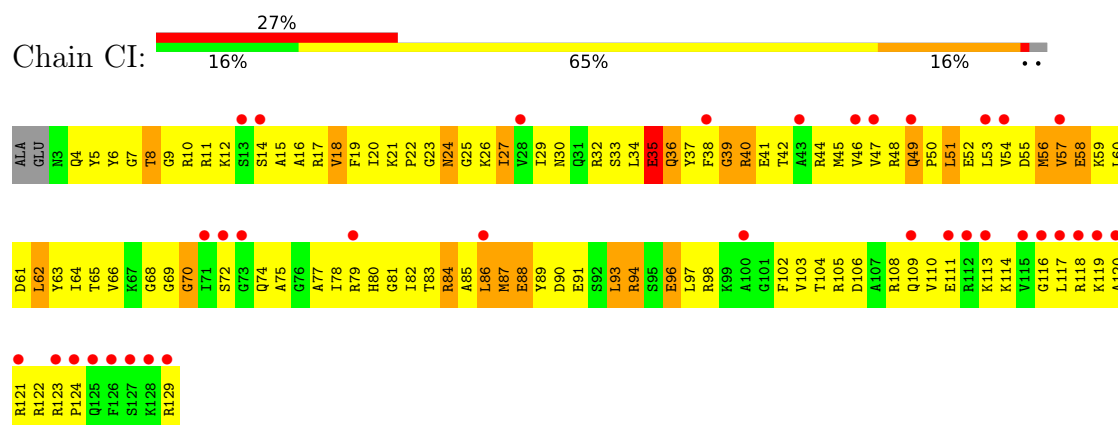
- Molecule 10: 30S ribosomal protein S8



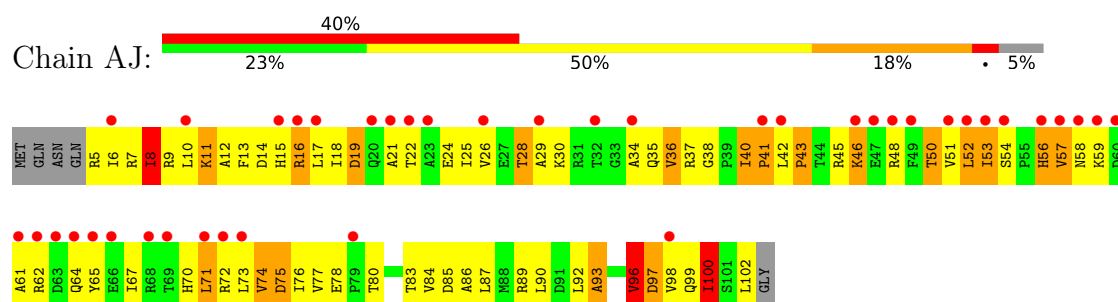
- Molecule 11: 30S ribosomal protein S9



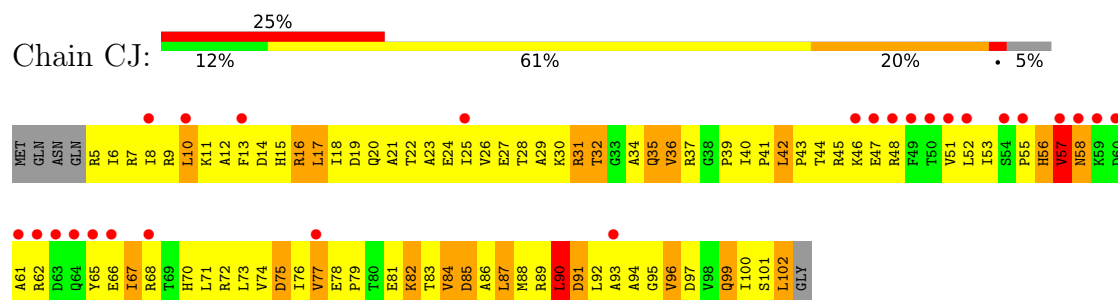
- Molecule 11: 30S ribosomal protein S9



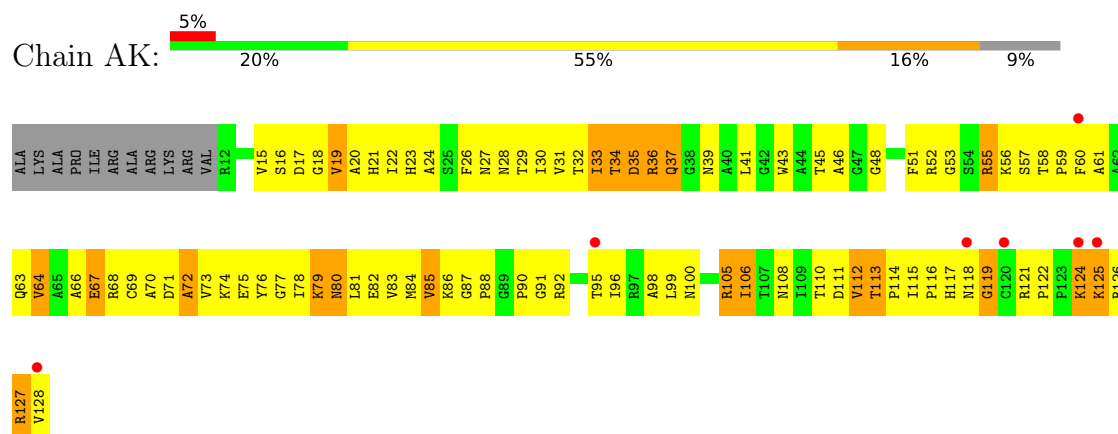
- Molecule 12: 30S ribosomal protein S10



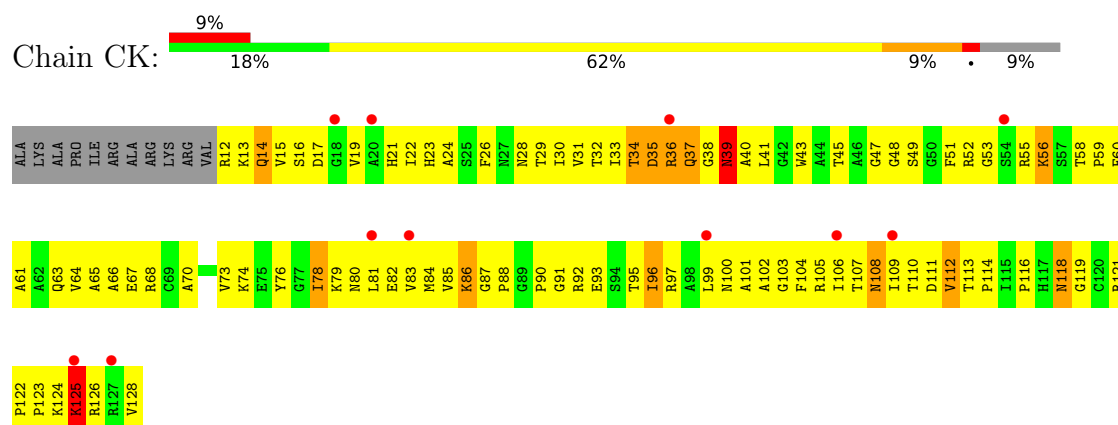
- Molecule 12: 30S ribosomal protein S10



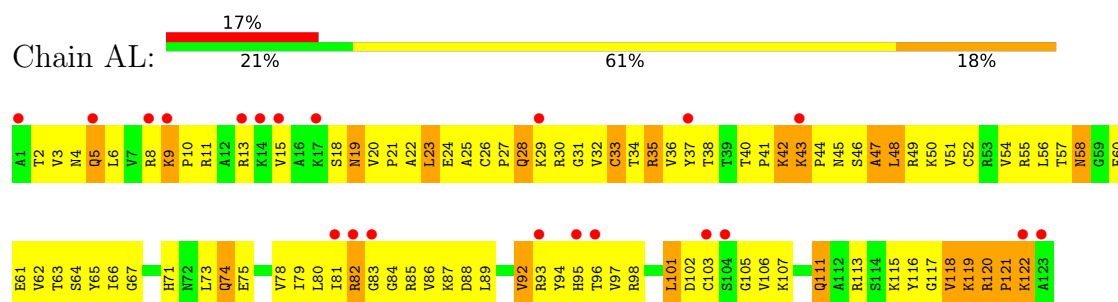
- Molecule 13: 30S ribosomal protein S11



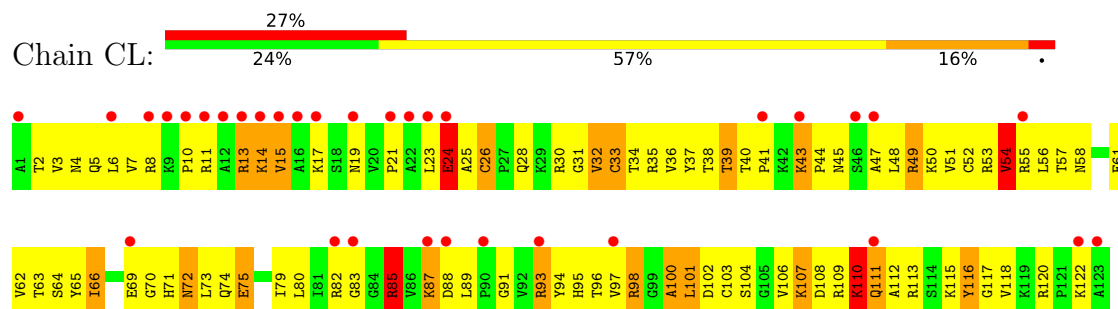
- Molecule 13: 30S ribosomal protein S11



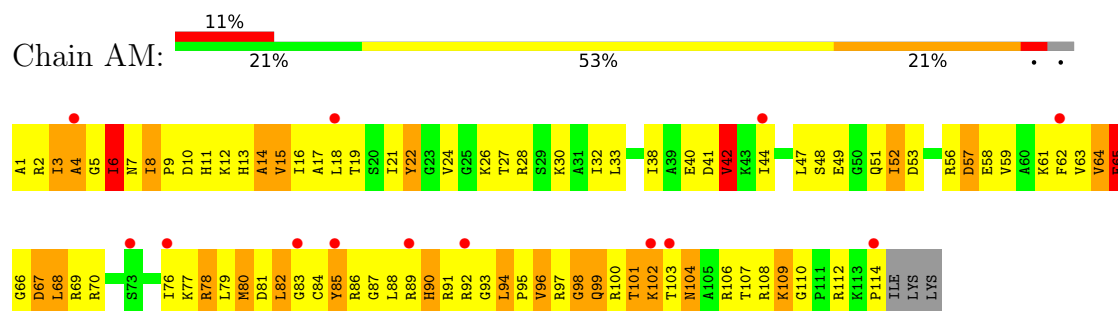
- Molecule 14: 30S ribosomal protein S12



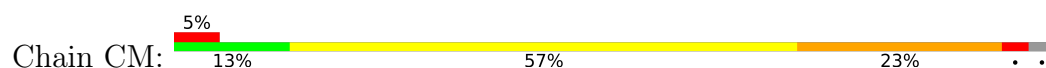
- Molecule 14: 30S ribosomal protein S12

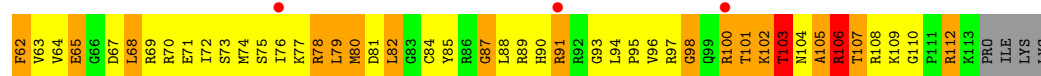
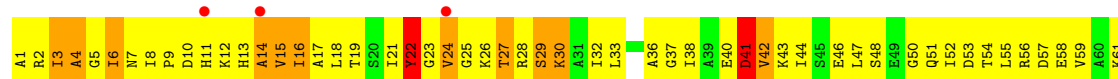


- Molecule 15: 30S ribosomal protein S13

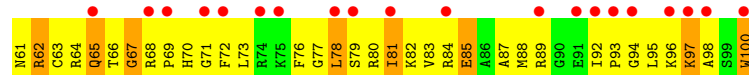
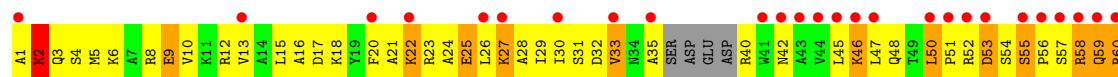
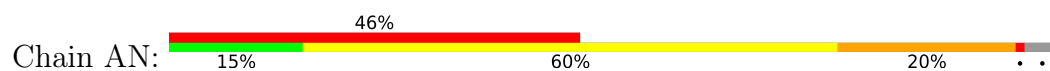


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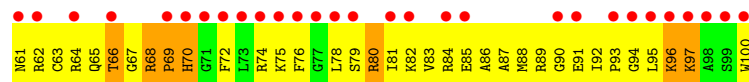
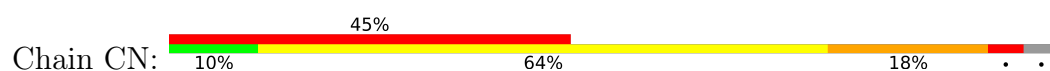




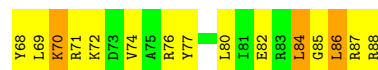
• Molecule 16: 30S ribosomal protein S14



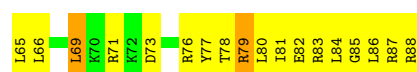
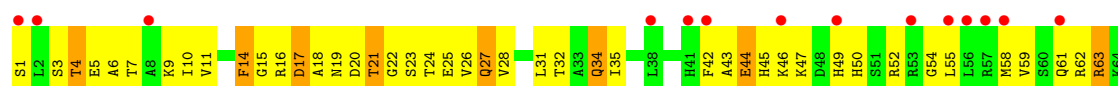
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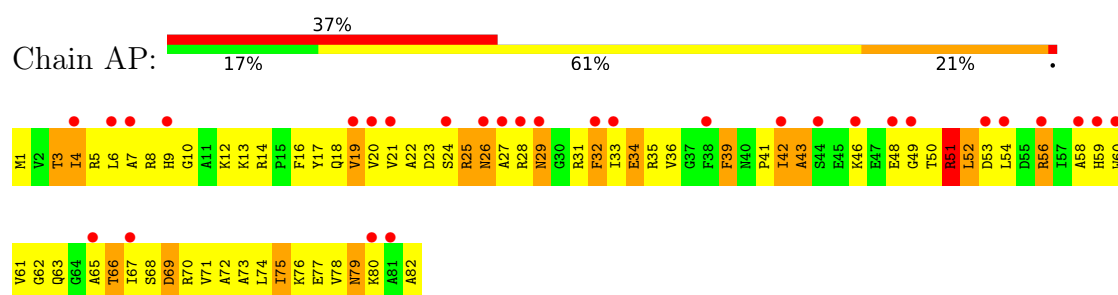
• Molecule 17: 30S ribosomal protein S15



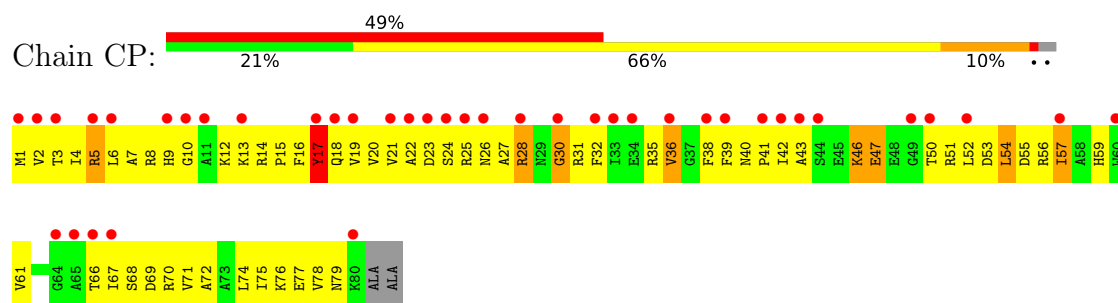
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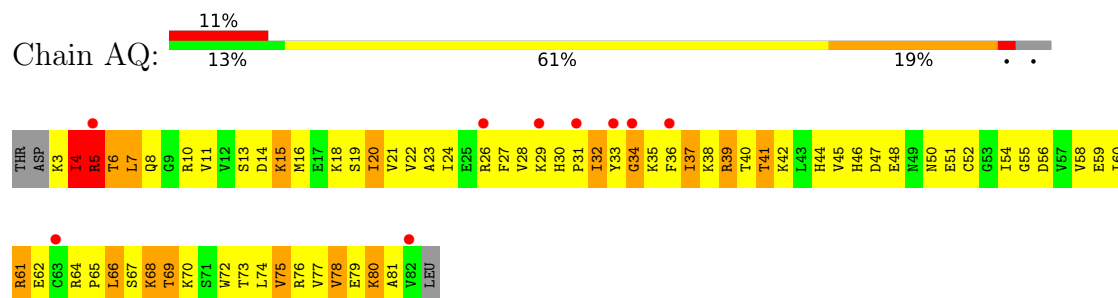
• Molecule 18: 30S ribosomal protein S16



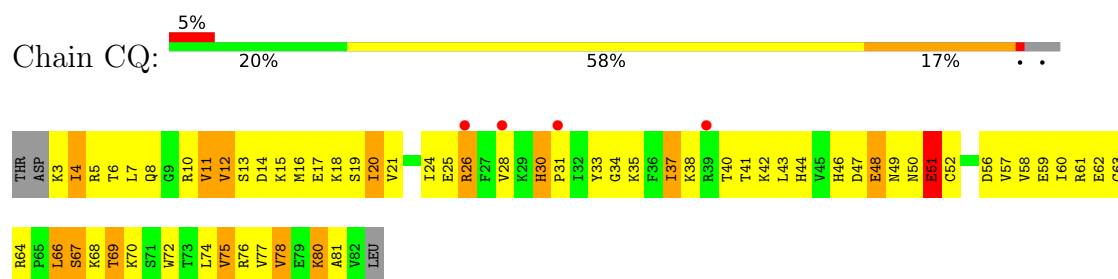
• Molecule 18: 30S ribosomal protein S16



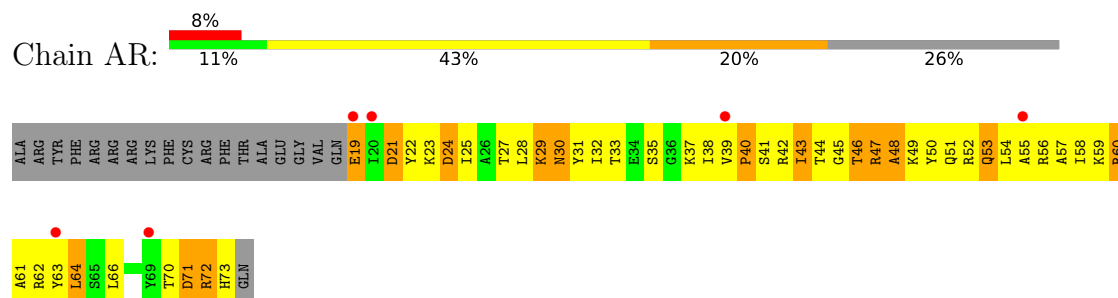
• Molecule 19: 30S ribosomal protein S17



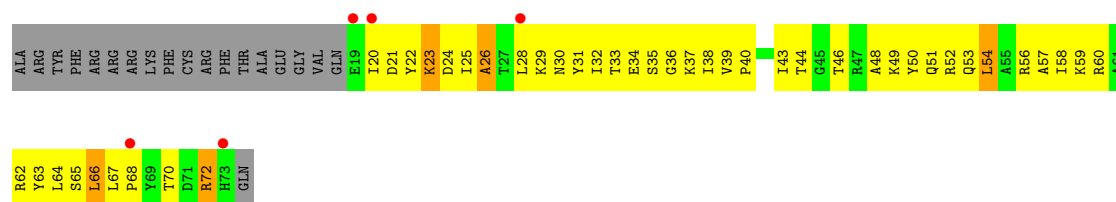
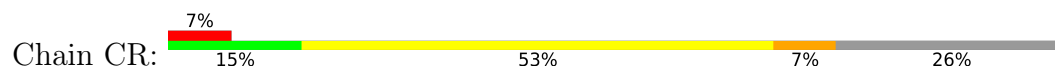
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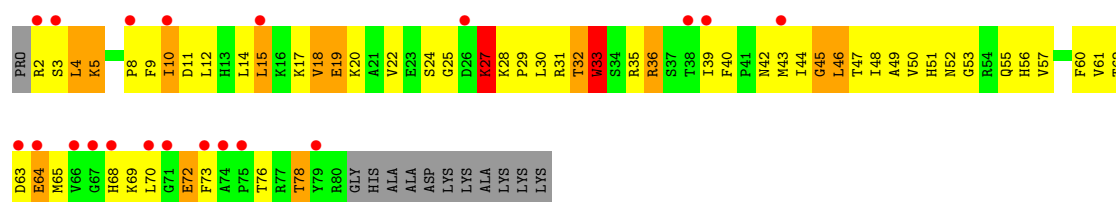
• Molecule 20: 30S ribosomal protein S18



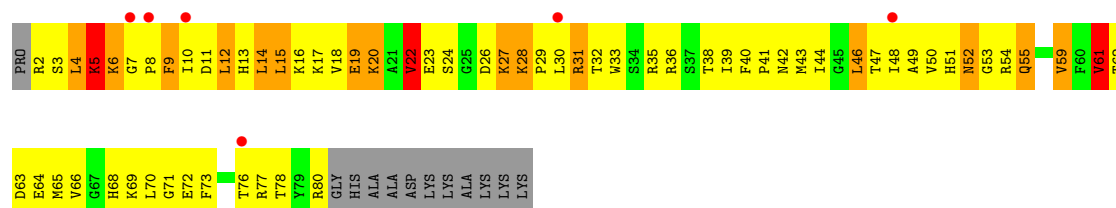
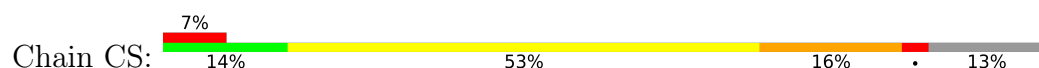
- Molecule 20: 30S ribosomal protein S18



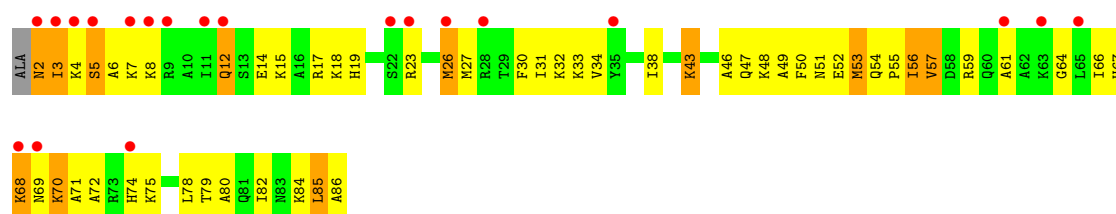
- Molecule 21: 30S ribosomal protein S19



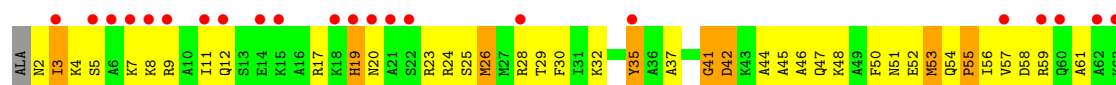
- Molecule 21: 30S ribosomal protein S19



- Molecule 22: 30S ribosomal protein S20



- Molecule 22: 30S ribosomal protein S20

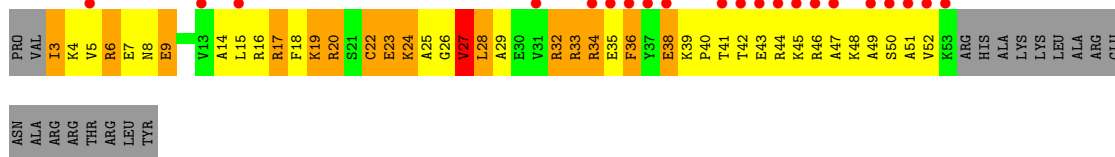




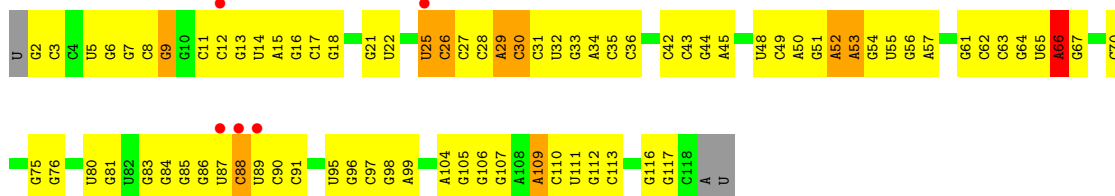
• Molecule 23: 30S ribosomal protein S21



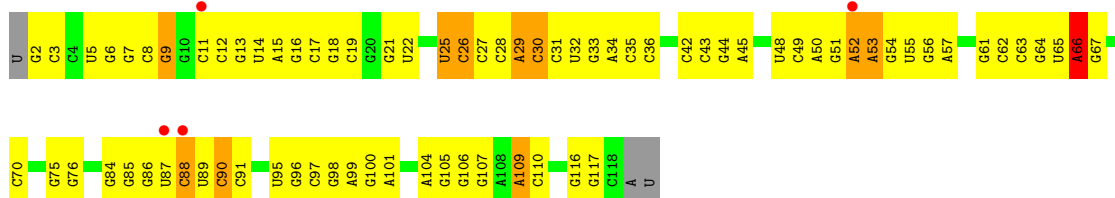
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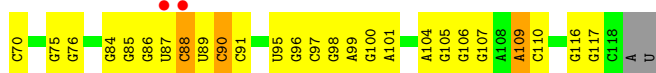
• Molecule 24: 5S ribosomal RNA



• Molecule 24: 5S ribosomal RNA



• Molecule 25: 23S ribosomal RNA





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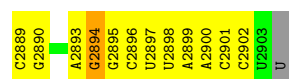
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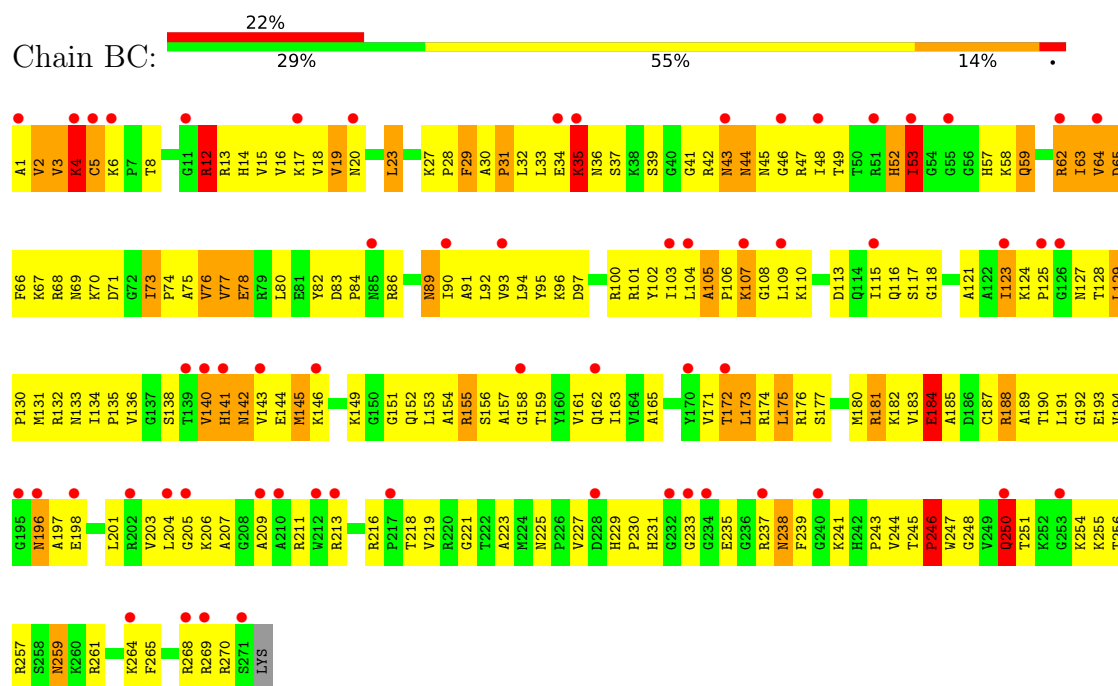




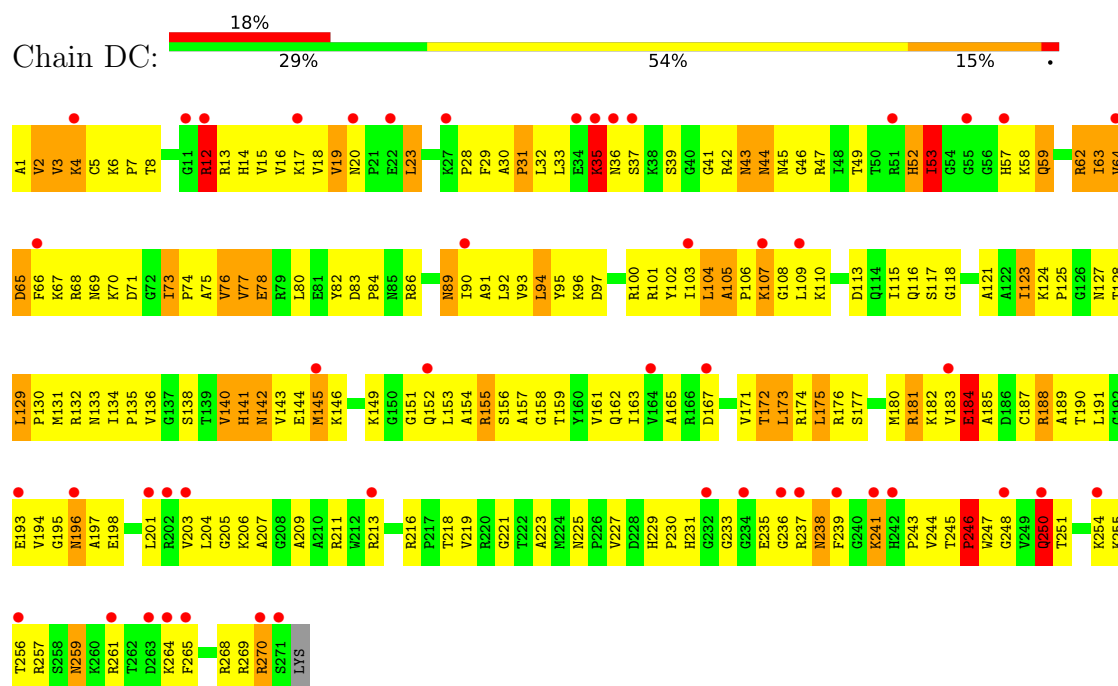
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G2846		U2584	U2585	A2506	G2378						
A2847		U2585	U2586	A2507	G2379						
U2848		U2586	U2587	A2508	G2380						
G2849		U2587	U2588	A2509	G2381						
A2850		U2588	U2589	A2510	G2382						
G2851		U2589	U2590	A2511	G2383						
U2852		U2590	U2591	A2512	G2384						
G2853		U2591	U2592	A2513	U2385						
A2854		U2592	U2593	A2514	A2386						
U2855		U2593	U2594	A2515	U2387						
G2856		U2594	U2595	A2516	G2388						
A2857		U2595	U2596	A2517	G2389						
U2858		U2596	U2597	A2518	G2390						
G2859		U2597	U2598	A2519	G2391						
A2860		U2598	U2599	A2520	A2392						
U2861		U2599	U2600	A2521	U2393						
G2862		U2600	U2601	A2522	G2394						
A2863		U2601	U2602	A2523	C2395						
U2864		U2602	U2603	A2524	G2396						
G2865		U2603	U2604	A2525	U2400						
U2866		U2604	U2605	A2526	U2401						
A2867		U2605	U2606	A2527	U2402						
U2868		U2606	U2607	A2528	U2403						
G2869		U2607	U2608	A2529	G2404						
A2870		U2608	U2609	A2530	U2405						
U2871		U2609	U2610	A2531	A2406						
G2872		U2610	U2611	A2532	U2407						
A2873		U2611	U2612	A2533	U2408						
U2874		U2612	U2613	A2534	G2409						
G2875		U2613	U2614	A2535	U2410						
A2876		U2614	U2615	A2536	G2411						
U2877		U2615	U2616	A2537	U2412						
G2878		U2616	U2617	A2538	G2413						
A2879		U2617	U2618	A2539	G2414						
U2880		U2618	U2619	A2540	G2415						
G2881		U2619	U2620	A2541	G2416						
A2882		U2620	U2621	A2542	G2417						
U2883		U2621	U2622	A2543	G2418						
G2884		U2622	U2623	A2544	G2419						
A2885		U2623	U2624	A2545	G2420						
U2886		U2624	U2625	A2546	G2421						
G2887		U2625	U2626	A2547	G2422						
A2888		U2626	U2627	A2548	G2423						
U2889		U2627	U2628	A2549	G2424						
G2890		U2628	U2629	A2550	G2425						
A2891		U2629	U2630	A2551	G2426						
U2892		U2630	U2631	A2552	G2427						
G2893		U2631	U2632	A2553	G2428						
A2894		U2632	U2633	A2554	G2429						



• Molecule 26: 50S ribosomal protein L2

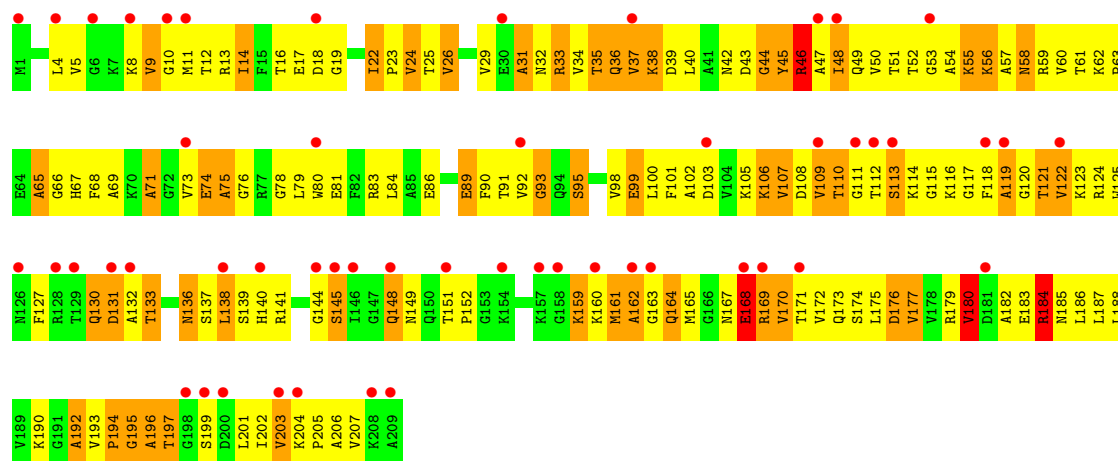


• Molecule 26: 50S ribosomal protein L2

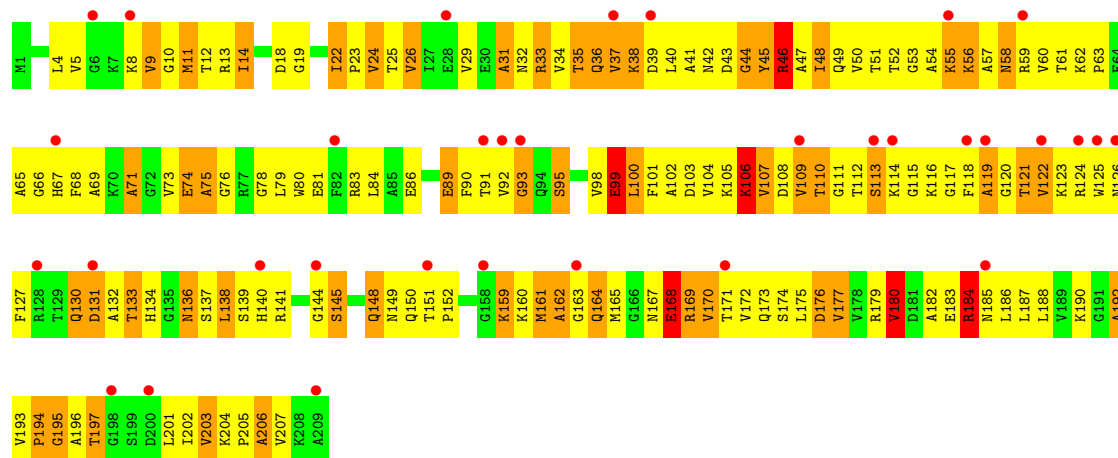


• Molecule 27: 50S ribosomal protein L3

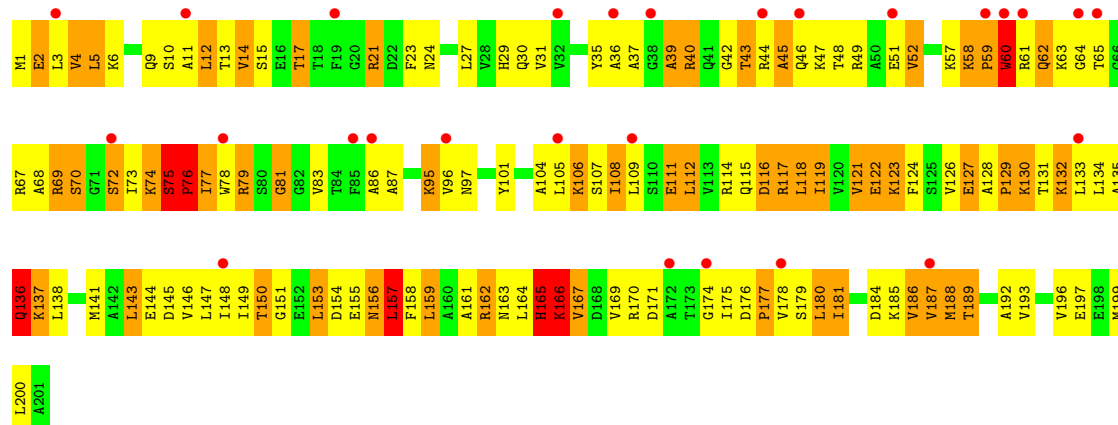




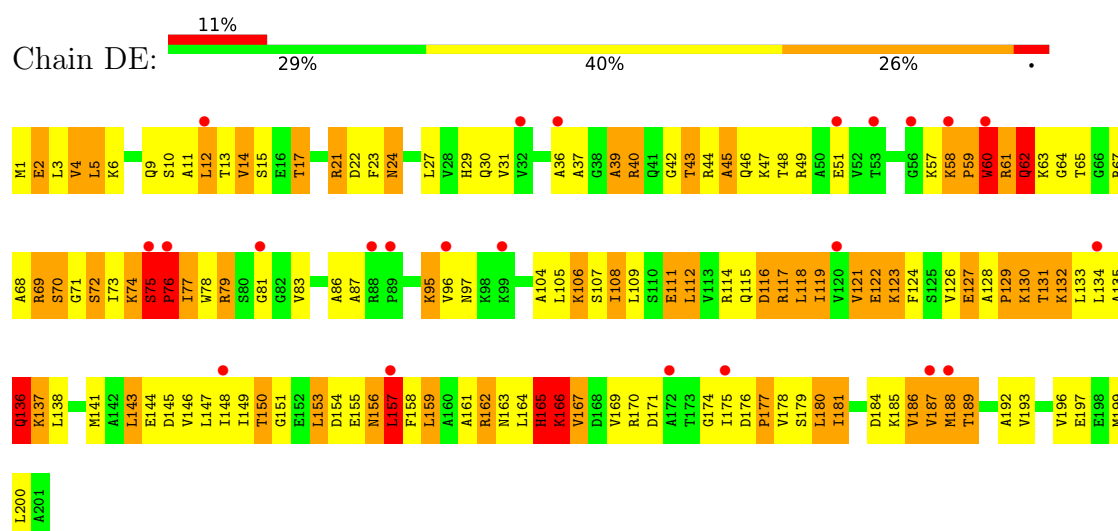
• Molecule 27: 50S ribosomal protein L3



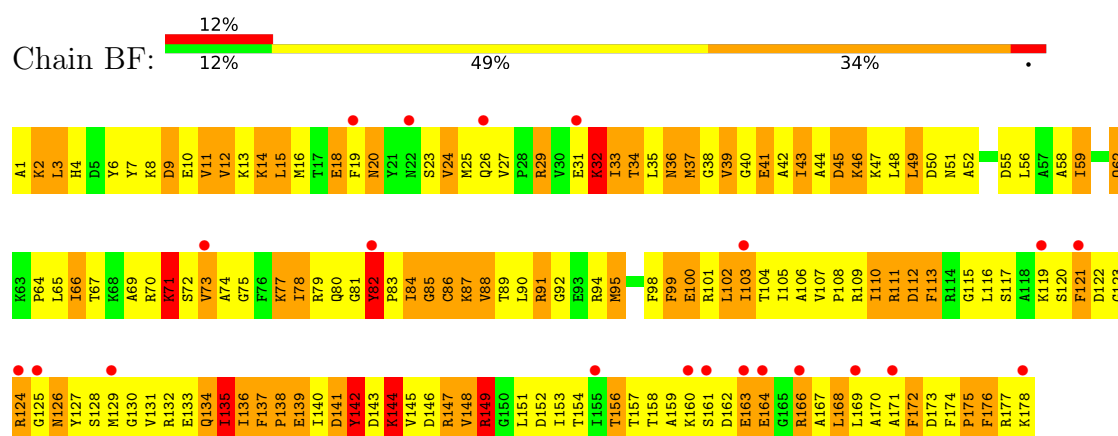
• Molecule 28: 50S ribosomal protein L4



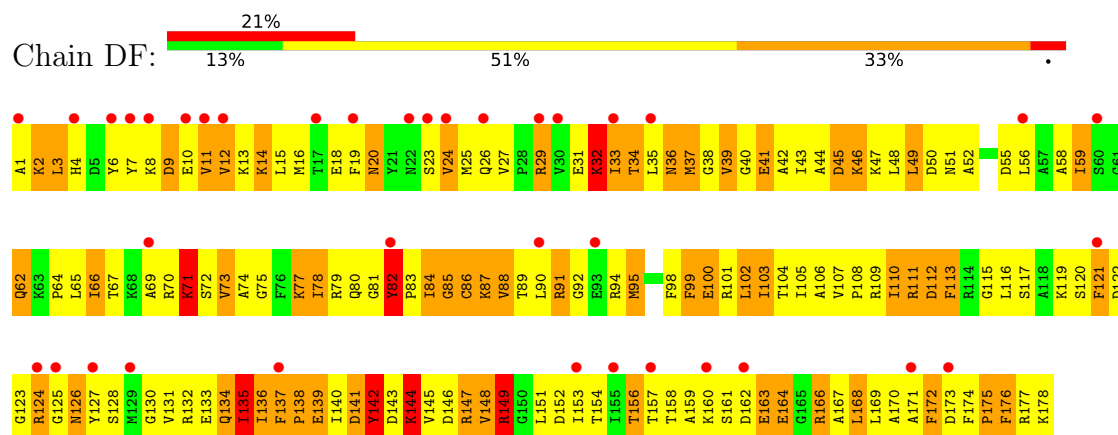
• Molecule 28: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L5

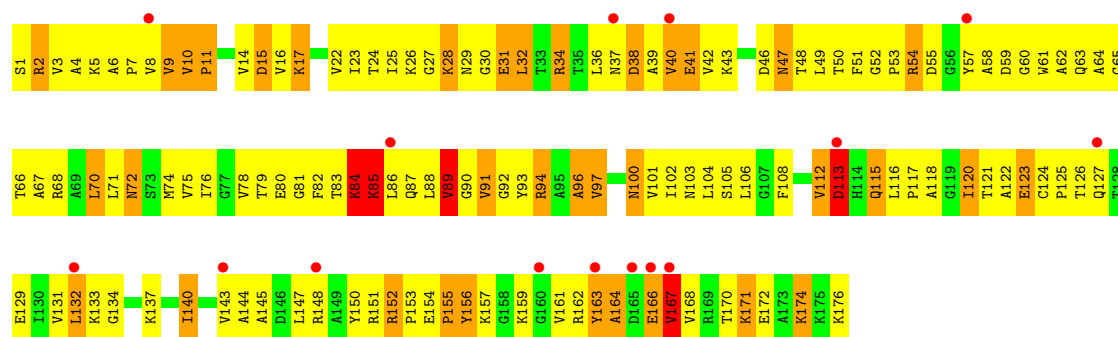


• Molecule 29: 50S ribosomal protein L5

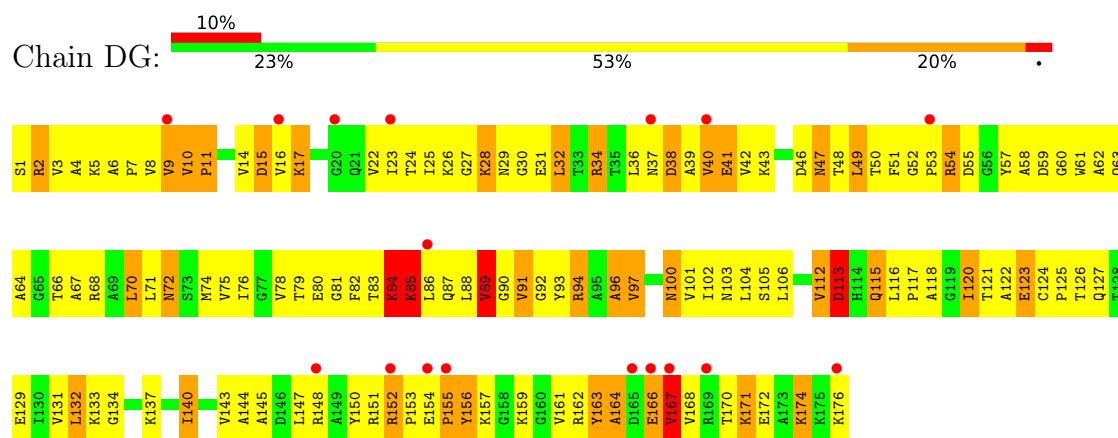


• Molecule 30: 50S ribosomal protein L6

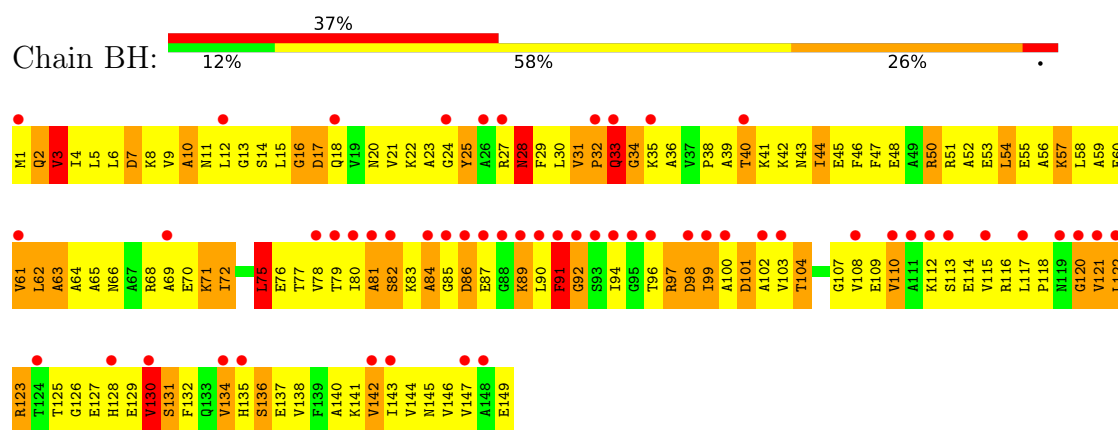




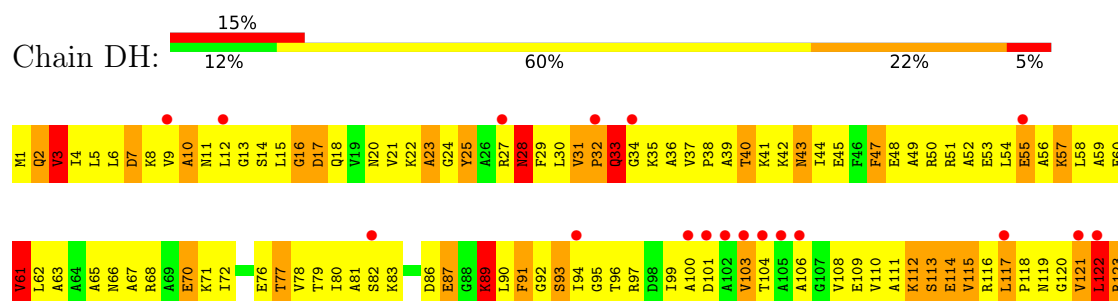
• Molecule 30: 50S ribosomal protein L6

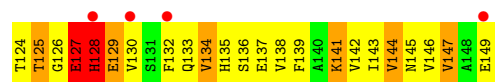


• Molecule 31: 50S ribosomal protein L9

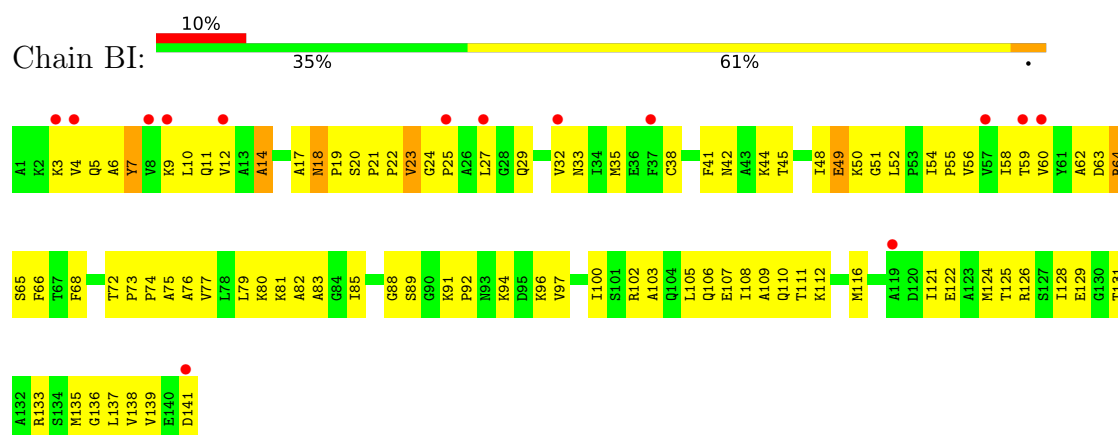


• Molecule 31: 50S ribosomal protein L9

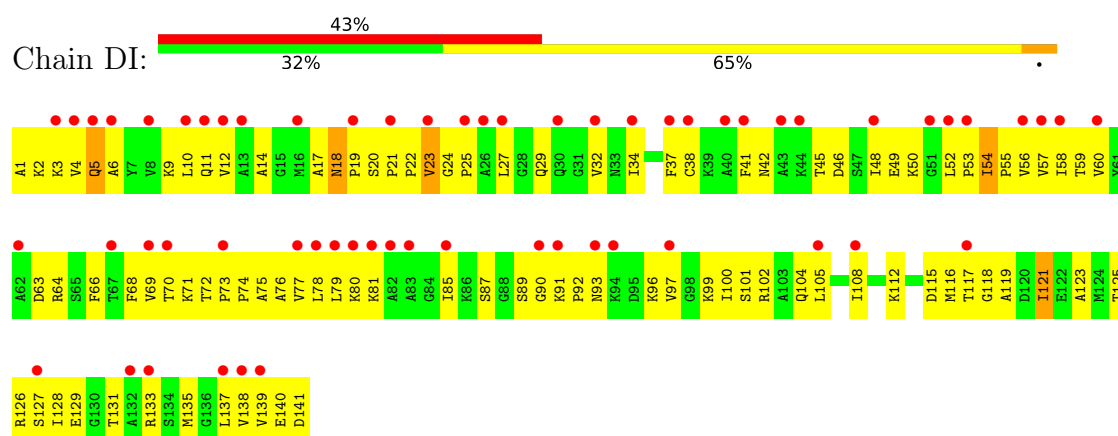




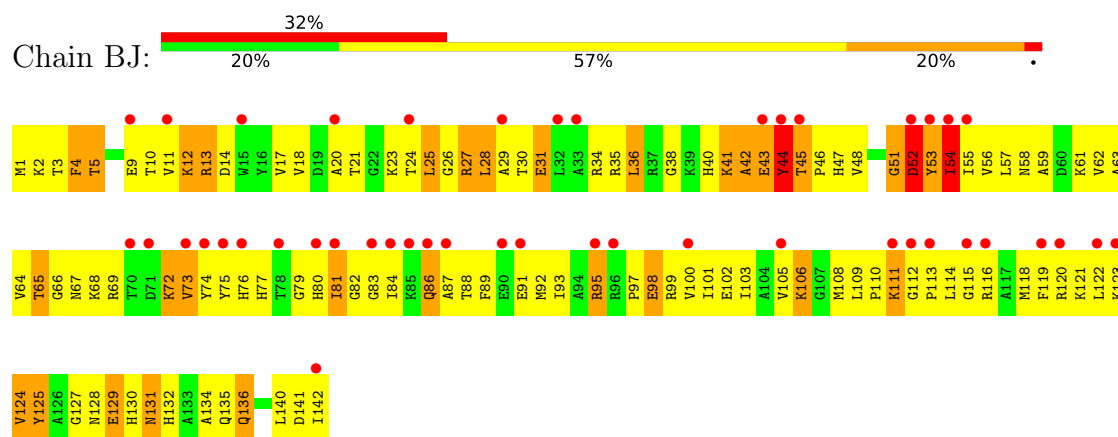
• Molecule 32: 50S ribosomal protein L11



• Molecule 32: 50S ribosomal protein L11

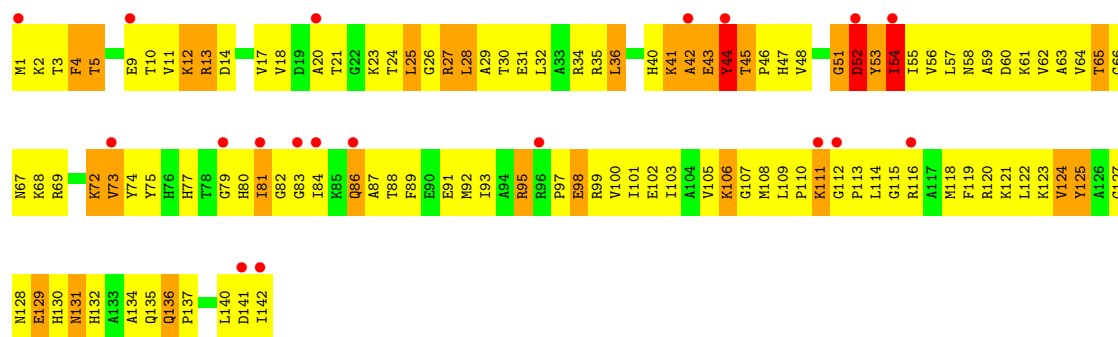


• Molecule 33: 50S ribosomal protein L13

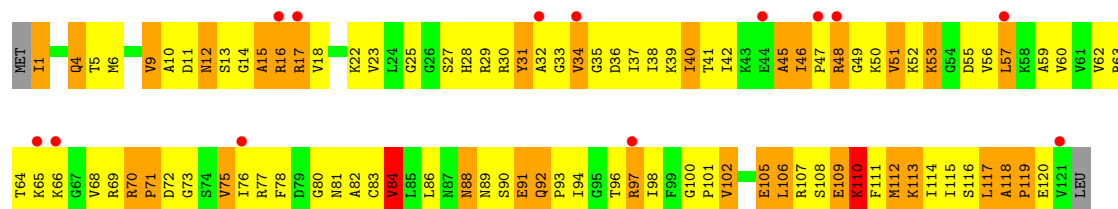
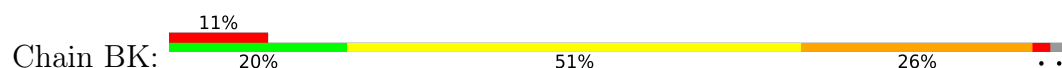


• Molecule 33: 50S ribosomal protein L13

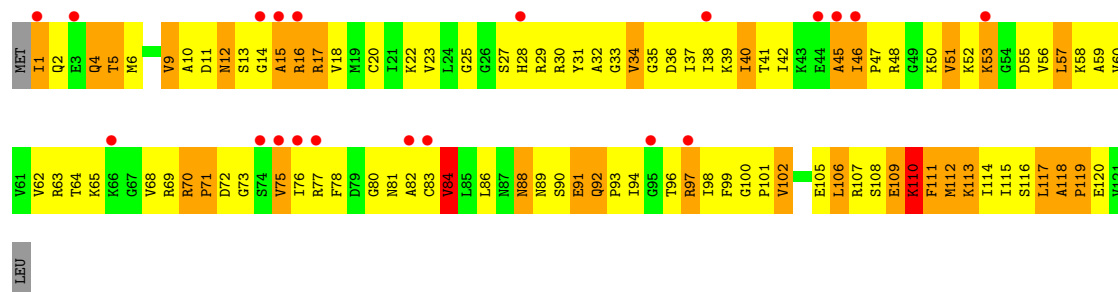
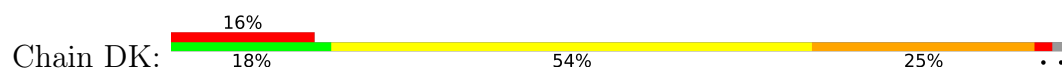




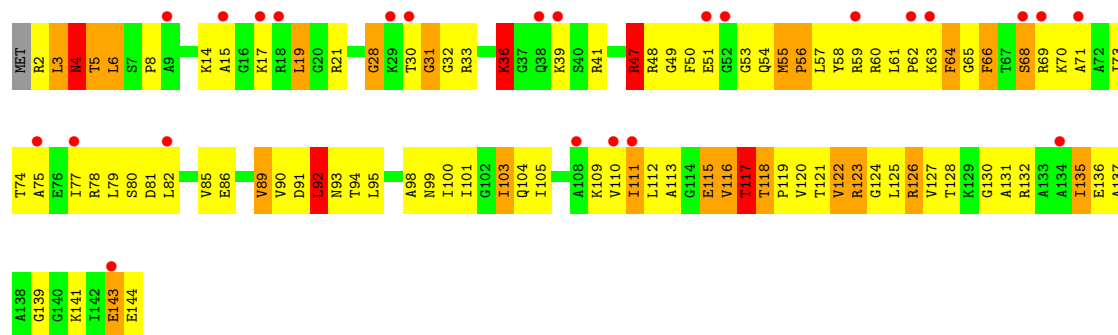
• Molecule 34: 50S ribosomal protein L14



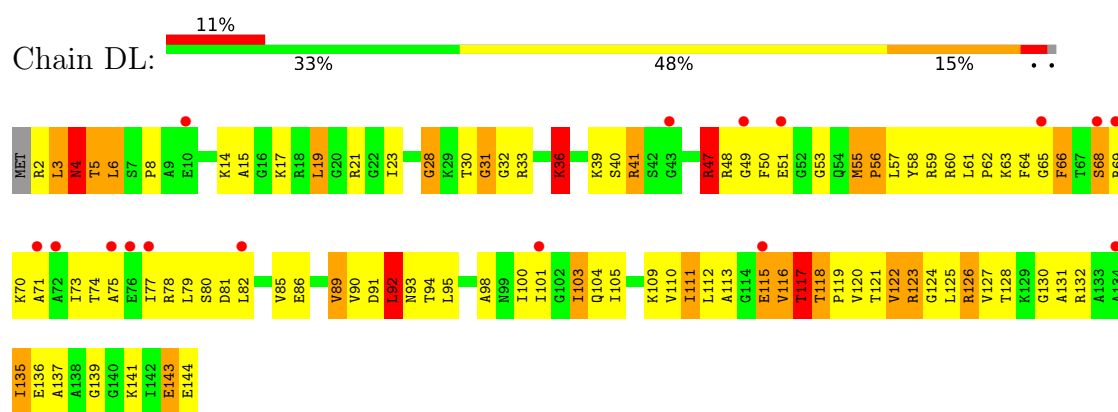
• Molecule 34: 50S ribosomal protein L14



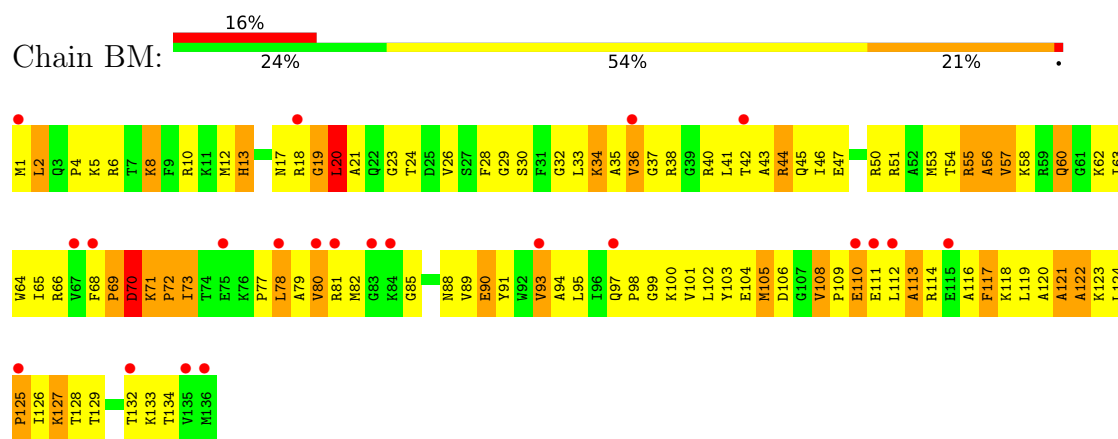
• Molecule 35: 50S ribosomal protein L15



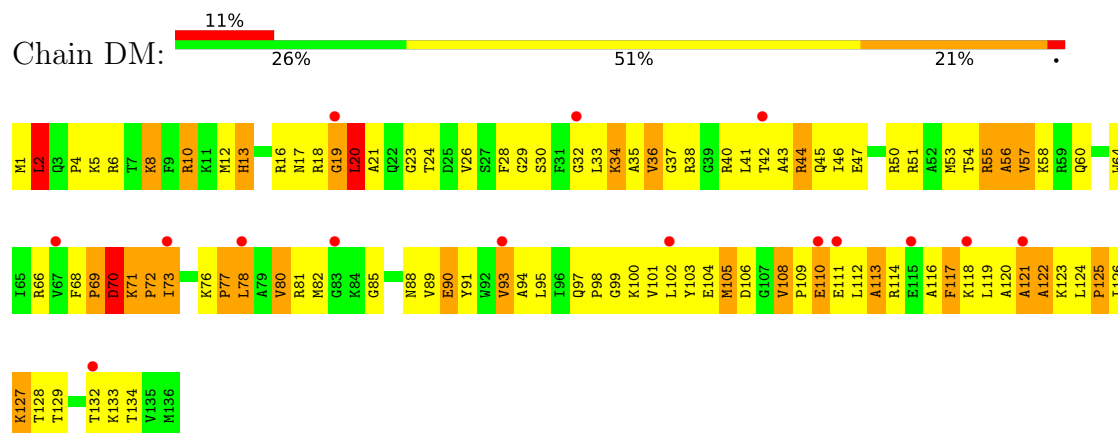
• Molecule 35: 50S ribosomal protein L15



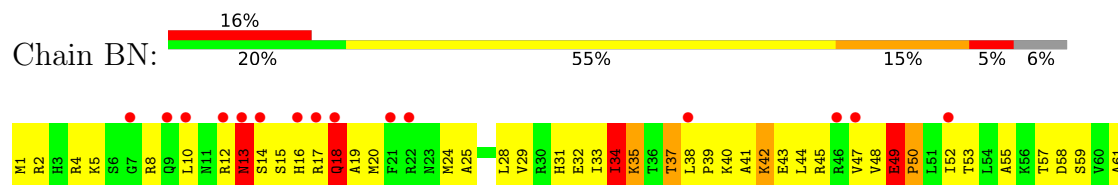
• Molecule 36: 50S ribosomal protein L16

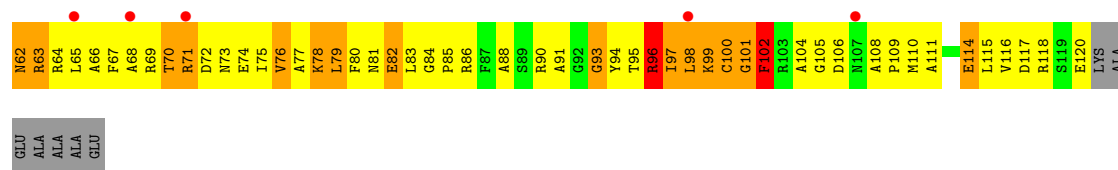


• Molecule 36: 50S ribosomal protein L16

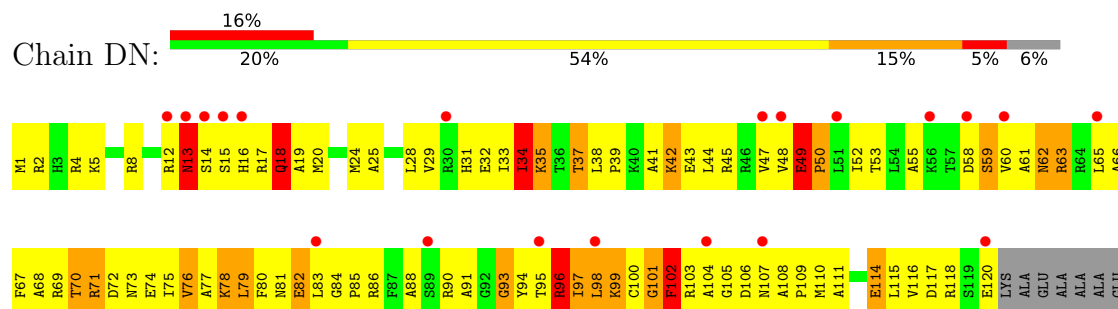


• Molecule 37: 50S ribosomal protein L17

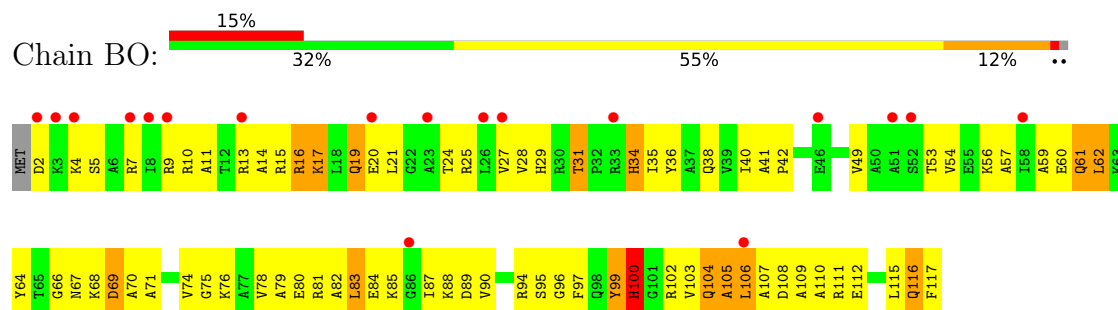




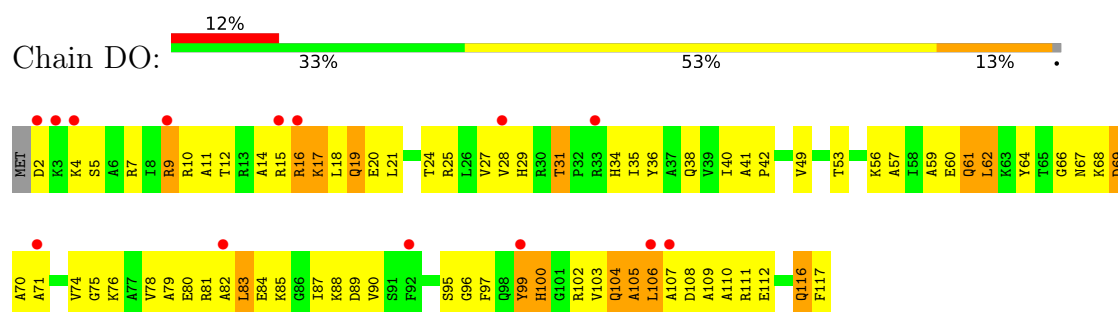
• Molecule 37: 50S ribosomal protein L17



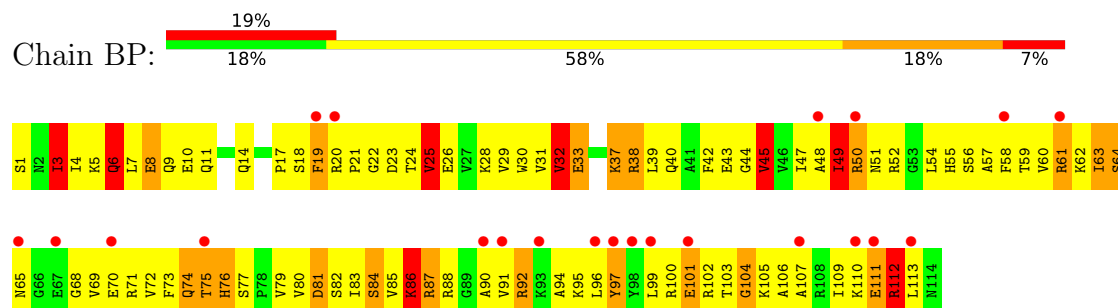
• Molecule 38: 50S ribosomal protein L18



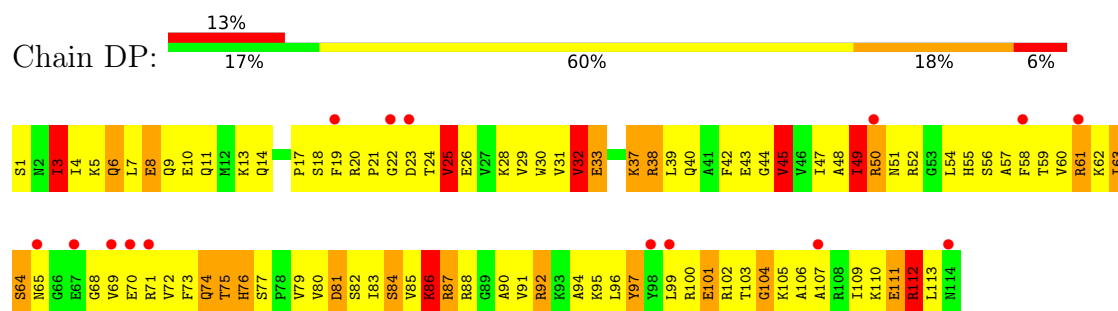
• Molecule 38: 50S ribosomal protein L18



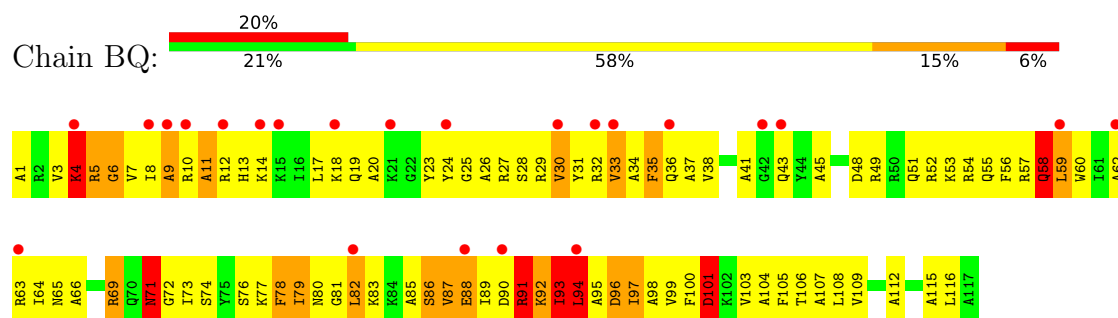
• Molecule 39: 50S ribosomal protein L19



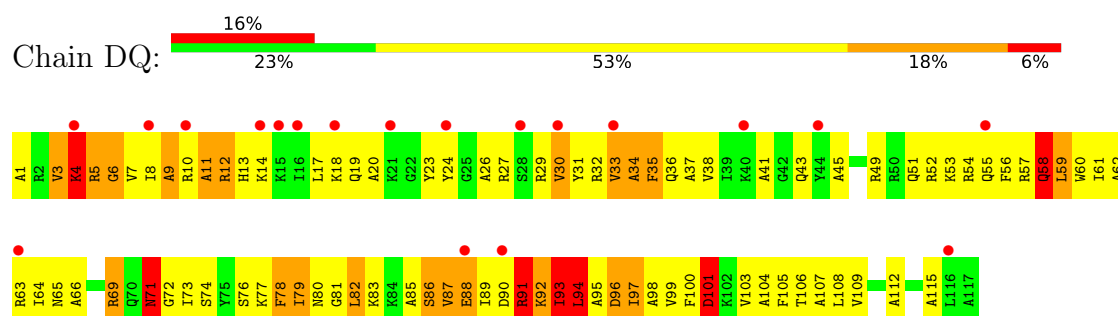
- Molecule 39: 50S ribosomal protein L19



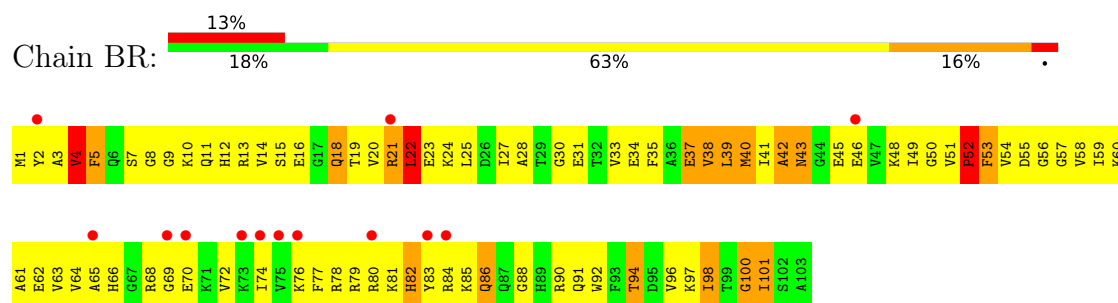
- Molecule 40: 50S ribosomal protein L20



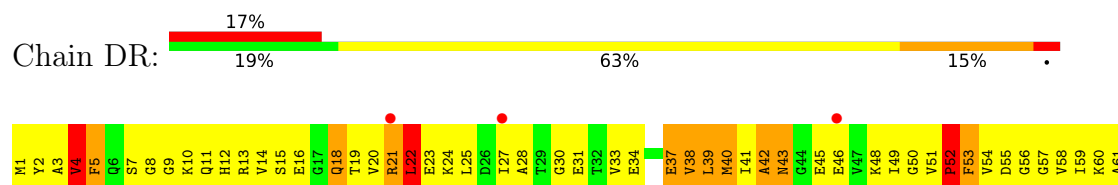
- Molecule 40: 50S ribosomal protein L20

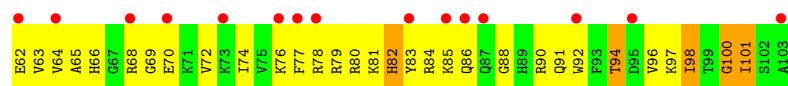


- Molecule 41: 50S ribosomal protein L21

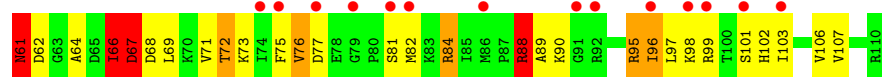


- Molecule 41: 50S ribosomal protein L21

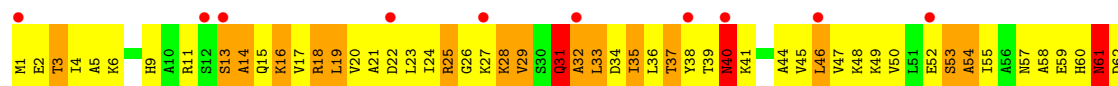




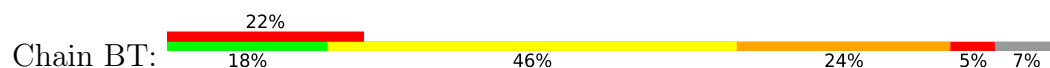
• Molecule 42: 50S ribosomal protein L22



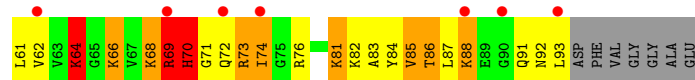
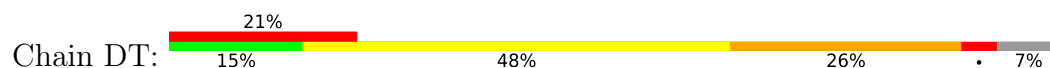
• Molecule 42: 50S ribosomal protein L22



• Molecule 43: 50S ribosomal protein L23

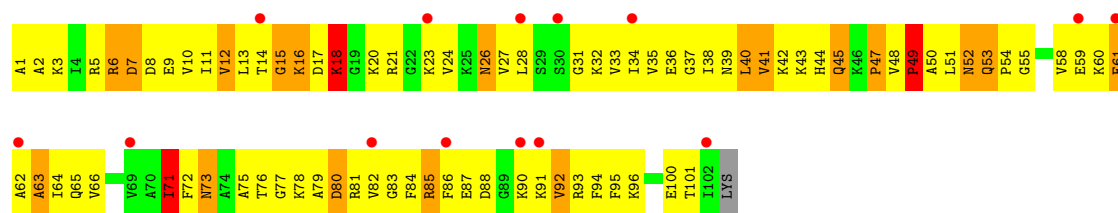


• Molecule 43: 50S ribosomal protein L23

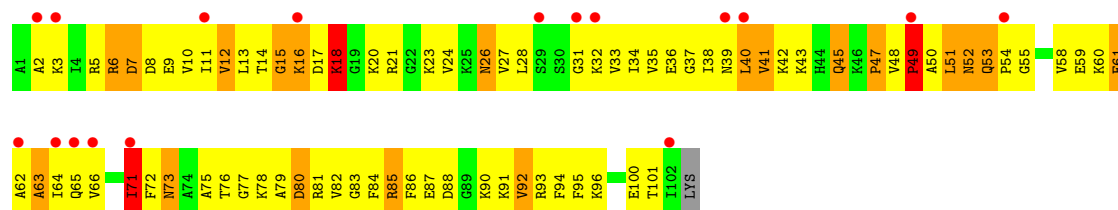


• Molecule 44: 50S ribosomal protein L24

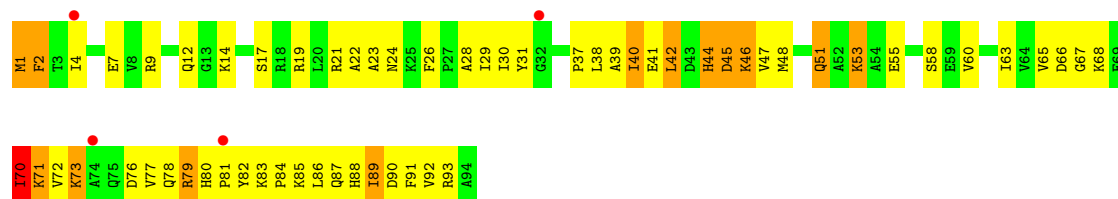




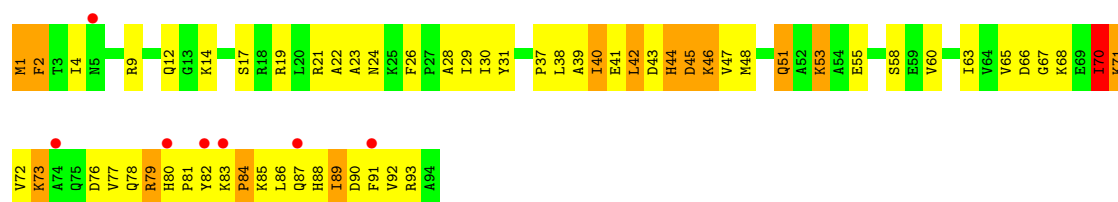
• Molecule 44: 50S ribosomal protein L24



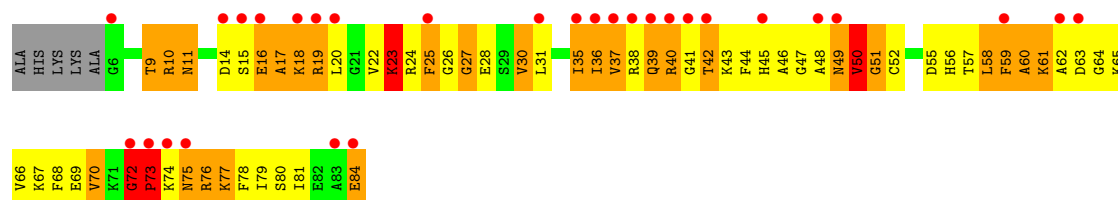
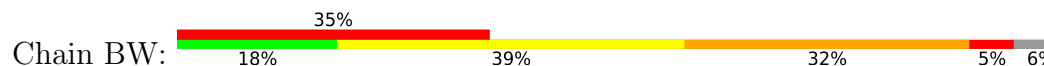
• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25

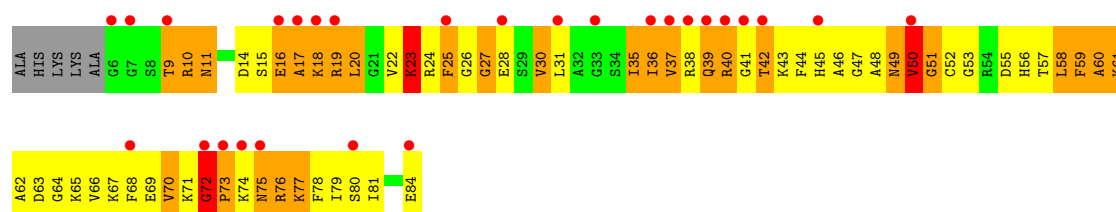


• Molecule 46: 50S ribosomal protein L27

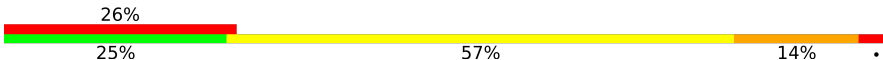


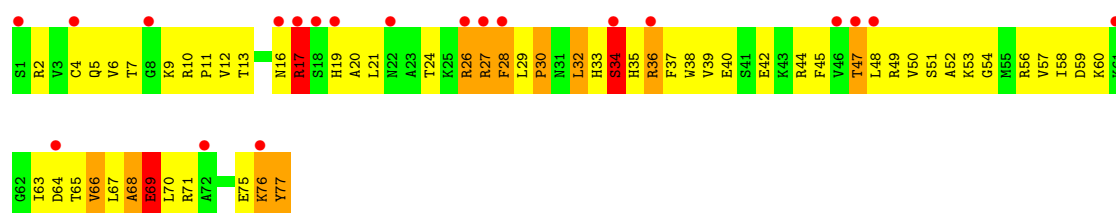
- Molecule 46: 50S ribosomal protein L27

Chain DW: 

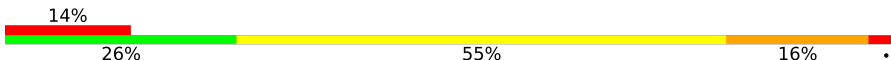


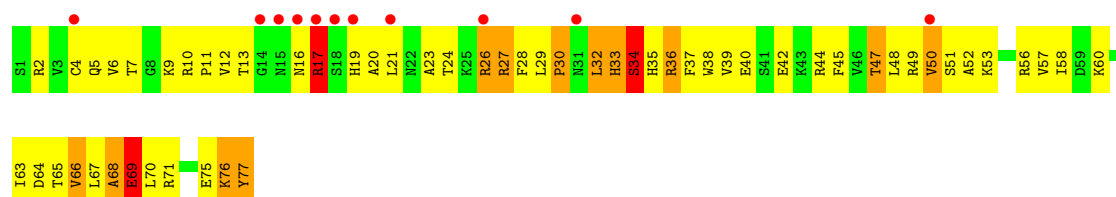
- Molecule 47: 50S ribosomal protein L28

Chain BX: 



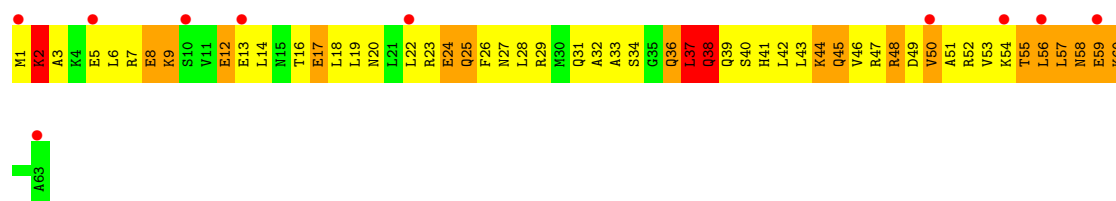
- Molecule 47: 50S ribosomal protein L28

Chain DX: 



- Molecule 48: 50S ribosomal protein L29

Chain BY: 



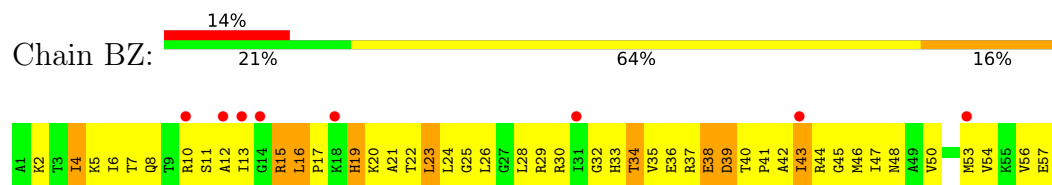
- Molecule 48: 50S ribosomal protein L29

Chain DY: 

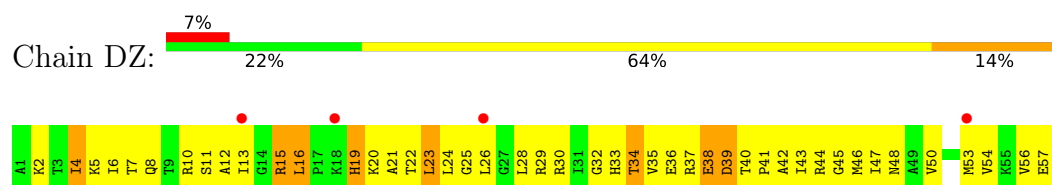




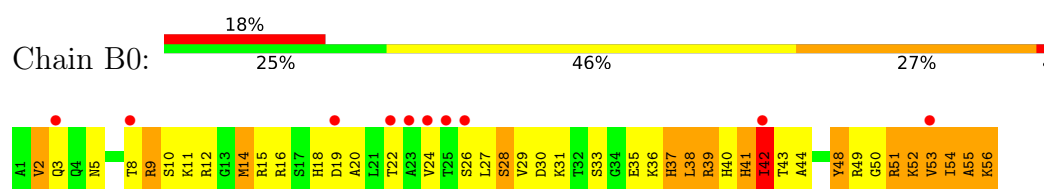
- Molecule 49: 50S ribosomal protein L30



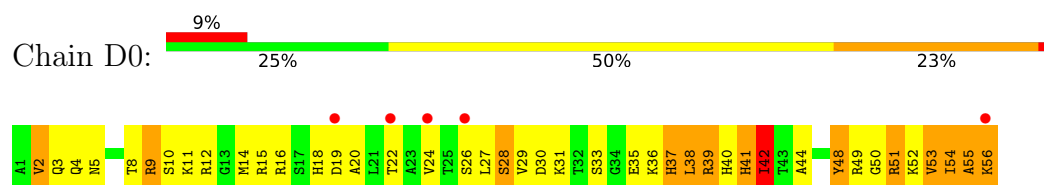
- Molecule 49: 50S ribosomal protein L30



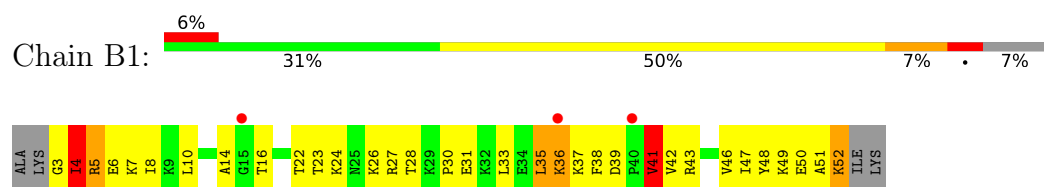
- Molecule 50: 50S ribosomal protein L32



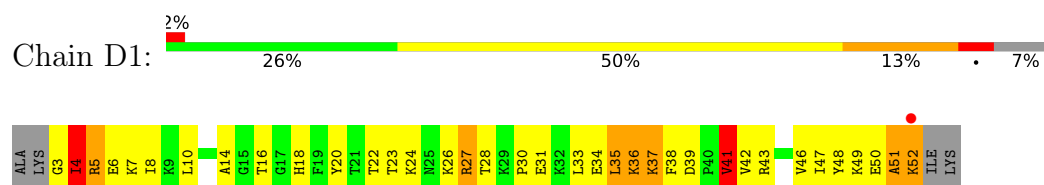
- Molecule 50: 50S ribosomal protein L32



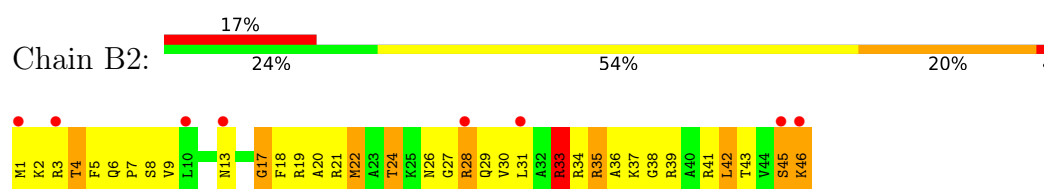
- Molecule 51: 50S ribosomal protein L33



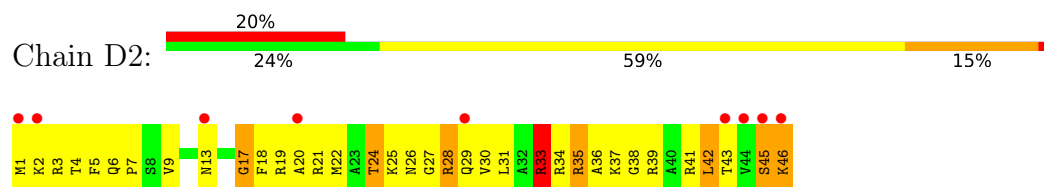
- Molecule 51: 50S ribosomal protein L33



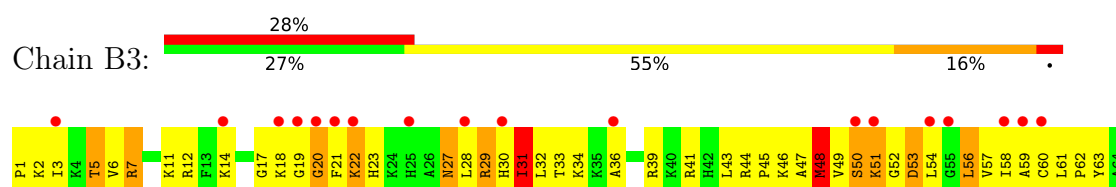
- Molecule 52: 50S ribosomal protein L34



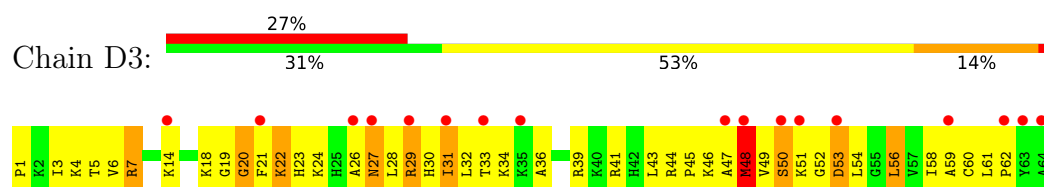
• Molecule 52: 50S ribosomal protein L34



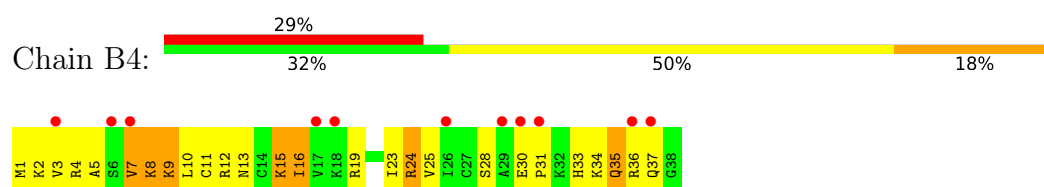
• Molecule 53: 50S ribosomal protein L35



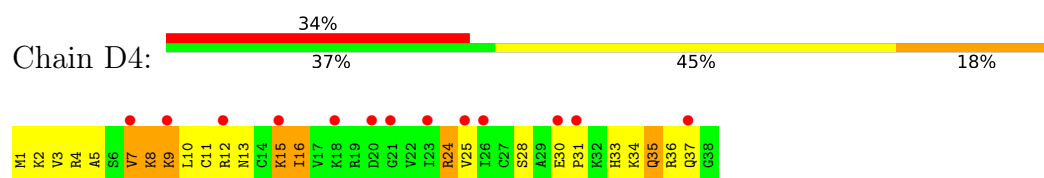
• Molecule 53: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L36



• Molecule 54: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 70.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.6 (70.00-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.320 0.259 , 0.287	Depositor DCC
R_{free} test set	37294 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	285033	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/36762	0.61	19/57350 (0.0%)
1	CA	0.26	0/36762	0.60	18/57350 (0.0%)
2	AW	0.32	0/401	0.63	0/622
2	CW	0.32	0/401	0.61	0/622
3	AX	0.42	0/138	0.85	1/212 (0.5%)
3	CX	0.43	0/138	0.87	1/212 (0.5%)
4	AB	0.30	0/1735	0.71	0/2338
4	CB	0.27	0/1735	0.69	0/2338
5	AC	0.28	0/1651	0.71	0/2225
5	CC	0.28	0/1651	0.69	0/2225
6	AD	0.26	0/1665	0.69	1/2227 (0.0%)
6	CD	0.26	0/1665	0.72	0/2227
7	AE	0.27	0/1118	0.71	1/1504 (0.1%)
7	CE	0.29	0/1118	0.73	0/1504
8	AF	0.28	0/835	0.69	1/1128 (0.1%)
8	CF	0.29	0/835	0.70	0/1128
9	AG	0.27	0/1187	0.73	1/1591 (0.1%)
9	CG	0.27	0/1187	0.75	0/1591
10	AH	0.27	0/989	0.75	0/1326
10	CH	0.27	0/989	0.70	2/1326 (0.2%)
11	AI	0.27	0/1034	0.70	0/1375
11	CI	0.27	0/1034	0.72	1/1375 (0.1%)
12	AJ	0.28	0/796	0.68	0/1077
12	CJ	0.29	0/796	0.75	1/1077 (0.1%)
13	AK	0.31	0/893	0.83	3/1205 (0.2%)
13	CK	0.30	0/893	0.77	1/1205 (0.1%)
14	AL	0.27	0/969	0.70	0/1300
14	CL	0.29	0/969	0.74	0/1300
15	AM	0.29	0/892	0.73	0/1193
15	CM	0.28	0/884	0.70	0/1181
16	AN	0.27	0/785	0.74	1/1043 (0.1%)
16	CN	0.27	0/786	0.72	0/1046

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AO	0.27	0/724	0.70	1/966 (0.1%)
17	CO	0.27	0/724	0.74	1/966 (0.1%)
18	AP	0.28	0/659	0.71	0/884
18	CP	0.27	0/648	0.69	0/870
19	AQ	0.26	0/657	0.67	0/881
19	CQ	0.28	0/657	0.68	0/881
20	AR	0.29	0/462	0.75	0/621
20	CR	0.28	0/462	0.68	0/621
21	AS	0.28	0/652	0.71	0/877
21	CS	0.29	0/652	0.71	1/877 (0.1%)
22	AT	0.28	0/671	0.71	0/888
22	CT	0.28	0/671	0.67	0/888
23	AU	0.28	0/430	0.78	0/570
23	CU	0.28	0/430	0.80	0/570
24	BA	0.27	0/2803	0.60	1/4371 (0.0%)
24	DA	0.27	0/2803	0.60	1/4371 (0.0%)
25	BB	0.27	1/68314 (0.0%)	0.62	71/106569 (0.1%)
25	DB	0.27	1/68314 (0.0%)	0.63	80/106569 (0.1%)
26	BC	0.28	0/2121	0.83	3/2852 (0.1%)
26	DC	0.27	0/2121	0.83	3/2852 (0.1%)
27	BD	0.30	0/1586	0.93	7/2134 (0.3%)
27	DD	0.30	0/1586	0.93	7/2134 (0.3%)
28	BE	0.30	0/1571	1.09	18/2113 (0.9%)
28	DE	0.29	0/1571	1.09	18/2113 (0.9%)
29	BF	0.29	0/1444	1.01	13/1937 (0.7%)
29	DF	0.29	0/1444	1.01	13/1937 (0.7%)
30	BG	0.29	0/1343	0.82	3/1816 (0.2%)
30	DG	0.29	0/1343	0.82	3/1816 (0.2%)
31	BH	0.32	0/1122	0.87	4/1515 (0.3%)
31	DH	0.29	0/1122	0.79	2/1515 (0.1%)
32	BI	0.31	0/1046	0.80	0/1410
32	DI	0.32	0/1046	0.83	0/1410
33	BJ	0.29	0/1152	0.90	4/1551 (0.3%)
33	DJ	0.29	0/1152	0.90	3/1551 (0.2%)
34	BK	0.31	0/939	1.30	17/1258 (1.4%)
34	DK	0.31	0/939	1.30	17/1258 (1.4%)
35	BL	0.29	0/1054	0.93	3/1403 (0.2%)
35	DL	0.29	0/1054	0.93	3/1403 (0.2%)
36	BM	0.28	0/1093	0.92	9/1460 (0.6%)
36	DM	0.28	0/1093	0.92	9/1460 (0.6%)
37	BN	0.29	0/973	1.10	12/1301 (0.9%)
37	DN	0.28	0/973	1.11	12/1301 (0.9%)
38	BO	0.28	0/902	0.97	8/1209 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DO	0.28	0/902	0.96	7/1209 (0.6%)
39	BP	0.29	0/929	0.94	5/1242 (0.4%)
39	DP	0.29	0/929	0.95	5/1242 (0.4%)
40	BQ	0.29	0/960	1.21	16/1278 (1.3%)
40	DQ	0.29	0/960	1.21	16/1278 (1.3%)
41	BR	0.27	0/829	0.86	2/1107 (0.2%)
41	DR	0.28	0/829	0.85	2/1107 (0.2%)
42	BS	0.31	0/864	1.04	8/1156 (0.7%)
42	DS	0.31	0/864	1.04	8/1156 (0.7%)
43	BT	0.28	0/744	1.14	10/994 (1.0%)
43	DT	0.29	0/744	1.14	10/994 (1.0%)
44	BU	0.29	0/787	0.84	0/1051
44	DU	0.29	0/787	0.83	1/1051 (0.1%)
45	BV	0.27	0/766	0.74	0/1025
45	DV	0.27	0/766	0.74	0/1025
46	BW	0.36	0/603	1.07	7/797 (0.9%)
46	DW	0.36	0/603	1.07	7/797 (0.9%)
47	BX	0.28	0/635	0.95	3/848 (0.4%)
47	DX	0.28	0/635	0.98	3/848 (0.4%)
48	BY	0.26	0/510	1.03	5/677 (0.7%)
48	DY	0.27	0/510	1.04	5/677 (0.7%)
49	BZ	0.30	0/453	0.96	4/605 (0.7%)
49	DZ	0.30	0/453	0.96	4/605 (0.7%)
50	B0	0.28	0/450	0.96	3/599 (0.5%)
50	D0	0.27	0/450	0.96	3/599 (0.5%)
51	B1	0.32	0/416	0.84	0/554
51	D1	0.32	0/416	0.84	0/554
52	B2	0.30	0/380	1.01	1/498 (0.2%)
52	D2	0.31	0/380	1.02	1/498 (0.2%)
53	B3	0.34	0/513	1.14	6/676 (0.9%)
53	D3	0.34	0/513	1.15	6/676 (0.9%)
54	B4	0.32	0/303	0.92	1/397 (0.3%)
54	D4	0.31	0/303	0.91	1/397 (0.3%)
All	All	0.27	2/307402 (0.0%)	0.69	549/459589 (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	AA	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	15
25	BB	0	37
25	DB	0	36
All	All	0	104

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BB	1086	A	C5-C6	-7.34	1.26	1.41
25	DB	1086	A	C5-C6	-7.29	1.26	1.41

The worst 5 of 549 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BE	60	TRP	N-CA-C	18.38	126.39	108.75
28	DE	60	TRP	N-CA-C	18.35	126.37	108.75
34	BK	118	ALA	CA-C-N	-13.65	102.78	119.84
34	BK	118	ALA	C-N-CA	-13.65	102.78	119.84
34	DK	118	ALA	CA-C-N	-13.64	102.78	119.84

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	82	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1483	0
1	CA	32831	0	16521	1483	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AW	360	0	185	9	0
2	CW	360	0	185	9	0
3	AX	125	0	63	6	0
3	CX	125	0	63	5	0
4	AB	1704	0	1732	286	0
4	CB	1704	0	1732	337	0
5	AC	1624	0	1699	220	0
5	CC	1624	0	1699	261	0
6	AD	1643	0	1710	213	0
6	CD	1643	0	1710	277	0
7	AE	1105	0	1148	167	0
7	CE	1105	0	1148	227	0
8	AF	817	0	808	97	0
8	CF	817	0	808	131	0
9	AG	1174	0	1230	151	0
9	CG	1174	0	1230	171	0
10	AH	979	0	1034	129	0
10	CH	979	0	1034	176	0
11	AI	1022	0	1070	195	0
11	CI	1022	0	1070	204	0
12	AJ	786	0	828	128	0
12	CJ	786	0	828	123	0
13	AK	877	0	887	119	0
13	CK	877	0	887	147	0
14	AL	955	0	1019	143	0
14	CL	955	0	1019	122	0
15	AM	883	0	944	134	0
15	CM	876	0	937	172	0
16	AN	774	0	827	137	0
16	CN	774	0	828	142	0
17	AO	716	0	742	66	0
17	CO	716	0	742	72	0
18	AP	649	0	666	108	0
18	CP	638	0	656	109	0
19	AQ	648	0	691	103	0
19	CQ	648	0	691	83	0
20	AR	455	0	478	82	0
20	CR	455	0	478	61	0
21	AS	637	0	665	92	0
21	CS	637	0	665	109	0
22	AT	665	0	714	64	0
22	CT	665	0	714	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AU	425	0	449	84	0
23	CU	425	0	449	89	0
24	BA	2507	0	1270	86	0
24	DA	2507	0	1270	75	0
25	BB	60995	0	30678	2086	0
25	DB	60995	0	30678	2164	0
26	BC	2082	0	2157	227	0
26	DC	2082	0	2157	224	0
27	BD	1565	0	1616	225	0
27	DD	1565	0	1616	227	0
28	BE	1552	0	1619	171	0
28	DE	1552	0	1619	175	0
29	BF	1420	0	1460	270	0
29	DF	1420	0	1460	260	0
30	BG	1323	0	1374	186	0
30	DG	1323	0	1374	184	0
31	BH	1111	0	1148	218	0
31	DH	1111	0	1148	187	0
32	BI	1032	0	1088	119	0
32	DI	1032	0	1088	194	0
33	BJ	1129	0	1162	161	0
33	DJ	1129	0	1162	177	0
34	BK	930	0	1003	106	0
34	DK	930	0	1003	102	0
35	BL	1045	0	1117	129	0
35	DL	1045	0	1117	128	0
36	BM	1074	0	1157	115	0
36	DM	1074	0	1157	113	0
37	BN	960	0	1000	108	0
37	DN	960	0	1000	108	0
38	BO	892	0	923	82	0
38	DO	892	0	923	78	0
39	BP	917	0	965	121	0
39	DP	917	0	965	114	0
40	BQ	947	0	1022	142	0
40	DQ	947	0	1022	145	0
41	BR	816	0	839	117	0
41	DR	816	0	839	121	0
42	BS	857	0	922	100	0
42	DS	857	0	922	102	0
43	BT	738	0	807	114	0
43	DT	738	0	807	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BU	779	0	834	115	0
44	DU	779	0	834	111	0
45	BV	753	0	780	77	0
45	DV	753	0	780	72	0
46	BW	596	0	610	149	0
46	DW	596	0	610	148	0
47	BX	625	0	655	84	0
47	DX	625	0	655	80	0
48	BY	509	0	543	89	0
48	DY	509	0	543	83	0
49	BZ	449	0	491	50	0
49	DZ	449	0	491	43	0
50	B0	444	0	461	46	0
50	D0	444	0	461	48	0
51	B1	409	0	440	31	0
51	D1	409	0	440	36	0
52	B2	377	0	418	37	0
52	D2	377	0	418	35	0
53	B3	504	0	574	54	0
53	D3	504	0	574	51	0
54	B4	302	0	340	28	0
54	D4	302	0	340	29	0
55	AA	60	0	0	0	0
55	AX	2	0	0	0	0
55	BB	118	0	0	0	0
55	BJ	1	0	0	0	0
55	CA	56	0	0	0	0
55	CN	1	0	0	0	0
55	CX	1	0	0	0	0
55	DB	119	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	5	0
57	AE	3	0	0	0	0
57	AI	1	0	0	0	0
57	AK	2	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	AX	9	0	0	1	0
57	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	5	0	0	0	0
57	BB	532	0	0	7	0
57	BC	7	0	0	0	0
57	BE	3	0	0	0	0
57	BH	3	0	0	0	0
57	BJ	3	0	0	0	0
57	BL	2	0	0	1	0
57	BN	3	0	0	0	0
57	CA	264	0	0	4	0
57	CE	2	0	0	0	0
57	CI	3	0	0	1	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CP	1	0	0	0	0
57	CT	3	0	0	0	0
57	CU	1	0	0	0	0
57	CX	6	0	0	1	0
57	D2	1	0	0	0	0
57	D4	4	0	0	0	0
57	DB	531	0	0	5	0
57	DC	7	0	0	0	0
57	DD	1	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	2	0	0	0	0
57	DL	3	0	0	0	0
57	DN	3	0	0	0	0
57	DT	1	0	0	0	0
All	All	285033	0	191150	18405	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 39.

The worst 5 of 18405 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)
37:DN:101:GLY:HA2	37:DN:110:MET:H	1.04	1.18
27:BD:148:GLN:HG3	27:BD:152:PRO:HG2	1.29	1.15
34:BK:70:ARG:HB3	34:BK:71:PRO:CD	1.76	1.14
37:BN:101:GLY:HA2	37:BN:110:MET:H	1.06	1.13
28:DE:46:GLN:HG3	28:DE:87:ALA:HB3	1.31	1.12

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	
4	AB	216/240 (90%)	133 (62%)	59 (27%)	24 (11%)	0	2
4	CB	216/240 (90%)	106 (49%)	71 (33%)	39 (18%)	0	0
5	AC	204/232 (88%)	134 (66%)	50 (24%)	20 (10%)	0	2
5	CC	204/232 (88%)	119 (58%)	57 (28%)	28 (14%)	0	1
6	AD	203/205 (99%)	123 (61%)	56 (28%)	24 (12%)	0	1
6	CD	203/205 (99%)	122 (60%)	54 (27%)	27 (13%)	0	1
7	AE	148/166 (89%)	101 (68%)	38 (26%)	9 (6%)	1	9
7	CE	148/166 (89%)	78 (53%)	50 (34%)	20 (14%)	0	1
8	AF	98/135 (73%)	63 (64%)	24 (24%)	11 (11%)	0	2
8	CF	98/135 (73%)	52 (53%)	30 (31%)	16 (16%)	0	0
9	AG	148/178 (83%)	107 (72%)	31 (21%)	10 (7%)	1	6
9	CG	148/178 (83%)	89 (60%)	40 (27%)	19 (13%)	0	1
10	AH	127/129 (98%)	83 (65%)	31 (24%)	13 (10%)	0	2
10	CH	127/129 (98%)	78 (61%)	35 (28%)	14 (11%)	0	2
11	AI	125/129 (97%)	78 (62%)	33 (26%)	14 (11%)	0	2
11	CI	125/129 (97%)	74 (59%)	44 (35%)	7 (6%)	1	10
12	AJ	96/103 (93%)	55 (57%)	27 (28%)	14 (15%)	0	1
12	CJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	1
13	AK	115/128 (90%)	75 (65%)	30 (26%)	10 (9%)	0	3
13	CK	115/128 (90%)	82 (71%)	25 (22%)	8 (7%)	1	6
14	AL	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	0	3
14	CL	121/123 (98%)	80 (66%)	24 (20%)	17 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AM	112/117 (96%)	75 (67%)	22 (20%)	15 (13%)	0	1
15	CM	111/117 (95%)	66 (60%)	29 (26%)	16 (14%)	0	1
16	AN	92/100 (92%)	61 (66%)	25 (27%)	6 (6%)	1	7
16	CN	94/100 (94%)	46 (49%)	29 (31%)	19 (20%)	0	0
17	AO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	3	19
17	CO	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	5	27
18	AP	80/82 (98%)	46 (58%)	26 (32%)	8 (10%)	0	2
18	CP	78/82 (95%)	53 (68%)	17 (22%)	8 (10%)	0	2
19	AQ	78/83 (94%)	51 (65%)	16 (20%)	11 (14%)	0	1
19	CQ	78/83 (94%)	51 (65%)	20 (26%)	7 (9%)	0	3
20	AR	53/74 (72%)	39 (74%)	9 (17%)	5 (9%)	0	3
20	CR	53/74 (72%)	37 (70%)	12 (23%)	4 (8%)	1	5
21	AS	77/91 (85%)	53 (69%)	19 (25%)	5 (6%)	1	7
21	CS	77/91 (85%)	55 (71%)	18 (23%)	4 (5%)	1	11
22	AT	83/86 (96%)	63 (76%)	11 (13%)	9 (11%)	0	2
22	CT	83/86 (96%)	59 (71%)	20 (24%)	4 (5%)	2	13
23	AU	49/70 (70%)	21 (43%)	17 (35%)	11 (22%)	0	0
23	CU	49/70 (70%)	27 (55%)	16 (33%)	6 (12%)	0	1
26	BC	269/272 (99%)	166 (62%)	68 (25%)	35 (13%)	0	1
26	DC	269/272 (99%)	168 (62%)	63 (23%)	38 (14%)	0	1
27	BD	207/209 (99%)	113 (55%)	56 (27%)	38 (18%)	0	0
27	DD	207/209 (99%)	110 (53%)	56 (27%)	41 (20%)	0	0
28	BE	199/201 (99%)	126 (63%)	43 (22%)	30 (15%)	0	1
28	DE	199/201 (99%)	127 (64%)	42 (21%)	30 (15%)	0	1
29	BF	176/178 (99%)	97 (55%)	40 (23%)	39 (22%)	0	0
29	DF	176/178 (99%)	95 (54%)	43 (24%)	38 (22%)	0	0
30	BG	174/176 (99%)	94 (54%)	54 (31%)	26 (15%)	0	1
30	DG	174/176 (99%)	93 (53%)	55 (32%)	26 (15%)	0	1
31	BH	147/149 (99%)	69 (47%)	50 (34%)	28 (19%)	0	0
31	DH	147/149 (99%)	68 (46%)	54 (37%)	25 (17%)	0	0
32	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	3	23
33	BJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	0
33	DJ	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	0
34	BK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
34	DK	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
35	BL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	0
35	DL	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	0
36	BM	134/136 (98%)	77 (58%)	32 (24%)	25 (19%)	0	0
36	DM	134/136 (98%)	77 (58%)	33 (25%)	24 (18%)	0	0
37	BN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	1
37	DN	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	1
38	BO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	2	14
38	DO	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	2	14
39	BP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
39	DP	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
40	BQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	2
40	DQ	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	0	2
41	BR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
41	DR	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	1
42	BS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
42	DS	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
43	BT	91/100 (91%)	54 (59%)	23 (25%)	14 (15%)	0	0
43	DT	91/100 (91%)	52 (57%)	25 (28%)	14 (15%)	0	0
44	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
44	DU	100/103 (97%)	57 (57%)	28 (28%)	15 (15%)	0	1
45	BV	92/94 (98%)	74 (80%)	11 (12%)	7 (8%)	1	5
45	DV	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	5
46	BW	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
46	DW	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
47	BX	75/77 (97%)	43 (57%)	26 (35%)	6 (8%)	1	4
47	DX	75/77 (97%)	41 (55%)	27 (36%)	7 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BY	61/63 (97%)	37 (61%)	18 (30%)	6 (10%)	0	2
48	DY	61/63 (97%)	34 (56%)	21 (34%)	6 (10%)	0	2
49	BZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	1	11
49	DZ	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	1	11
50	B0	54/56 (96%)	35 (65%)	8 (15%)	11 (20%)	0	0
50	D0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	0
51	B1	48/54 (89%)	33 (69%)	7 (15%)	8 (17%)	0	0
51	D1	48/54 (89%)	33 (69%)	6 (12%)	9 (19%)	0	0
52	B2	44/46 (96%)	26 (59%)	13 (30%)	5 (11%)	0	2
52	D2	44/46 (96%)	26 (59%)	14 (32%)	4 (9%)	0	3
53	B3	62/64 (97%)	42 (68%)	15 (24%)	5 (8%)	1	4
53	D3	62/64 (97%)	41 (66%)	17 (27%)	4 (6%)	1	7
54	B4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	2
54	D4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	0	2
All	All	11239/11910 (94%)	6961 (62%)	2802 (25%)	1476 (13%)	0	1

5 of 1476 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AB	19	THR
4	AB	22	TRP
4	AB	75	ALA
4	AB	76	SER
4	AB	91	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AB	180/198 (91%)	140 (78%)	40 (22%)	1	5
4	CB	180/198 (91%)	147 (82%)	33 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AC	170/189 (90%)	134 (79%)	36 (21%)	1	6
5	CC	170/189 (90%)	136 (80%)	34 (20%)	1	7
6	AD	172/172 (100%)	147 (86%)	25 (14%)	3	15
6	CD	172/172 (100%)	127 (74%)	45 (26%)	0	3
7	AE	113/125 (90%)	98 (87%)	15 (13%)	4	18
7	CE	113/125 (90%)	87 (77%)	26 (23%)	1	4
8	AF	87/116 (75%)	72 (83%)	15 (17%)	2	10
8	CF	87/116 (75%)	78 (90%)	9 (10%)	7	27
9	AG	123/146 (84%)	99 (80%)	24 (20%)	1	7
9	CG	123/146 (84%)	98 (80%)	25 (20%)	1	6
10	AH	104/104 (100%)	86 (83%)	18 (17%)	2	9
10	CH	104/104 (100%)	82 (79%)	22 (21%)	1	6
11	AI	105/106 (99%)	81 (77%)	24 (23%)	1	4
11	CI	105/106 (99%)	87 (83%)	18 (17%)	2	10
12	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	13
12	CJ	86/90 (96%)	70 (81%)	16 (19%)	1	8
13	AK	90/98 (92%)	74 (82%)	16 (18%)	2	9
13	CK	90/98 (92%)	78 (87%)	12 (13%)	4	18
14	AL	103/103 (100%)	88 (85%)	15 (15%)	3	15
14	CL	103/103 (100%)	79 (77%)	24 (23%)	1	4
15	AM	92/95 (97%)	74 (80%)	18 (20%)	1	7
15	CM	91/95 (96%)	71 (78%)	20 (22%)	1	5
16	AN	79/83 (95%)	57 (72%)	22 (28%)	0	2
16	CN	79/83 (95%)	64 (81%)	15 (19%)	1	8
17	AO	76/76 (100%)	68 (90%)	8 (10%)	6	27
17	CO	76/76 (100%)	66 (87%)	10 (13%)	4	19
18	AP	65/65 (100%)	53 (82%)	12 (18%)	1	8
18	CP	65/65 (100%)	60 (92%)	5 (8%)	12	40
19	AQ	74/77 (96%)	60 (81%)	14 (19%)	1	8
19	CQ	74/77 (96%)	64 (86%)	10 (14%)	4	18
20	AR	48/64 (75%)	37 (77%)	11 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CR	48/64 (75%)	44 (92%)	4 (8%)	10	37
21	AS	70/78 (90%)	57 (81%)	13 (19%)	1	8
21	CS	70/78 (90%)	52 (74%)	18 (26%)	0	3
22	AT	65/65 (100%)	55 (85%)	10 (15%)	2	13
22	CT	65/65 (100%)	55 (85%)	10 (15%)	2	13
23	AU	44/60 (73%)	37 (84%)	7 (16%)	2	12
23	CU	44/60 (73%)	31 (70%)	13 (30%)	0	1
26	BC	216/217 (100%)	186 (86%)	30 (14%)	3	16
26	DC	216/217 (100%)	186 (86%)	30 (14%)	3	16
27	BD	164/164 (100%)	136 (83%)	28 (17%)	2	10
27	DD	164/164 (100%)	136 (83%)	28 (17%)	2	10
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	6
28	DE	165/165 (100%)	128 (78%)	37 (22%)	1	5
29	BF	149/149 (100%)	113 (76%)	36 (24%)	1	3
29	DF	149/149 (100%)	115 (77%)	34 (23%)	1	4
30	BG	137/137 (100%)	112 (82%)	25 (18%)	2	8
30	DG	137/137 (100%)	112 (82%)	25 (18%)	2	8
31	BH	114/114 (100%)	85 (75%)	29 (25%)	0	3
31	DH	114/114 (100%)	87 (76%)	27 (24%)	1	4
32	BI	109/109 (100%)	108 (99%)	1 (1%)	70	79
32	DI	109/109 (100%)	107 (98%)	2 (2%)	51	72
33	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	17
33	DJ	116/116 (100%)	101 (87%)	15 (13%)	4	19
34	BK	102/104 (98%)	86 (84%)	16 (16%)	2	12
34	DK	102/104 (98%)	84 (82%)	18 (18%)	2	9
35	BL	102/103 (99%)	88 (86%)	14 (14%)	3	17
35	DL	102/103 (99%)	89 (87%)	13 (13%)	4	20
36	BM	109/109 (100%)	91 (84%)	18 (16%)	2	10
36	DM	109/109 (100%)	90 (83%)	19 (17%)	2	9
37	BN	100/103 (97%)	86 (86%)	14 (14%)	3	16
37	DN	100/103 (97%)	85 (85%)	15 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BO	86/87 (99%)	76 (88%)	10 (12%)	5	23
38	DO	86/87 (99%)	76 (88%)	10 (12%)	5	23
39	BP	99/99 (100%)	76 (77%)	23 (23%)	1	4
39	DP	99/99 (100%)	77 (78%)	22 (22%)	1	5
40	BQ	89/89 (100%)	74 (83%)	15 (17%)	2	10
40	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	10
41	BR	84/84 (100%)	69 (82%)	15 (18%)	2	9
41	DR	84/84 (100%)	69 (82%)	15 (18%)	2	9
42	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
42	DS	93/93 (100%)	79 (85%)	14 (15%)	3	13
43	BT	80/84 (95%)	60 (75%)	20 (25%)	0	3
43	DT	80/84 (95%)	60 (75%)	20 (25%)	0	3
44	BU	83/84 (99%)	69 (83%)	14 (17%)	2	10
44	DU	83/84 (99%)	69 (83%)	14 (17%)	2	10
45	BV	78/78 (100%)	67 (86%)	11 (14%)	3	16
45	DV	78/78 (100%)	67 (86%)	11 (14%)	3	16
46	BW	59/62 (95%)	49 (83%)	10 (17%)	2	10
46	DW	59/62 (95%)	49 (83%)	10 (17%)	2	10
47	BX	67/67 (100%)	56 (84%)	11 (16%)	2	11
47	DX	67/67 (100%)	56 (84%)	11 (16%)	2	11
48	BY	55/55 (100%)	43 (78%)	12 (22%)	1	5
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
49	BZ	48/48 (100%)	42 (88%)	6 (12%)	4	20
49	DZ	48/48 (100%)	43 (90%)	5 (10%)	7	27
50	B0	47/47 (100%)	39 (83%)	8 (17%)	2	10
50	D0	47/47 (100%)	39 (83%)	8 (17%)	2	10
51	B1	45/48 (94%)	38 (84%)	7 (16%)	2	12
51	D1	45/48 (94%)	38 (84%)	7 (16%)	2	12
52	B2	38/38 (100%)	32 (84%)	6 (16%)	2	12
52	D2	38/38 (100%)	32 (84%)	6 (16%)	2	12
53	B3	51/51 (100%)	43 (84%)	8 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D3	51/51 (100%)	44 (86%)	7 (14%)	3	17
54	B4	34/34 (100%)	28 (82%)	6 (18%)	2	9
54	D4	34/34 (100%)	28 (82%)	6 (18%)	2	9
All	All	9329/9696 (96%)	7690 (82%)	1639 (18%)	2	9

5 of 1639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CE	10	LEU
21	CS	12	LEU
48	DY	60	LYS
8	CF	6	ILE
6	CD	189	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 391 such sidechains are listed below:

Mol	Chain	Res	Type
9	CG	96	ASN
26	DC	89	ASN
10	CH	75	GLN
17	CO	27	GLN
27	DD	136	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	278 (18%)	20 (1%)
1	CA	1529/1542 (99%)	272 (17%)	19 (1%)
2	AW	16/17 (94%)	0	0
2	CW	16/17 (94%)	0	0
24	BA	116/120 (96%)	19 (16%)	2 (1%)
24	DA	116/120 (96%)	19 (16%)	2 (1%)
25	BB	2837/2904 (97%)	416 (14%)	13 (0%)
25	DB	2837/2904 (97%)	420 (14%)	17 (0%)
3	AX	5/6 (83%)	3 (60%)	0
3	CX	5/6 (83%)	3 (60%)	0
All	All	9006/9178 (98%)	1430 (15%)	73 (0%)

5 of 1430 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	15	G

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DB	544	C
25	DB	2756	U
25	DB	784	G
25	DB	2076	U
25	BB	858	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 360 ligands modelled in this entry, 360 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	0.17	44 (2%)	53	35	41, 98, 164, 180	0
1	CA	1530/1542 (99%)	0.29	71 (4%)	37	23	41, 109, 167, 180	0
2	AW	17/17 (100%)	-0.15	0	100	100	73, 87, 132, 177	0
2	CW	17/17 (100%)	-0.06	0	100	100	63, 86, 126, 150	0
3	AX	6/6 (100%)	0.72	0	100	100	63, 78, 113, 127	0
3	CX	6/6 (100%)	0.69	0	100	100	76, 83, 113, 115	0
4	AB	218/240 (90%)	0.54	18 (8%)	17	11	59, 127, 169, 180	0
4	CB	218/240 (90%)	1.37	63 (28%)	1	1	67, 141, 180, 180	0
5	AC	206/232 (88%)	1.06	30 (14%)	6	4	61, 104, 153, 180	0
5	CC	206/232 (88%)	0.82	34 (16%)	4	3	69, 121, 161, 180	0
6	AD	205/205 (100%)	1.27	51 (24%)	2	2	44, 106, 149, 180	0
6	CD	205/205 (100%)	1.43	54 (26%)	1	2	67, 120, 164, 180	0
7	AE	150/166 (90%)	1.28	32 (21%)	2	2	39, 98, 148, 180	0
7	CE	150/166 (90%)	2.59	81 (54%)	0	1	46, 129, 180, 180	0
8	AF	100/135 (74%)	0.36	5 (5%)	34	22	52, 100, 148, 180	0
8	CF	100/135 (74%)	0.73	8 (8%)	18	12	33, 101, 144, 165	0
9	AG	150/178 (84%)	1.10	27 (18%)	3	3	55, 113, 167, 180	0
9	CG	150/178 (84%)	1.11	35 (23%)	2	2	71, 122, 165, 180	0
10	AH	129/129 (100%)	0.85	17 (13%)	7	6	51, 100, 143, 179	0
10	CH	129/129 (100%)	1.12	24 (18%)	3	3	37, 106, 149, 176	0
11	AI	127/129 (98%)	1.28	30 (23%)	2	2	84, 120, 166, 180	0
11	CI	127/129 (98%)	1.47	35 (27%)	1	1	68, 128, 167, 180	0
12	AJ	98/103 (95%)	2.00	41 (41%)	0	1	56, 124, 172, 180	0
12	CJ	98/103 (95%)	1.54	26 (26%)	1	1	76, 131, 164, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AK	117/128 (91%)	0.54	7 (5%) 27 17	36, 91, 142, 180	0
13	CK	117/128 (91%)	0.73	11 (9%) 14 9	48, 91, 131, 159	0
14	AL	123/123 (100%)	1.07	21 (17%) 4 3	31, 80, 130, 169	0
14	CL	123/123 (100%)	1.45	33 (26%) 1 1	42, 91, 138, 172	0
15	AM	114/117 (97%)	0.96	13 (11%) 10 7	63, 119, 165, 180	0
15	CM	113/117 (96%)	0.60	6 (5%) 32 20	58, 121, 165, 176	0
16	AN	96/100 (96%)	2.24	46 (47%) 0 1	56, 112, 155, 180	0
16	CN	96/100 (96%)	2.19	45 (46%) 0 1	65, 124, 154, 180	0
17	AO	88/88 (100%)	0.65	5 (5%) 29 19	54, 91, 138, 180	0
17	CO	88/88 (100%)	0.84	14 (15%) 5 4	37, 96, 143, 160	0
18	AP	82/82 (100%)	1.64	30 (36%) 1 1	49, 95, 163, 180	0
18	CP	80/82 (97%)	2.02	40 (50%) 0 1	68, 113, 155, 180	0
19	AQ	80/83 (96%)	0.72	9 (11%) 10 7	54, 107, 155, 169	0
19	CQ	80/83 (96%)	0.57	4 (5%) 34 22	50, 104, 145, 155	0
20	AR	55/74 (74%)	0.92	6 (10%) 10 7	52, 98, 134, 158	0
20	CR	55/74 (74%)	0.57	5 (9%) 15 10	46, 101, 144, 157	0
21	AS	79/91 (86%)	1.26	20 (25%) 1 2	80, 133, 169, 180	0
21	CS	79/91 (86%)	0.65	6 (7%) 20 13	75, 128, 160, 180	0
22	AT	85/86 (98%)	1.28	20 (23%) 2 2	62, 101, 151, 162	0
22	CT	85/86 (98%)	1.56	28 (32%) 1 1	65, 104, 154, 180	0
23	AU	51/70 (72%)	1.74	18 (35%) 1 1	54, 110, 154, 180	0
23	CU	51/70 (72%)	2.20	21 (41%) 0 1	63, 125, 169, 180	0
24	BA	117/120 (97%)	-0.09	5 (4%) 40 25	44, 75, 109, 180	0
24	DA	117/120 (97%)	-0.20	4 (3%) 48 30	33, 66, 105, 180	0
25	BB	2841/2904 (97%)	-0.11	59 (2%) 63 43	13, 70, 147, 180	0
25	DB	2841/2904 (97%)	-0.31	63 (2%) 62 42	12, 55, 149, 180	0
26	BC	271/272 (99%)	1.28	60 (22%) 2 2	16, 66, 111, 151	0
26	DC	271/272 (99%)	0.98	48 (17%) 4 3	9, 52, 97, 153	0
27	BD	209/209 (100%)	1.33	52 (24%) 2 2	25, 83, 146, 180	0
27	DD	209/209 (100%)	0.99	33 (15%) 5 4	20, 59, 119, 166	0
28	BE	201/201 (100%)	0.77	27 (13%) 7 6	22, 78, 139, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	201/201 (100%)	0.72	23 (11%) 10 7	11, 76, 143, 178	0
29	BF	178/178 (100%)	0.78	21 (11%) 9 7	49, 111, 174, 180	0
29	DF	178/178 (100%)	1.22	37 (20%) 2 2	49, 110, 166, 180	0
30	BG	176/176 (100%)	0.63	15 (8%) 16 11	47, 112, 165, 176	0
30	DG	176/176 (100%)	0.63	17 (9%) 13 9	38, 88, 155, 174	0
31	BH	149/149 (100%)	1.93	55 (36%) 1 1	52, 131, 180, 180	0
31	DH	149/149 (100%)	0.80	22 (14%) 5 4	35, 109, 150, 180	0
32	BI	141/141 (100%)	0.82	14 (9%) 13 9	110, 167, 180, 180	0
32	DI	141/141 (100%)	1.94	60 (42%) 0 1	105, 179, 180, 180	0
33	BJ	142/142 (100%)	1.56	45 (31%) 1 1	32, 86, 133, 180	0
33	DJ	142/142 (100%)	0.78	19 (13%) 7 6	19, 53, 108, 175	0
34	BK	121/123 (98%)	1.03	13 (10%) 11 7	32, 74, 148, 180	0
34	DK	121/123 (98%)	0.97	20 (16%) 4 3	27, 64, 130, 163	0
35	BL	143/144 (99%)	1.17	24 (16%) 4 3	27, 69, 121, 180	0
35	DL	143/144 (99%)	0.82	16 (11%) 10 7	17, 64, 115, 180	0
36	BM	136/136 (100%)	1.00	22 (16%) 4 3	33, 65, 132, 168	0
36	DM	136/136 (100%)	0.80	15 (11%) 10 7	11, 56, 109, 176	0
37	BN	120/127 (94%)	1.09	20 (16%) 4 3	43, 88, 131, 169	0
37	DN	120/127 (94%)	1.08	20 (16%) 4 3	19, 57, 97, 180	0
38	BO	116/117 (99%)	1.03	18 (15%) 5 4	34, 77, 118, 138	0
38	DO	116/117 (99%)	0.71	14 (12%) 8 6	28, 71, 129, 157	0
39	BP	114/114 (100%)	1.12	22 (19%) 3 2	43, 84, 145, 164	0
39	DP	114/114 (100%)	0.93	15 (13%) 7 6	26, 73, 123, 174	0
40	BQ	117/117 (100%)	1.13	23 (19%) 3 2	34, 73, 135, 149	0
40	DQ	117/117 (100%)	0.77	19 (16%) 4 3	22, 53, 104, 158	0
41	BR	103/103 (100%)	0.63	13 (12%) 8 6	44, 95, 146, 177	0
41	DR	103/103 (100%)	0.93	18 (17%) 4 3	23, 72, 131, 156	0
42	BS	110/110 (100%)	1.32	23 (20%) 2 2	47, 84, 138, 180	0
42	DS	110/110 (100%)	0.93	17 (15%) 5 4	18, 53, 108, 152	0
43	BT	93/100 (93%)	1.12	22 (23%) 2 2	44, 93, 163, 180	0
43	DT	93/100 (93%)	1.35	21 (22%) 2 2	35, 72, 141, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BU	102/103 (99%)	1.10	14 (13%) 6 5	48, 106, 162, 175	0
44	DU	102/103 (99%)	0.98	17 (16%) 4 3	41, 94, 154, 180	0
45	BV	94/94 (100%)	0.33	4 (4%) 40 25	37, 84, 140, 180	0
45	DV	94/94 (100%)	0.50	7 (7%) 20 13	31, 70, 138, 156	0
46	BW	79/84 (94%)	1.89	29 (36%) 1 1	6, 53, 116, 154	0
46	DW	79/84 (94%)	1.58	27 (34%) 1 1	7, 42, 103, 180	0
47	BX	77/77 (100%)	1.32	20 (25%) 1 2	24, 63, 107, 157	0
47	DX	77/77 (100%)	1.05	11 (14%) 6 5	23, 60, 112, 152	0
48	BY	63/63 (100%)	0.79	10 (15%) 5 4	47, 108, 165, 180	0
48	DY	63/63 (100%)	0.62	4 (6%) 26 16	34, 92, 158, 180	0
49	BZ	58/58 (100%)	0.97	8 (13%) 6 5	40, 74, 124, 150	0
49	DZ	58/58 (100%)	0.56	4 (6%) 23 15	22, 58, 110, 114	0
50	B0	56/56 (100%)	1.00	10 (17%) 3 3	35, 87, 152, 180	0
50	D0	56/56 (100%)	0.97	5 (8%) 15 10	19, 56, 118, 135	0
51	B1	50/54 (92%)	0.50	3 (6%) 27 17	43, 72, 122, 140	0
51	D1	50/54 (92%)	0.45	1 (2%) 65 45	26, 76, 119, 163	0
52	B2	46/46 (100%)	1.42	8 (17%) 4 3	42, 61, 97, 162	0
52	D2	46/46 (100%)	1.20	9 (19%) 3 2	17, 47, 97, 131	0
53	B3	64/64 (100%)	1.61	18 (28%) 1 1	21, 56, 99, 136	0
53	D3	64/64 (100%)	1.44	17 (26%) 1 1	27, 49, 85, 105	0
54	B4	38/38 (100%)	1.48	11 (28%) 1 1	36, 86, 126, 146	0
54	D4	38/38 (100%)	1.54	13 (34%) 1 1	44, 68, 126, 165	0
All	All	20459/21088 (97%)	0.59	2438 (11%) 9 6	6, 86, 162, 180	0

The worst 5 of 2438 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CE	114	LEU	35.2
24	BA	88	C	14.5
11	CI	129	ARG	13.0
7	CE	130	THR	12.1
6	CD	8	LEU	11.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1658	1/1	0.18	0.64	147,147,147,147	0
55	MG	AA	1625	1/1	0.34	0.23	145,145,145,145	0
55	MG	AA	1614	1/1	0.36	0.17	174,174,174,174	0
55	MG	CA	1646	1/1	0.36	0.26	155,155,155,155	0
55	MG	AA	1626	1/1	0.38	0.21	139,139,139,139	0
55	MG	AA	1637	1/1	0.38	0.51	134,134,134,134	0
55	MG	CA	1639	1/1	0.49	0.30	99,99,99,99	0
55	MG	CA	1640	1/1	0.54	0.33	138,138,138,138	0
55	MG	BJ	201	1/1	0.58	0.37	160,160,160,160	0
55	MG	DB	3115	1/1	0.58	0.35	132,132,132,132	0
55	MG	BB	3047	1/1	0.61	0.11	131,131,131,131	0
55	MG	AA	1630	1/1	0.61	0.12	114,114,114,114	0
55	MG	DB	3052	1/1	0.65	0.22	137,137,137,137	0
55	MG	CA	1641	1/1	0.67	0.12	123,123,123,123	0
55	MG	AA	1639	1/1	0.70	0.16	126,126,126,126	0
55	MG	CA	1614	1/1	0.71	0.18	171,171,171,171	0
55	MG	CA	1632	1/1	0.74	0.11	154,154,154,154	0
55	MG	CA	1655	1/1	0.75	0.49	153,153,153,153	0
55	MG	CA	1644	1/1	0.75	0.18	131,131,131,131	0
55	MG	CA	1643	1/1	0.75	0.08	138,138,138,138	0
55	MG	CA	1613	1/1	0.76	0.25	140,140,140,140	0
55	MG	BB	3093	1/1	0.76	0.22	120,120,120,120	0
55	MG	BB	3063	1/1	0.77	0.18	95,95,95,95	0
55	MG	BB	3057	1/1	0.79	0.28	100,100,100,100	0
55	MG	AA	1643	1/1	0.79	0.12	112,112,112,112	0
55	MG	AA	1628	1/1	0.80	0.11	100,100,100,100	0
55	MG	CA	1656	1/1	0.81	0.12	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1656	1/1	0.82	0.27	101,101,101,101	0
55	MG	CA	1638	1/1	0.82	0.27	102,102,102,102	0
55	MG	CA	1606	1/1	0.83	0.13	139,139,139,139	0
55	MG	CA	1653	1/1	0.83	0.10	149,149,149,149	0
55	MG	BB	3034	1/1	0.83	0.14	70,70,70,70	0
55	MG	CA	1647	1/1	0.84	0.12	109,109,109,109	0
55	MG	AA	1617	1/1	0.84	0.07	123,123,123,123	0
55	MG	BB	3100	1/1	0.84	0.18	128,128,128,128	0
55	MG	CA	1603	1/1	0.85	0.08	124,124,124,124	0
55	MG	BB	3097	1/1	0.85	0.11	112,112,112,112	0
55	MG	AA	1655	1/1	0.85	0.22	82,82,82,82	0
55	MG	BB	3107	1/1	0.85	0.07	86,86,86,86	0
55	MG	DB	3034	1/1	0.85	0.10	87,87,87,87	0
55	MG	BB	3115	1/1	0.85	0.16	106,106,106,106	0
55	MG	AA	1641	1/1	0.85	0.10	111,111,111,111	0
55	MG	CA	1615	1/1	0.86	0.20	156,156,156,156	0
55	MG	CA	1652	1/1	0.86	0.07	117,117,117,117	0
55	MG	AA	1652	1/1	0.86	0.10	103,103,103,103	0
55	MG	BB	3010	1/1	0.86	0.10	95,95,95,95	0
55	MG	CA	1649	1/1	0.87	0.07	100,100,100,100	0
55	MG	AX	101	1/1	0.88	0.19	84,84,84,84	0
55	MG	CN	201	1/1	0.88	0.08	104,104,104,104	0
55	MG	AA	1635	1/1	0.88	0.06	129,129,129,129	0
55	MG	BB	3076	1/1	0.88	0.08	56,56,56,56	0
55	MG	CA	1636	1/1	0.88	0.09	127,127,127,127	0
55	MG	BB	3046	1/1	0.89	0.08	90,90,90,90	0
55	MG	AA	1627	1/1	0.89	0.10	91,91,91,91	0
55	MG	CA	1610	1/1	0.89	0.06	130,130,130,130	0
55	MG	AA	1608	1/1	0.89	0.14	113,113,113,113	0
55	MG	BB	3030	1/1	0.89	0.08	111,111,111,111	0
55	MG	AA	1660	1/1	0.89	0.09	95,95,95,95	0
55	MG	CA	1617	1/1	0.89	0.10	149,149,149,149	0
55	MG	CA	1629	1/1	0.89	0.07	94,94,94,94	0
55	MG	DB	3059	1/1	0.89	0.12	110,110,110,110	0
55	MG	BB	3091	1/1	0.89	0.10	44,44,44,44	0
55	MG	AA	1632	1/1	0.90	0.14	106,106,106,106	0
55	MG	CA	1642	1/1	0.90	0.06	110,110,110,110	0
55	MG	BB	3014	1/1	0.90	0.24	76,76,76,76	0
55	MG	CA	1635	1/1	0.90	0.10	129,129,129,129	0
55	MG	DB	3029	1/1	0.90	0.15	92,92,92,92	0
55	MG	AA	1644	1/1	0.90	0.07	99,99,99,99	0
55	MG	DB	3045	1/1	0.90	0.07	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AA	1633	1/1	0.90	0.08	85,85,85,85	0
55	MG	BB	3038	1/1	0.90	0.07	125,125,125,125	0
55	MG	AA	1605	1/1	0.90	0.11	87,87,87,87	0
55	MG	CA	1645	1/1	0.91	0.17	119,119,119,119	0
55	MG	CA	1627	1/1	0.91	0.07	122,122,122,122	0
55	MG	CA	1607	1/1	0.91	0.07	108,108,108,108	0
55	MG	AA	1613	1/1	0.91	0.07	106,106,106,106	0
55	MG	DB	3065	1/1	0.91	0.15	67,67,67,67	0
55	MG	DB	3082	1/1	0.91	0.11	104,104,104,104	0
55	MG	CA	1621	1/1	0.91	0.10	161,161,161,161	0
55	MG	CA	1612	1/1	0.92	0.07	95,95,95,95	0
55	MG	CA	1623	1/1	0.92	0.09	136,136,136,136	0
55	MG	AA	1619	1/1	0.92	0.10	92,92,92,92	0
55	MG	CA	1648	1/1	0.92	0.11	119,119,119,119	0
55	MG	AA	1623	1/1	0.92	0.10	115,115,115,115	0
55	MG	DB	3058	1/1	0.92	0.09	136,136,136,136	0
55	MG	CA	1631	1/1	0.92	0.07	91,91,91,91	0
55	MG	AA	1624	1/1	0.92	0.16	88,88,88,88	0
55	MG	DB	3070	1/1	0.92	0.09	61,61,61,61	0
55	MG	CA	1633	1/1	0.92	0.07	136,136,136,136	0
55	MG	BB	3042	1/1	0.92	0.10	90,90,90,90	0
55	MG	DB	3032	1/1	0.93	0.09	111,111,111,111	0
55	MG	CA	1650	1/1	0.93	0.06	103,103,103,103	0
55	MG	DB	3037	1/1	0.93	0.06	32,32,32,32	0
55	MG	BB	3007	1/1	0.93	0.11	115,115,115,115	0
55	MG	BB	3118	1/1	0.93	0.09	113,113,113,113	0
55	MG	CA	1654	1/1	0.93	0.21	78,78,78,78	0
55	MG	CA	1626	1/1	0.93	0.07	154,154,154,154	0
55	MG	BB	3043	1/1	0.93	0.10	107,107,107,107	0
55	MG	AA	1611	1/1	0.93	0.16	148,148,148,148	0
55	MG	DB	3013	1/1	0.93	0.10	62,62,62,62	0
55	MG	DB	3088	1/1	0.93	0.11	83,83,83,83	0
55	MG	CA	1637	1/1	0.93	0.11	81,81,81,81	0
55	MG	DB	3030	1/1	0.94	0.14	46,46,46,46	0
55	MG	BB	3081	1/1	0.94	0.09	85,85,85,85	0
55	MG	CA	1620	1/1	0.94	0.06	103,103,103,103	0
55	MG	AA	1642	1/1	0.94	0.08	63,63,63,63	0
55	MG	DB	3039	1/1	0.94	0.07	95,95,95,95	0
55	MG	AA	1638	1/1	0.94	0.06	95,95,95,95	0
55	MG	CA	1625	1/1	0.94	0.10	54,54,54,54	0
55	MG	BB	3050	1/1	0.94	0.08	54,54,54,54	0
55	MG	BB	3051	1/1	0.94	0.06	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	CA	1628	1/1	0.94	0.10	106,106,106,106	0
55	MG	BB	3102	1/1	0.94	0.07	71,71,71,71	0
55	MG	AA	1615	1/1	0.94	0.07	85,85,85,85	0
55	MG	AA	1618	1/1	0.94	0.08	92,92,92,92	0
55	MG	BB	3029	1/1	0.94	0.09	81,81,81,81	0
55	MG	BB	3090	1/1	0.95	0.06	71,71,71,71	0
55	MG	BB	3031	1/1	0.95	0.10	83,83,83,83	0
55	MG	BB	3033	1/1	0.95	0.15	86,86,86,86	0
55	MG	AA	1612	1/1	0.95	0.08	117,117,117,117	0
55	MG	AA	1657	1/1	0.95	0.06	85,85,85,85	0
55	MG	AA	1606	1/1	0.95	0.05	114,114,114,114	0
55	MG	CA	1622	1/1	0.95	0.04	98,98,98,98	0
55	MG	AA	1616	1/1	0.95	0.07	104,104,104,104	0
55	MG	AA	1631	1/1	0.95	0.06	91,91,91,91	0
55	MG	BB	3004	1/1	0.95	0.13	65,65,65,65	0
55	MG	AA	1646	1/1	0.95	0.10	74,74,74,74	0
55	MG	CA	1602	1/1	0.95	0.09	87,87,87,87	0
55	MG	AA	1647	1/1	0.95	0.13	79,79,79,79	0
55	MG	AA	1650	1/1	0.95	0.05	92,92,92,92	0
55	MG	DB	3067	1/1	0.95	0.06	33,33,33,33	0
55	MG	BB	3019	1/1	0.95	0.06	62,62,62,62	0
55	MG	CA	1609	1/1	0.95	0.13	60,60,60,60	0
55	MG	AA	1622	1/1	0.95	0.12	87,87,87,87	0
55	MG	AA	1640	1/1	0.95	0.12	99,99,99,99	0
55	MG	BB	3045	1/1	0.96	0.06	60,60,60,60	0
55	MG	BB	3092	1/1	0.96	0.05	62,62,62,62	0
55	MG	CA	1634	1/1	0.96	0.09	80,80,80,80	0
55	MG	BB	3008	1/1	0.96	0.06	63,63,63,63	0
55	MG	BB	3094	1/1	0.96	0.08	81,81,81,81	0
55	MG	CA	1604	1/1	0.96	0.06	58,58,58,58	0
55	MG	BB	3096	1/1	0.96	0.06	49,49,49,49	0
55	MG	BB	3068	1/1	0.96	0.06	40,40,40,40	0
55	MG	AA	1653	1/1	0.96	0.09	84,84,84,84	0
55	MG	AA	1602	1/1	0.96	0.11	83,83,83,83	0
55	MG	BB	3082	1/1	0.96	0.08	80,80,80,80	0
55	MG	CX	101	1/1	0.96	0.05	73,73,73,73	0
55	MG	AA	1645	1/1	0.96	0.09	127,127,127,127	0
55	MG	BB	3117	1/1	0.96	0.07	82,82,82,82	0
55	MG	DB	3020	1/1	0.96	0.06	25,25,25,25	0
55	MG	DB	3028	1/1	0.96	0.06	42,42,42,42	0
55	MG	CA	1624	1/1	0.97	0.07	103,103,103,103	0
55	MG	AA	1604	1/1	0.97	0.05	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	AX	102	1/1	0.97	0.05	66,66,66,66	0
55	MG	BB	3001	1/1	0.97	0.06	57,57,57,57	0
55	MG	BB	3078	1/1	0.97	0.05	71,71,71,71	0
55	MG	CA	1601	1/1	0.97	0.08	48,48,48,48	0
55	MG	BB	3080	1/1	0.97	0.04	65,65,65,65	0
55	MG	DB	3002	1/1	0.97	0.06	44,44,44,44	0
55	MG	DB	3005	1/1	0.97	0.05	66,66,66,66	0
55	MG	AA	1634	1/1	0.97	0.05	55,55,55,55	0
55	MG	DB	3018	1/1	0.97	0.05	32,32,32,32	0
55	MG	BB	3005	1/1	0.97	0.09	52,52,52,52	0
55	MG	DB	3026	1/1	0.97	0.06	38,38,38,38	0
55	MG	CA	1605	1/1	0.97	0.04	98,98,98,98	0
55	MG	BB	3083	1/1	0.97	0.11	47,47,47,47	0
55	MG	BB	3087	1/1	0.97	0.06	63,63,63,63	0
55	MG	CA	1608	1/1	0.97	0.06	82,82,82,82	0
55	MG	BB	3037	1/1	0.97	0.08	56,56,56,56	0
55	MG	AA	1648	1/1	0.97	0.05	67,67,67,67	0
55	MG	CA	1611	1/1	0.97	0.04	102,102,102,102	0
55	MG	DB	3043	1/1	0.97	0.09	49,49,49,49	0
55	MG	AA	1649	1/1	0.97	0.05	84,84,84,84	0
55	MG	DB	3051	1/1	0.97	0.05	48,48,48,48	0
55	MG	BB	3009	1/1	0.97	0.05	92,92,92,92	0
55	MG	AA	1621	1/1	0.97	0.10	36,36,36,36	0
55	MG	BB	3011	1/1	0.97	0.10	45,45,45,45	0
55	MG	DB	3061	1/1	0.97	0.06	97,97,97,97	0
55	MG	AA	1659	1/1	0.97	0.05	86,86,86,86	0
55	MG	CA	1618	1/1	0.97	0.04	87,87,87,87	0
55	MG	BB	3016	1/1	0.97	0.12	91,91,91,91	0
55	MG	DB	3071	1/1	0.97	0.05	30,30,30,30	0
55	MG	DB	3077	1/1	0.97	0.06	57,57,57,57	0
55	MG	BB	3101	1/1	0.97	0.06	50,50,50,50	0
55	MG	AA	1601	1/1	0.97	0.06	62,62,62,62	0
55	MG	DB	3094	1/1	0.97	0.07	77,77,77,77	0
55	MG	DB	3104	1/1	0.97	0.04	50,50,50,50	0
55	MG	DB	3107	1/1	0.97	0.07	24,24,24,24	0
55	MG	DB	3108	1/1	0.97	0.05	36,36,36,36	0
55	MG	DB	3109	1/1	0.97	0.12	28,28,28,28	0
55	MG	DB	3112	1/1	0.97	0.05	52,52,52,52	0
55	MG	BB	3028	1/1	0.97	0.05	54,54,54,54	0
55	MG	DB	3119	1/1	0.97	0.15	64,64,64,64	0
55	MG	DB	3027	1/1	0.98	0.07	43,43,43,43	0
55	MG	BB	3072	1/1	0.98	0.03	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	BB	3073	1/1	0.98	0.05	30,30,30,30	0
55	MG	CA	1616	1/1	0.98	0.04	80,80,80,80	0
55	MG	BB	3106	1/1	0.98	0.06	53,53,53,53	0
55	MG	DB	3033	1/1	0.98	0.04	43,43,43,43	0
55	MG	BB	3074	1/1	0.98	0.06	25,25,25,25	0
55	MG	CA	1619	1/1	0.98	0.04	79,79,79,79	0
55	MG	BB	3112	1/1	0.98	0.14	27,27,27,27	0
55	MG	BB	3044	1/1	0.98	0.04	62,62,62,62	0
55	MG	DB	3044	1/1	0.98	0.05	20,20,20,20	0
55	MG	AA	1629	1/1	0.98	0.07	53,53,53,53	0
55	MG	DB	3046	1/1	0.98	0.06	47,47,47,47	0
55	MG	DB	3047	1/1	0.98	0.07	36,36,36,36	0
55	MG	DB	3050	1/1	0.98	0.05	51,51,51,51	0
55	MG	AA	1651	1/1	0.98	0.03	83,83,83,83	0
55	MG	AA	1609	1/1	0.98	0.08	67,67,67,67	0
55	MG	DB	3053	1/1	0.98	0.12	37,37,37,37	0
55	MG	DB	3056	1/1	0.98	0.06	28,28,28,28	0
55	MG	DB	3057	1/1	0.98	0.07	63,63,63,63	0
55	MG	BB	3048	1/1	0.98	0.05	38,38,38,38	0
55	MG	CA	1651	1/1	0.98	0.11	66,66,66,66	0
55	MG	DB	3060	1/1	0.98	0.14	35,35,35,35	0
55	MG	BB	3049	1/1	0.98	0.04	40,40,40,40	0
55	MG	DB	3064	1/1	0.98	0.05	32,32,32,32	0
55	MG	BB	3084	1/1	0.98	0.08	61,61,61,61	0
55	MG	BB	3024	1/1	0.98	0.04	47,47,47,47	0
55	MG	BB	3088	1/1	0.98	0.04	76,76,76,76	0
55	MG	CA	1630	1/1	0.98	0.03	97,97,97,97	0
55	MG	DB	3075	1/1	0.98	0.07	46,46,46,46	0
55	MG	AA	1607	1/1	0.98	0.05	93,93,93,93	0
55	MG	BB	3056	1/1	0.98	0.04	49,49,49,49	0
55	MG	DB	3083	1/1	0.98	0.11	31,31,31,31	0
55	MG	DB	3087	1/1	0.98	0.06	28,28,28,28	0
55	MG	BB	3039	1/1	0.98	0.05	55,55,55,55	0
55	MG	DB	3089	1/1	0.98	0.10	51,51,51,51	0
55	MG	DB	3090	1/1	0.98	0.07	62,62,62,62	0
55	MG	DB	3091	1/1	0.98	0.05	39,39,39,39	0
55	MG	BB	3058	1/1	0.98	0.05	62,62,62,62	0
55	MG	DB	3101	1/1	0.98	0.05	44,44,44,44	0
55	MG	DB	3008	1/1	0.98	0.05	55,55,55,55	0
55	MG	AA	1603	1/1	0.98	0.04	55,55,55,55	0
55	MG	DB	3016	1/1	0.98	0.09	43,43,43,43	0
55	MG	BB	3064	1/1	0.98	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DB	3110	1/1	0.98	0.05	41,41,41,41	0
55	MG	DB	3111	1/1	0.98	0.04	38,38,38,38	0
55	MG	BB	3012	1/1	0.98	0.05	32,32,32,32	0
55	MG	DB	3114	1/1	0.98	0.09	43,43,43,43	0
55	MG	DB	3021	1/1	0.98	0.05	50,50,50,50	0
55	MG	DB	3116	1/1	0.98	0.12	54,54,54,54	0
55	MG	BB	3070	1/1	0.98	0.05	52,52,52,52	0
56	ZN	B4	101	1/1	0.98	0.09	72,72,72,72	0
55	MG	DB	3024	1/1	0.99	0.07	22,22,22,22	0
55	MG	BB	3099	1/1	0.99	0.03	41,41,41,41	0
55	MG	AA	1620	1/1	0.99	0.03	74,74,74,74	0
55	MG	BB	3022	1/1	0.99	0.02	56,56,56,56	0
55	MG	BB	3065	1/1	0.99	0.04	46,46,46,46	0
55	MG	BB	3103	1/1	0.99	0.03	38,38,38,38	0
55	MG	BB	3104	1/1	0.99	0.03	38,38,38,38	0
55	MG	BB	3105	1/1	0.99	0.04	64,64,64,64	0
55	MG	BB	3066	1/1	0.99	0.03	51,51,51,51	0
55	MG	DB	3036	1/1	0.99	0.03	36,36,36,36	0
55	MG	BB	3067	1/1	0.99	0.09	39,39,39,39	0
55	MG	DB	3038	1/1	0.99	0.03	19,19,19,19	0
55	MG	BB	3108	1/1	0.99	0.03	30,30,30,30	0
55	MG	DB	3041	1/1	0.99	0.04	32,32,32,32	0
55	MG	DB	3042	1/1	0.99	0.04	56,56,56,56	0
55	MG	BB	3109	1/1	0.99	0.06	52,52,52,52	0
55	MG	BB	3110	1/1	0.99	0.04	56,56,56,56	0
55	MG	BB	3111	1/1	0.99	0.02	43,43,43,43	0
55	MG	BB	3040	1/1	0.99	0.09	64,64,64,64	0
55	MG	BB	3069	1/1	0.99	0.04	28,28,28,28	0
55	MG	DB	3048	1/1	0.99	0.06	45,45,45,45	0
55	MG	BB	3041	1/1	0.99	0.06	28,28,28,28	0
55	MG	BB	3071	1/1	0.99	0.10	41,41,41,41	0
55	MG	AA	1610	1/1	0.99	0.02	61,61,61,61	0
55	MG	BB	3025	1/1	0.99	0.06	63,63,63,63	0
55	MG	DB	3054	1/1	0.99	0.05	53,53,53,53	0
55	MG	DB	3055	1/1	0.99	0.03	30,30,30,30	0
55	MG	BB	3027	1/1	0.99	0.12	40,40,40,40	0
55	MG	BB	3075	1/1	0.99	0.11	44,44,44,44	0
55	MG	AA	1654	1/1	0.99	0.04	49,49,49,49	0
55	MG	BB	3077	1/1	0.99	0.04	50,50,50,50	0
55	MG	BB	3013	1/1	0.99	0.06	52,52,52,52	0
55	MG	BB	3079	1/1	0.99	0.06	46,46,46,46	0
55	MG	DB	3062	1/1	0.99	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DB	3063	1/1	0.99	0.06	45,45,45,45	0
55	MG	AA	1636	1/1	0.99	0.05	61,61,61,61	0
55	MG	BB	3015	1/1	0.99	0.04	69,69,69,69	0
55	MG	DB	3066	1/1	0.99	0.05	30,30,30,30	0
55	MG	BB	3032	1/1	0.99	0.05	53,53,53,53	0
55	MG	DB	3068	1/1	0.99	0.05	35,35,35,35	0
55	MG	DB	3069	1/1	0.99	0.03	48,48,48,48	0
55	MG	BB	3003	1/1	0.99	0.08	20,20,20,20	0
55	MG	BB	3017	1/1	0.99	0.09	35,35,35,35	0
55	MG	DB	3072	1/1	0.99	0.04	39,39,39,39	0
55	MG	BB	3052	1/1	0.99	0.04	33,33,33,33	0
55	MG	DB	3076	1/1	0.99	0.03	49,49,49,49	0
55	MG	BB	3054	1/1	0.99	0.03	56,56,56,56	0
55	MG	DB	3079	1/1	0.99	0.04	18,18,18,18	0
55	MG	DB	3080	1/1	0.99	0.07	29,29,29,29	0
55	MG	BB	3089	1/1	0.99	0.07	51,51,51,51	0
55	MG	BB	3055	1/1	0.99	0.07	72,72,72,72	0
55	MG	DB	3084	1/1	0.99	0.07	26,26,26,26	0
55	MG	DB	3086	1/1	0.99	0.04	57,57,57,57	0
55	MG	BB	3035	1/1	0.99	0.05	40,40,40,40	0
55	MG	DB	3004	1/1	0.99	0.03	21,21,21,21	0
55	MG	BB	3036	1/1	0.99	0.04	52,52,52,52	0
55	MG	DB	3006	1/1	0.99	0.04	38,38,38,38	0
55	MG	DB	3007	1/1	0.99	0.04	49,49,49,49	0
55	MG	DB	3092	1/1	0.99	0.09	44,44,44,44	0
55	MG	DB	3093	1/1	0.99	0.04	54,54,54,54	0
55	MG	BB	3018	1/1	0.99	0.04	42,42,42,42	0
55	MG	DB	3096	1/1	0.99	0.03	46,46,46,46	0
55	MG	DB	3097	1/1	0.99	0.06	39,39,39,39	0
55	MG	DB	3098	1/1	0.99	0.08	42,42,42,42	0
55	MG	DB	3099	1/1	0.99	0.06	19,19,19,19	0
55	MG	DB	3010	1/1	0.99	0.04	20,20,20,20	0
55	MG	DB	3102	1/1	0.99	0.05	67,67,67,67	0
55	MG	DB	3011	1/1	0.99	0.03	16,16,16,16	0
55	MG	DB	3105	1/1	0.99	0.05	18,18,18,18	0
55	MG	DB	3106	1/1	0.99	0.04	29,29,29,29	0
55	MG	BB	3059	1/1	0.99	0.03	37,37,37,37	0
55	MG	DB	3014	1/1	0.99	0.06	32,32,32,32	0
55	MG	DB	3015	1/1	0.99	0.02	49,49,49,49	0
55	MG	BB	3095	1/1	0.99	0.03	48,48,48,48	0
55	MG	DB	3017	1/1	0.99	0.03	34,34,34,34	0
55	MG	BB	3060	1/1	0.99	0.03	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	DB	3019	1/1	0.99	0.03	43,43,43,43	0
55	MG	BB	3061	1/1	0.99	0.04	57,57,57,57	0
55	MG	BB	3098	1/1	0.99	0.05	73,73,73,73	0
55	MG	DB	3118	1/1	0.99	0.03	35,35,35,35	0
55	MG	DB	3022	1/1	0.99	0.03	42,42,42,42	0
55	MG	DB	3023	1/1	0.99	0.04	46,46,46,46	0
56	ZN	D4	401	1/1	0.99	0.04	72,72,72,72	0
55	MG	DB	3003	1/1	1.00	0.02	24,24,24,24	0
55	MG	BB	3114	1/1	1.00	0.02	57,57,57,57	0
55	MG	BB	3006	1/1	1.00	0.03	35,35,35,35	0
55	MG	BB	3116	1/1	1.00	0.01	24,24,24,24	0
55	MG	BB	3053	1/1	1.00	0.04	43,43,43,43	0
55	MG	DB	3095	1/1	1.00	0.07	26,26,26,26	0
55	MG	DB	3025	1/1	1.00	0.04	40,40,40,40	0
55	MG	BB	3085	1/1	1.00	0.03	57,57,57,57	0
55	MG	DB	3009	1/1	1.00	0.01	48,48,48,48	0
55	MG	DB	3049	1/1	1.00	0.03	42,42,42,42	0
55	MG	DB	3100	1/1	1.00	0.02	10,10,10,10	0
55	MG	BB	3086	1/1	1.00	0.12	50,50,50,50	0
55	MG	DB	3073	1/1	1.00	0.03	7,7,7,7	0
55	MG	DB	3103	1/1	1.00	0.03	46,46,46,46	0
55	MG	DB	3074	1/1	1.00	0.02	9,9,9,9	0
55	MG	BB	3023	1/1	1.00	0.02	15,15,15,15	0
55	MG	DB	3012	1/1	1.00	0.09	37,37,37,37	0
55	MG	DB	3031	1/1	1.00	0.04	16,16,16,16	0
55	MG	DB	3078	1/1	1.00	0.02	28,28,28,28	0
55	MG	BB	3062	1/1	1.00	0.05	42,42,42,42	0
55	MG	BB	3002	1/1	1.00	0.03	31,31,31,31	0
55	MG	DB	3081	1/1	1.00	0.03	36,36,36,36	0
55	MG	BB	3020	1/1	1.00	0.06	45,45,45,45	0
55	MG	DB	3113	1/1	1.00	0.04	27,27,27,27	0
55	MG	DB	3035	1/1	1.00	0.09	27,27,27,27	0
55	MG	BB	3026	1/1	1.00	0.02	26,26,26,26	0
55	MG	DB	3085	1/1	1.00	0.05	21,21,21,21	0
55	MG	DB	3117	1/1	1.00	0.02	26,26,26,26	0
55	MG	BB	3021	1/1	1.00	0.02	45,45,45,45	0
55	MG	DB	3001	1/1	1.00	0.02	14,14,14,14	0
55	MG	BB	3113	1/1	1.00	0.03	41,41,41,41	0
55	MG	DB	3040	1/1	1.00	0.02	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.