



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 03:14 pm BST

PDB ID : 4V4Q
Title : Crystal structure of the bacterial ribosome from Escherichia coli at 3.5 Å resolution.
Authors : Schuwirth, B.S.; Borovinskaya, M.A.; Hau, C.W.; Zhang, W.; Vila-Sanjurjo, A.; Holton, J.M.; Cate, J.H.D.
Deposited on : 2005-08-30
Resolution : 3.46 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

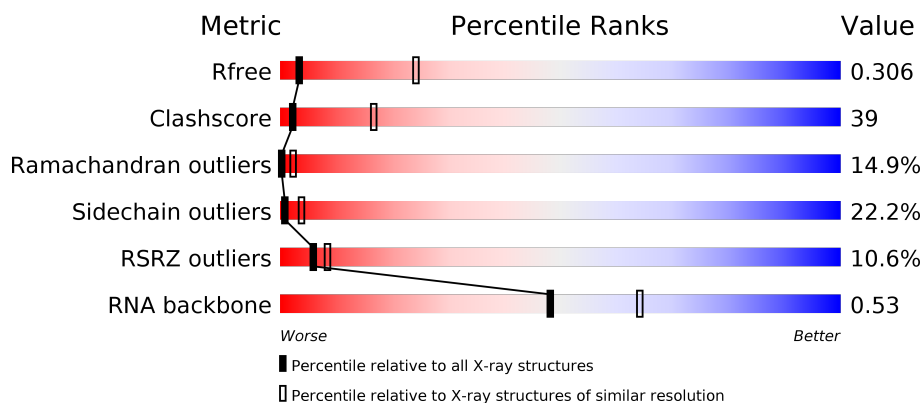
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>3%</div> <div>25%</div> <div>59%</div> <div>14%</div> <div>.</div> </div>
1	CA	1542	<div> <div>26%</div> <div>60%</div> <div>13%</div> <div>..</div> </div>
2	AC	232	<div> <div>3%</div> <div>26%</div> <div>49%</div> <div>13%</div> <div>.</div> <div>11%</div> </div>
2	CC	232	<div> <div>3%</div> <div>27%</div> <div>50%</div> <div>12%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	

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Mol	Chain	Length	Quality of chain
28	BF	178	
28	DF	178	
29	BG	176	
29	DG	176	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	103	
42	DU	103	
43	BW	84	
43	DW	84	
44	BX	63	
44	DX	63	
45	BY	58	
45	DY	58	
46	BZ	70	
46	DZ	70	
47	B0	56	
47	D0	56	
48	B1	54	
48	D1	54	
49	B2	46	
49	D2	46	
50	B3	64	
50	D3	64	
51	B4	38	
51	D4	38	
52	BI	141	
52	DI	141	

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
53	MG	AA	1636	-	-	-	X

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 284107 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 protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			656	417	122	114	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

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

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

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

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

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

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

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			
25	DC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

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

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			
31	DJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
35	DN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
36	DO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			
41	DT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

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

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

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0
43	DW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0
44	DX	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0
45	DY	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0
46	DZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	54	Total	C	N	O	0	0	0
			441	284	81	76			
48	D1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 49 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L36.

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

- Molecule 52 is a protein called 50S ribosomal protein L11.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	AP	1	Total Mg 1 1	0	0
53	BB	110	Total Mg 110 110	0	0
53	CA	62	Total Mg 62 62	0	0
53	AA	59	Total Mg 59 59	0	0
53	DN	1	Total Mg 1 1	0	0
53	DB	110	Total Mg 110 110	0	0

- Molecule 54 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	AA	290	Total O 290 290	0	0
54	AE	3	Total O 3 3	0	0
54	AK	2	Total O 2 2	0	0
54	AN	4	Total O 4 4	0	0
54	AP	1	Total O 1 1	0	0
54	BB	497	Total O 497 497	0	0
54	BC	1	Total O 1 1	0	0
54	BE	5	Total O 5 5	0	0
54	BH	1	Total O 1 1	0	0
54	BL	2	Total O 2 2	0	0
54	BN	1	Total O 1 1	0	0
54	CA	295	Total O 295 295	0	0
54	CE	3	Total O 3 3	0	0
54	CK	1	Total O 1 1	0	0

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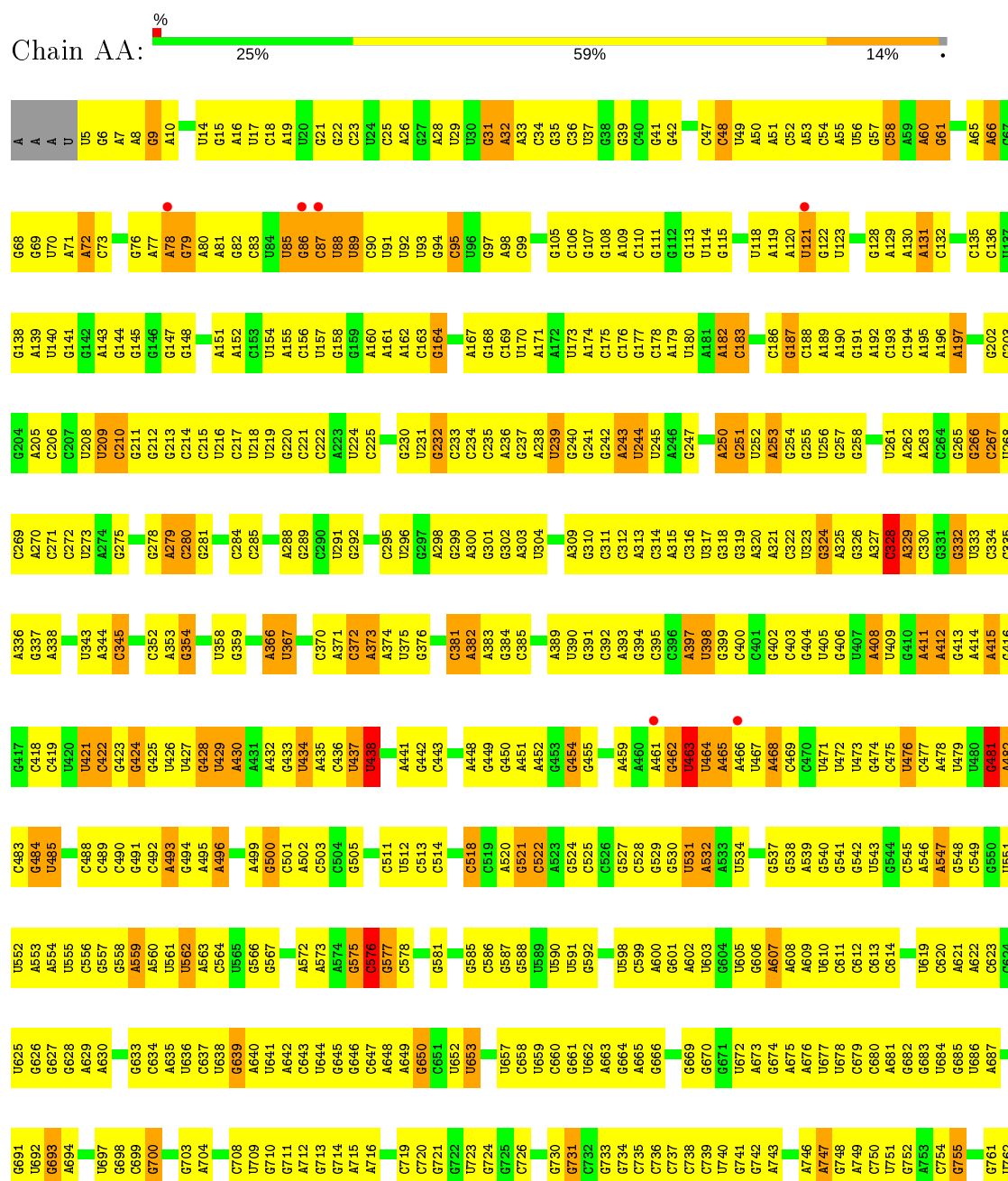
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CL	4	Total 4	O 4	0	0
54	CN	2	Total 2	O 2	0	0
54	CP	1	Total 1	O 1	0	0
54	CT	2	Total 2	O 2	0	0
54	DB	499	Total 499	O 499	0	0
54	DC	1	Total 1	O 1	0	0
54	DD	1	Total 1	O 1	0	0
54	DE	3	Total 3	O 3	0	0
54	DJ	2	Total 2	O 2	0	0
54	DL	1	Total 1	O 1	0	0
54	DN	2	Total 2	O 2	0	0
54	DQ	1	Total 1	O 1	0	0
54	D2	2	Total 2	O 2	0	0

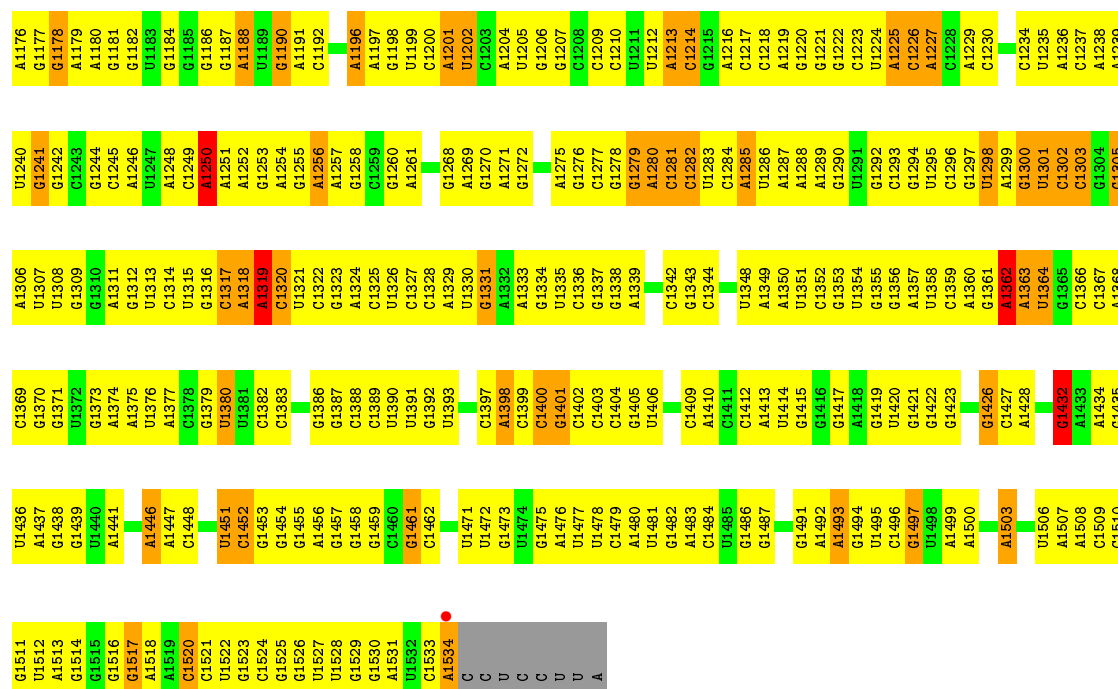
3 Residue-property plots

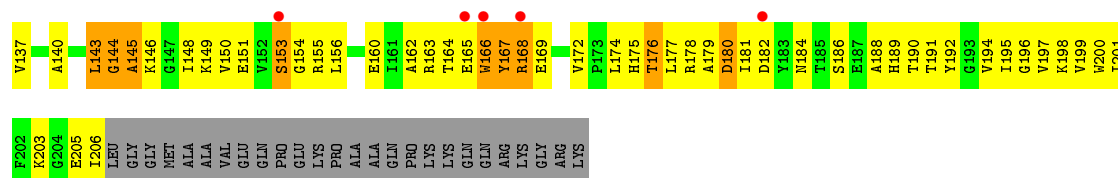
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S ribosomal RNA

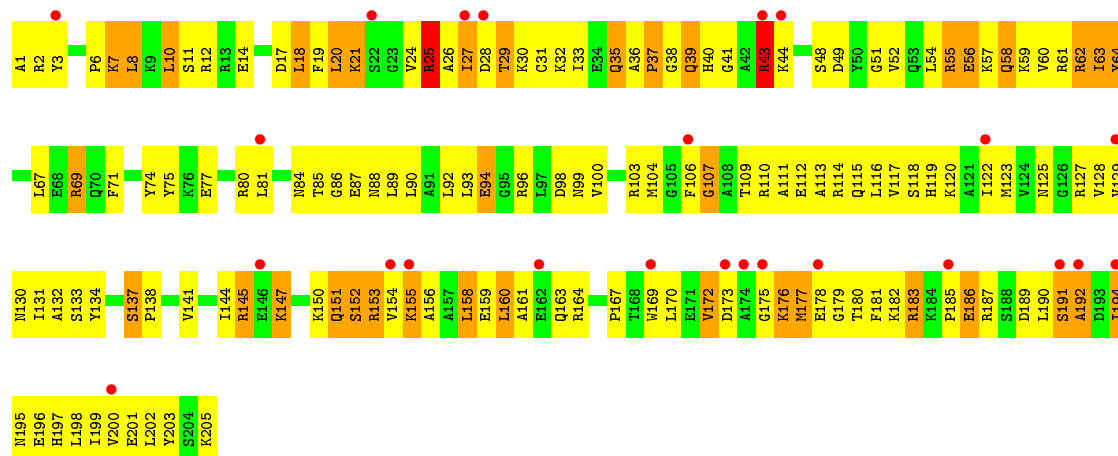


G1108	A1042	C980	G838	A767	A695	G628	A553	C483	C419	C345	U273	U208	G144
A1111	G1043	U981	C839	A768		A629	A554	G484	U420	C345	A274	U209	G142
C1113	A1044	U982	C840	G769	C699	A630	U555	U485	U421	C352	G275	C210	A143
C1114		A983	C941	C770	G700		C556	C422	C422	A353	G276	G211	G144
	U1048	C984	U843	G771	G703	G633	C557	C423	G423	C354	G277	G212	G145
	U1049	C985	U844	G772	A704	G634	C558	G424	G424		G278	G213	G146
	G1050	U986	G844	G773	G705	A635	C559	G425	G425	U358	A279	C214	G147
	C1051	G987	A845	A777	A706	U636	A560	G426	U426	C280	G280	C215	G148
C1119	U1052	G988	G846	G778	A707	G637	U561	C492	U427	G360	G281	U216	A149
C1120	G1053	U989	G847	C779	G708	U638	U562	A493	G428	A366	C284	C217	U150
U1121	C1054	C990	C848	A780	C708	G639	A563	G494	U429	U367	G285	U218	A151
U1122	A1055	U991		A781	G709		G566	A495	A430			U219	A152
U1123	U1056	C930	C857	A782	G710	A642	G567	A496	A431			G220	
G1124	G1057	C931	G858	C783	G711	C643	G567		A432	C370	A288	C221	A155
U1125	G1058	G932	G859	A784	G712	U644	G568	A499	A433	A371	G289	C222	C156
U1126	C1059	A984	A860	G785	G713	U645		U500	U434	C372		G223	U157
		U997	G861		G714	G646	A572	C501	A435	A373	C295	U224	G158
	U1060	C998	C862	A792	A715	G647	A573	A502	G436	A374	U296	C225	G159
	G1127	C999	U863	U793	A716	A648	A574	C503	U437	U375	G297		
C1129	U1062	C936	A864	U794		A649	G575	G504	U438	G376	A298	G230	A160
A1130	G1063	A937	A865	C795	C719	G650	G576	G505	U439	G377	G299	U231	A161
G1131	U1064	A938	C866	C796	G720	C651	G577		G440	A300	A300	G232	A162
C1132	C1065	G939	C866	C797	G721	U652	C578	C511	A441	C381	G301	C233	C163
G1133	G1066	C940		U798	G722	U653	C578	U512	G442	A382	G302	C234	G164
	A1067	G941	G869		G724		G585	C513	C443	A383	G303	C235	
	C1068		U875	U801	G725	C658	C586	C514	A448	G384	U304	A236	A167
	G1069		U876	A802	C726	U659	G587		A449	C385		G237	G168
	U1070		A878	G803	G727	C660		C518	G449	C386	A309	U239	C169
	C1071	U1008	C879	U804	G730	U661	U590		G450	U387	G310	G240	U170
	U1072	U1009	C880	C805	G731	U662	U591	G521	A451		C311	U241	U173
	C1073	U1010	G881	C806	C732	A663	G592	C522	A452		C312	G242	A174
	G1074	C1011	C882	A807	G733	G664	A596	A523	G453	U390	A313	G243	C175
	U1075	A1012	G883	C808	G734	A665	G597	G524	U454	G391	C314	U244	C176
		G1013	U884	G809	C735	G666	G598	C525	G455	C392	A315	U245	G177
		A1014	G885	C810	C736	G667	U599	C526	A456	C393	C316	U246	C178
		G1015		C811	C737	G668	C527	G527		G394	U317	A247	A179
		A1016	G890	G812	C738	G669	A600	C528	A459	C395	G318	G247	U180
			U897	U813	C739	G670	G601	G529	A460	C396	G319		A181
		A1019	C893	A814	U740	G671	A602	G530	A461	A397	A320	A250	A182
		G1020	U894	A815	G741	U672	U603	U531	G462	U398	A321	G251	C183
		A1021	G895	A816	G742	A673	G604	A532	U463	G399	C322	U252	
		U1022	C896	C817	A743	G674	U605	A533	U464	C400	U323	A253	C186
		G1023	C897	G818		A675	G606	U534	A465	G401	G324	G254	G187
		U1024	C962	G819	A746	A676	A607		A466	G402	A325	G255	C188
		G1025	G863	U820	A747	U677	A608	G537	U467	C403	G326	U256	A189
		A1026	A964	G821	G748	U678	A609	G538	A468	G404	A327	G257	A190
		C1027	U965	A822	A749	C679	U610	A539	C469	A405	C328	G258	G191
		G1028	G902	G824	G750		C611	G540	U470	G406	A329		A192
		U1029	G903	G825	U751	G682	C612	G541	U471	U407	C330	U261	C193
		U1030	U904	A825	G752	U683	C613	G542	U472	A408	G331	C194	A194
		C1031	U905		A753	U684	C614	U543	U473	U409	G332	A262	A195
		G1032	A906	U828	G754	G685		G544	G474	G409	G333	A263	A196
		U1033	U907	G829	C755	U686	U619	G545	A411	G410	U334	G264	A197
		A1034	A908	G830	G755	A687	C620	A546	C475	A412	C335	G265	
		C1035	G973	A831		U688	A621	A547	U476	G413	G336	G266	G202
		U1036	C910	G832	G761	G688	A622	G548	C477	G414	G337	U268	G203
		A1037	G974	G833	U762		A622	G549	A478	A415	A338	C269	G204
		C1038	U834	U834	G763	G691		U551	U479	G416	U343	A270	A205
		G1039	U835	G763	G765	U692	U625	G550	U480	G417	G337	C271	C206
		U1040	G836	G765	G766	U693	G626	G431	G481	G418		A272	C207
		C979	G917	A766		A694	G627	U552	A482	C418	A344	C272	

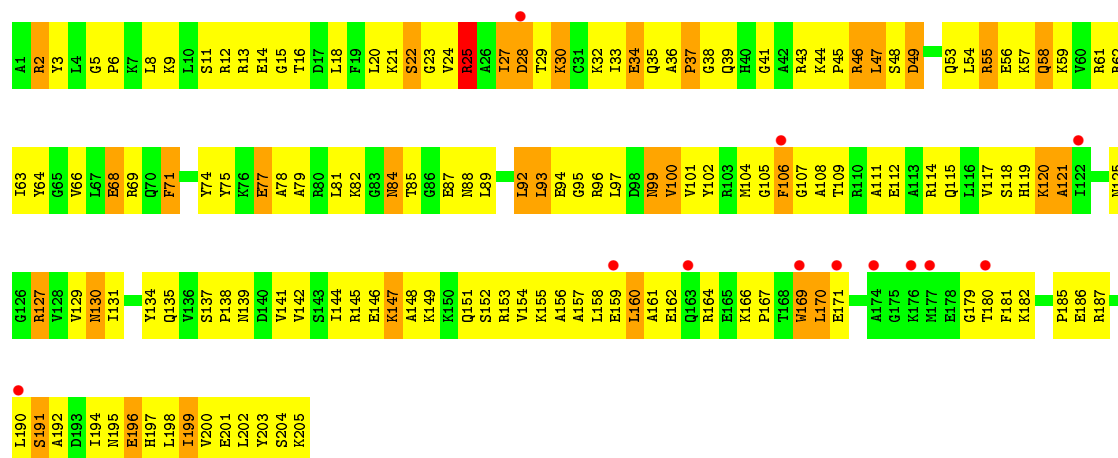




• Molecule 3: 30S ribosomal protein S4

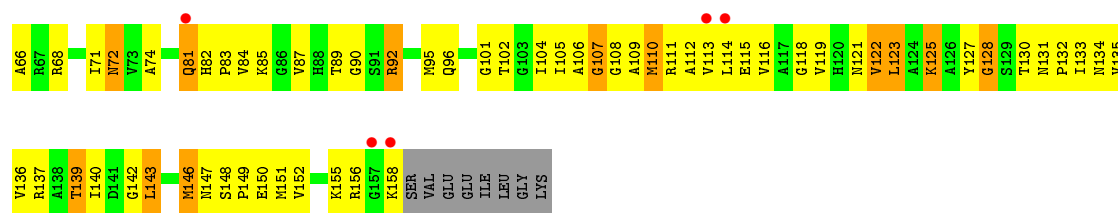


• Molecule 3: 30S ribosomal protein S4

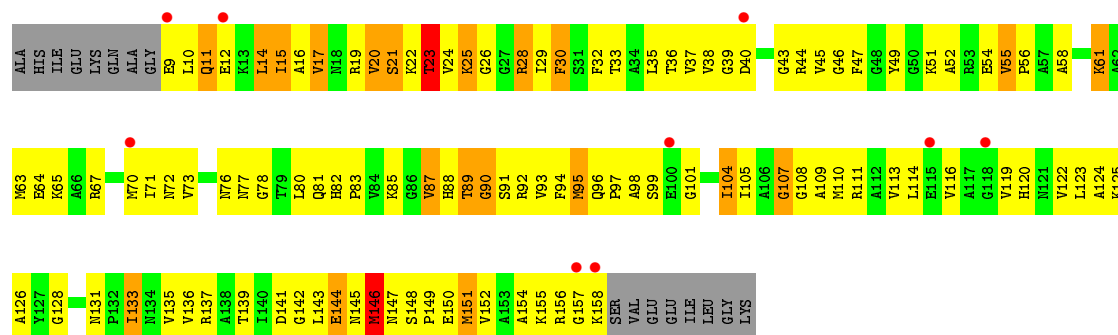


• Molecule 4: 30S ribosomal protein S5

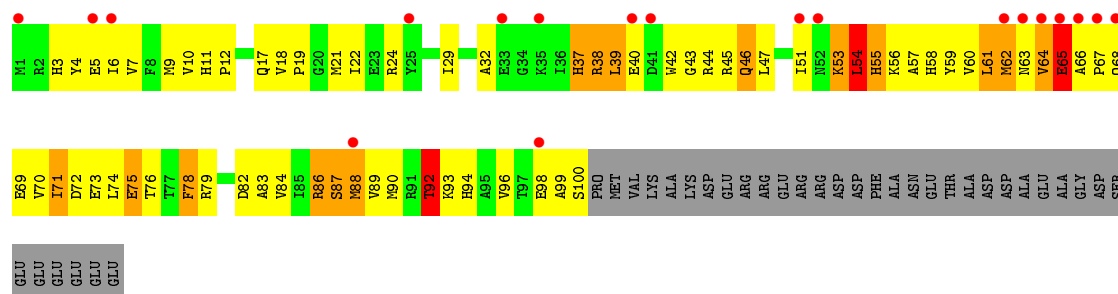
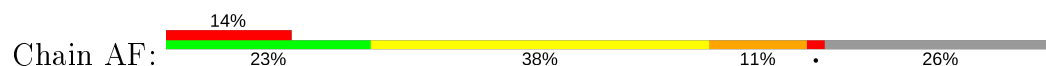




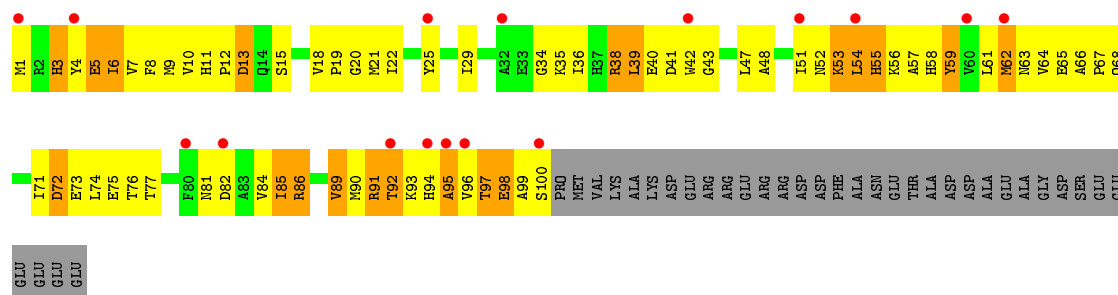
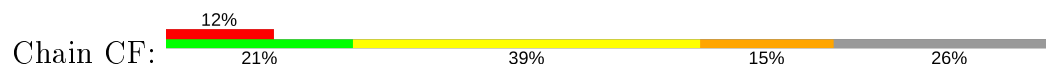
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

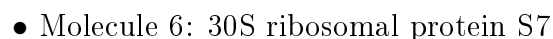


• Molecule 5: 30S ribosomal protein S6

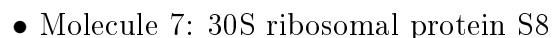


• Molecule 6: 30S ribosomal protein S7

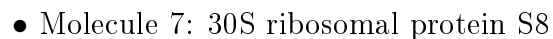
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5%	5%
25%	25%
47%	47%
12%	12%
16%	16%



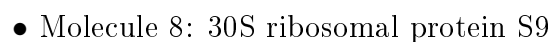
Response	Percentage
Not at all	2%
A little	25%
A lot	49%
Not sure	11%
Don't know	15%

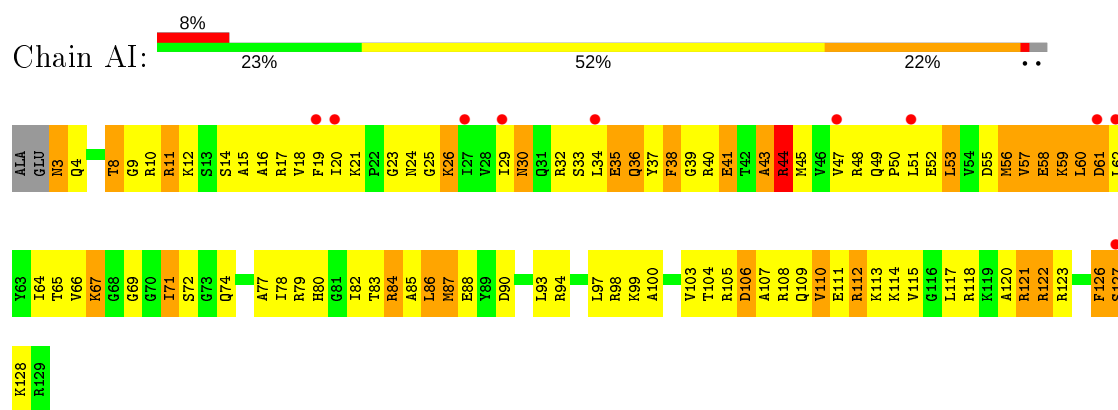


Government	Percentage
Current Government	13%
Opposition	43%
Current Government	47%
Opposition	9%

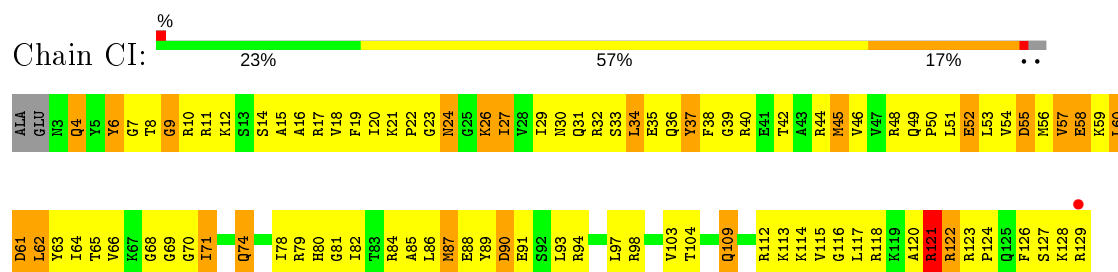


Frequency	Percentage
Daily	12%
Often	35%
Sometimes	53%
Never	12%

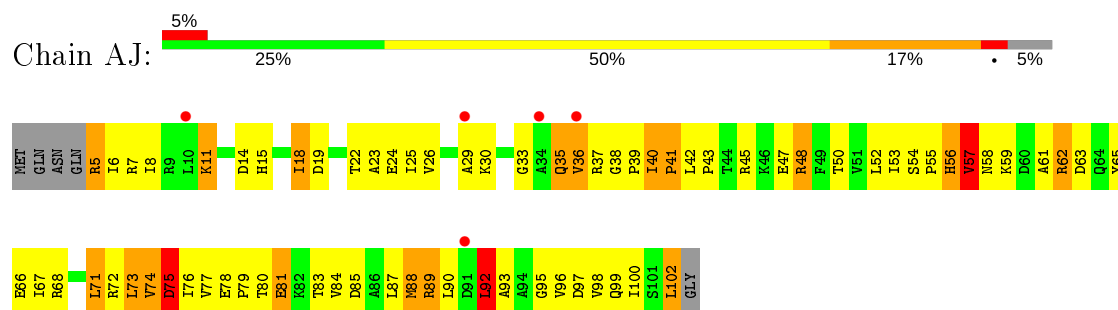




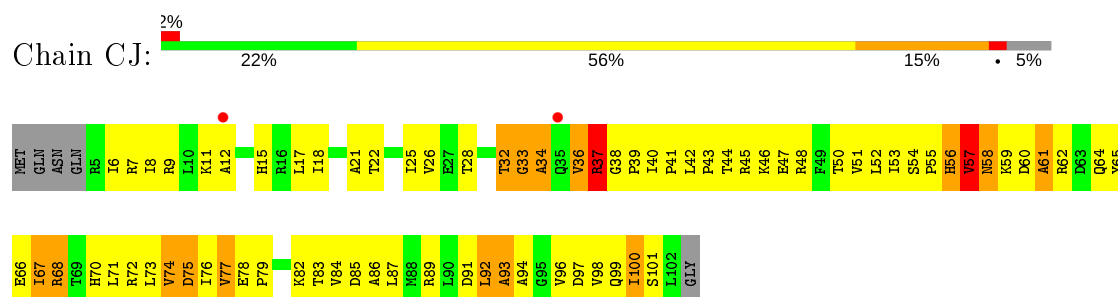
• Molecule 8: 30S ribosomal protein S9



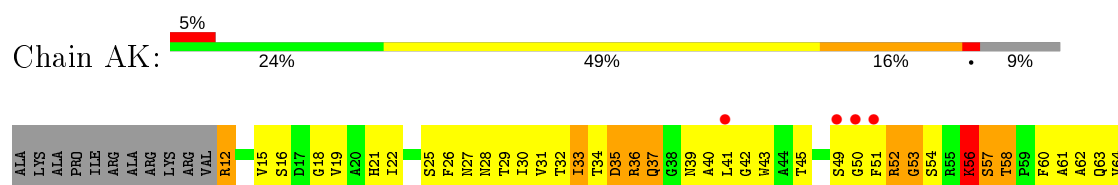
• Molecule 9: 30S ribosomal protein S10



• Molecule 9: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S11

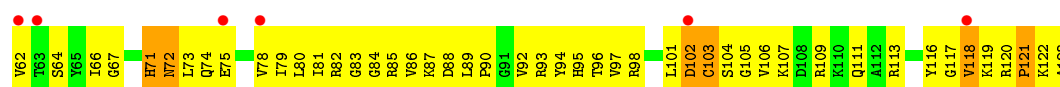
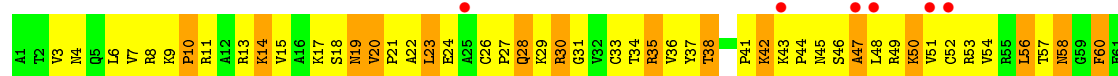




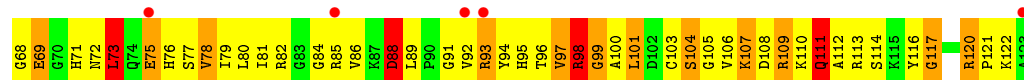
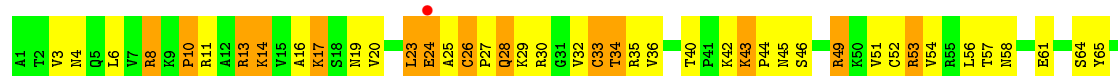
- Molecule 10: 30S ribosomal protein S11



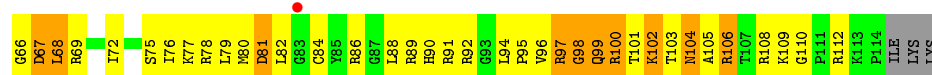
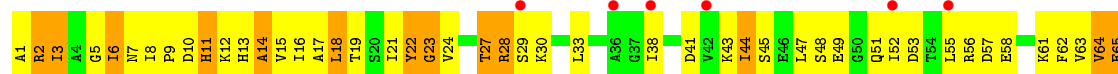
- Molecule 11: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S12

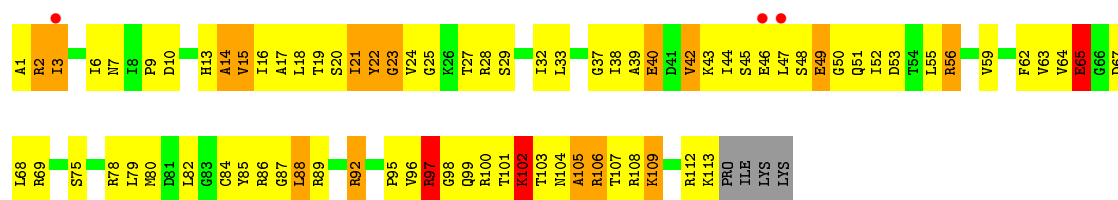


- Molecule 12: 30S ribosomal protein S13

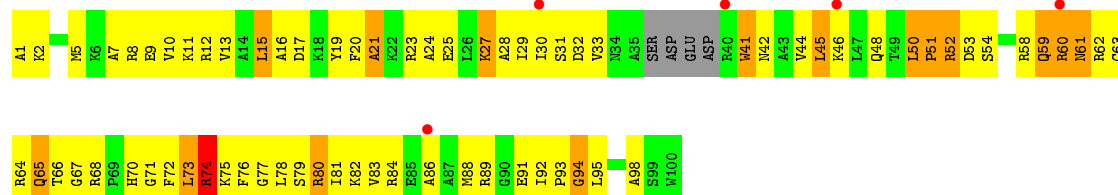


- Molecule 12: 30S ribosomal protein S13

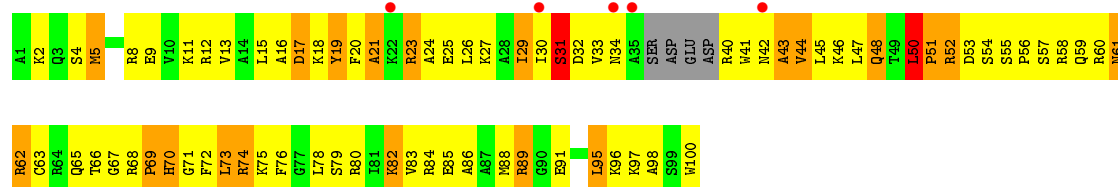




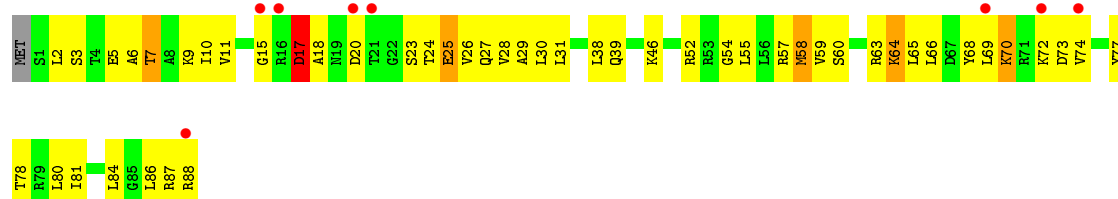
• Molecule 13: 30S ribosomal protein S14



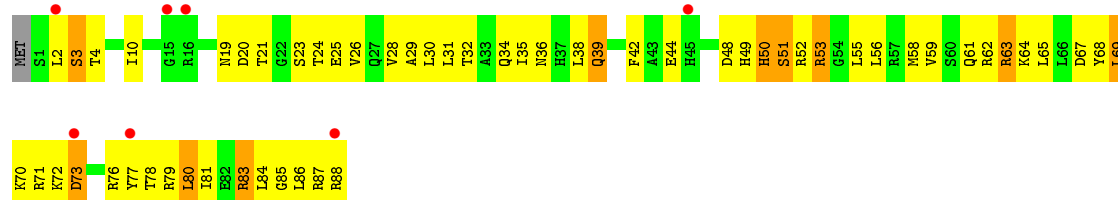
• Molecule 13: 30S ribosomal protein S14



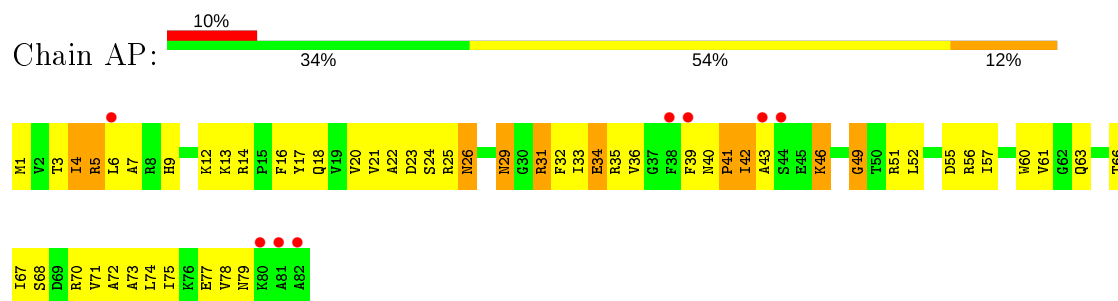
• Molecule 14: 30S ribosomal protein S15



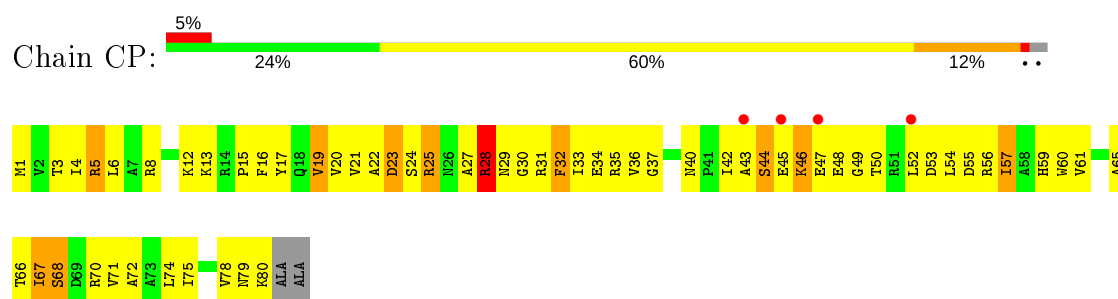
• Molecule 14: 30S ribosomal protein S15



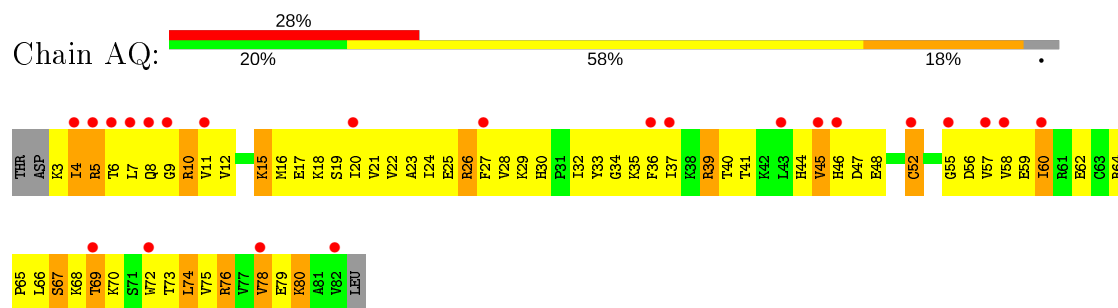
• Molecule 15: 30S ribosomal protein S16



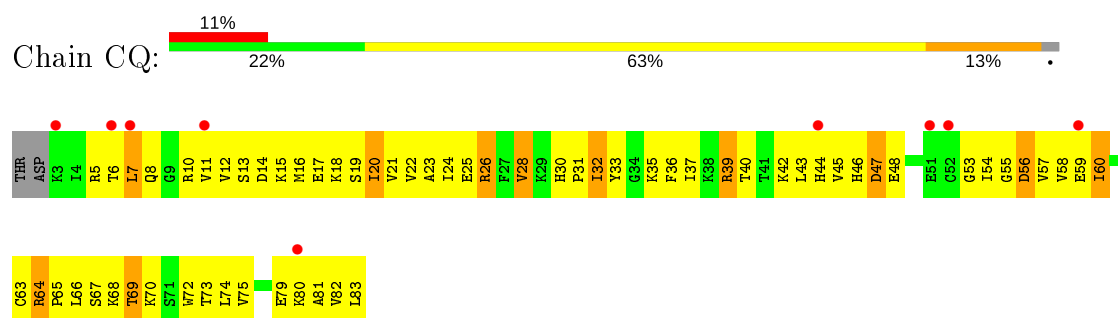
• Molecule 15: 30S ribosomal protein S16



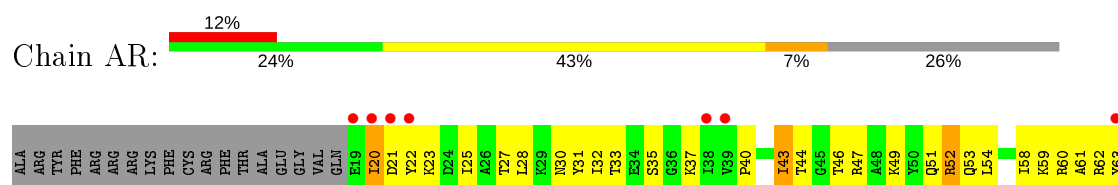
• Molecule 16: 30S ribosomal protein S17

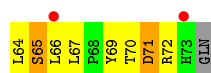


• Molecule 16: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S18

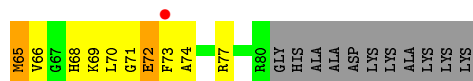
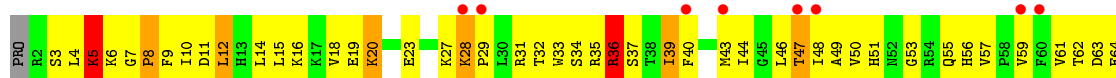




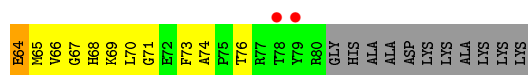
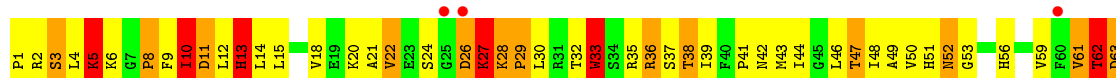
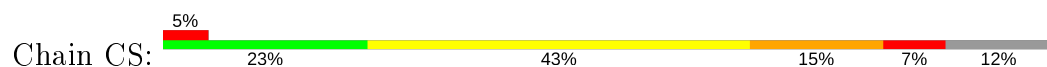
- Molecule 17: 30S ribosomal protein S18



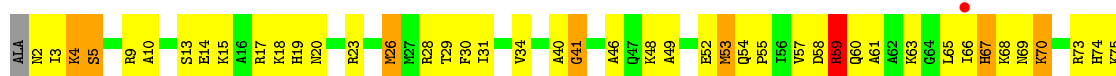
- Molecule 18: 30S ribosomal protein S19



- Molecule 18: 30S ribosomal protein S19

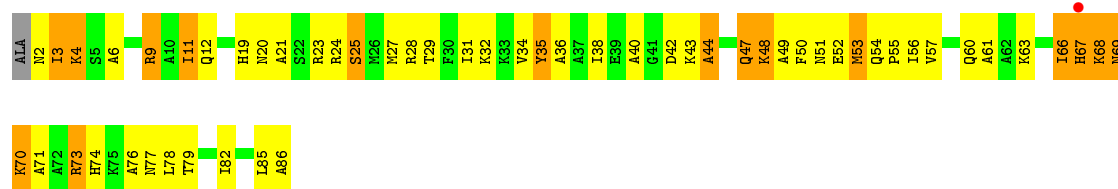


- Molecule 19: 30S ribosomal protein S20

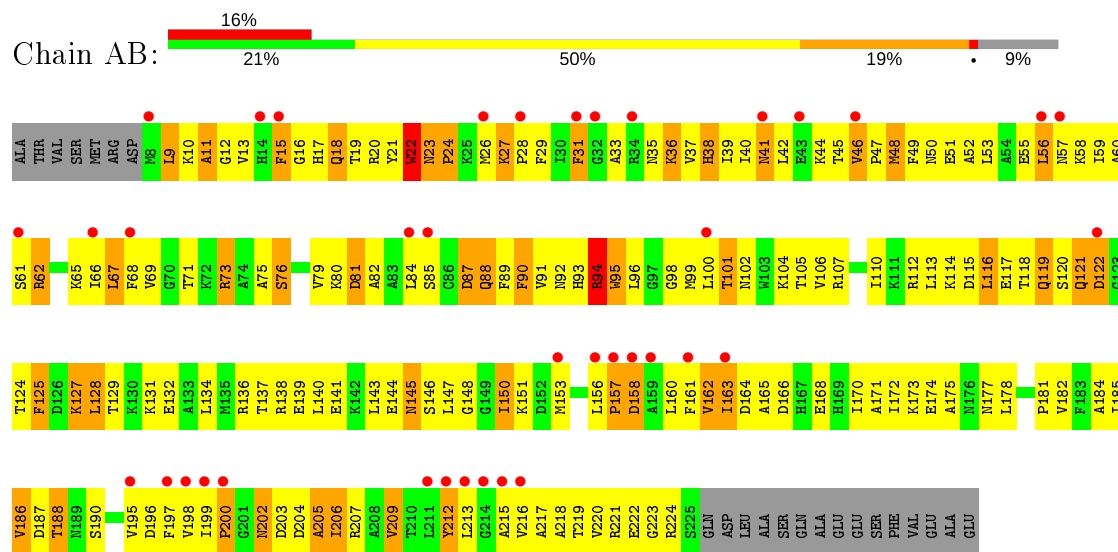


- Molecule 19: 30S ribosomal protein S20

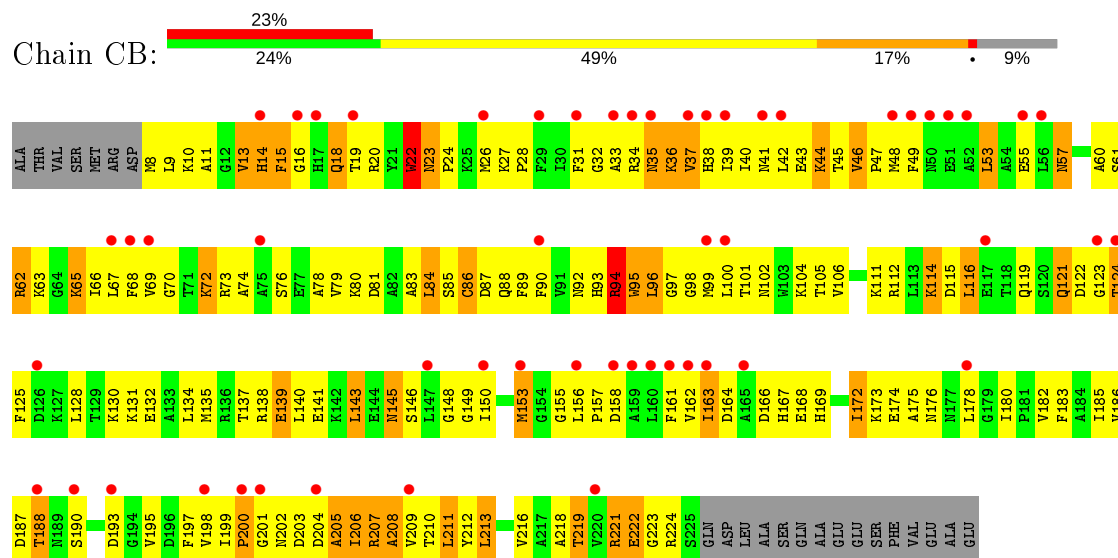




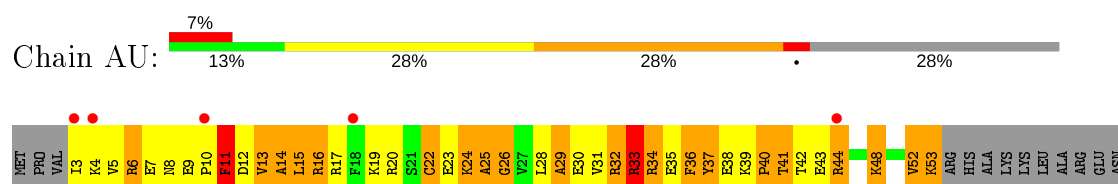
• Molecule 20: 30S ribosomal protein S2



• Molecule 20: 30S ribosomal protein S2



• Molecule 21: 30S ribosomal protein S21



ALA
ARG
ARG
THR
ARG
LEU
TYR

• Molecule 21: 30S ribosomal protein S21



MET PRO VAL I3 K4 V5 R6 E7 R8 P10 F11 D12 V13 A14 L15 R16 R17 F18 K19 R20 S21 C22 E23 K24 A25 L28 R32 R33 R34 E35 F36 Y37 E38 K39 P40 T41 T42 E43 R44 K45 R46 A47 K48 A49 S50 A51 V52 K53 ARG HIS ALA LYS LYS LEU ALA ARG GLU

ASN
ALA
ARG
THR
ARG
LEU
TYR

• Molecule 22: 5S ribosomal RNA



U G2 C3 C4 U5 G6 G7 G10 C11 C12 G13 G14 A15 G16 C17 G18 C19 G20 G21 G22 G23 G24 U25 C26 C27 C28 A29 A30 C31 U32 G33 A34 C35 A39 U40 G41 C42 C43 C44 A45 A46 G47 U48 C49 A50 A51 G51 A52 A53 G54 U55 A56 A57 A58 A59 C60 G61 C63

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• Molecule 22: 5S ribosomal RNA



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• Molecule 23: 23S ribosomal RNA



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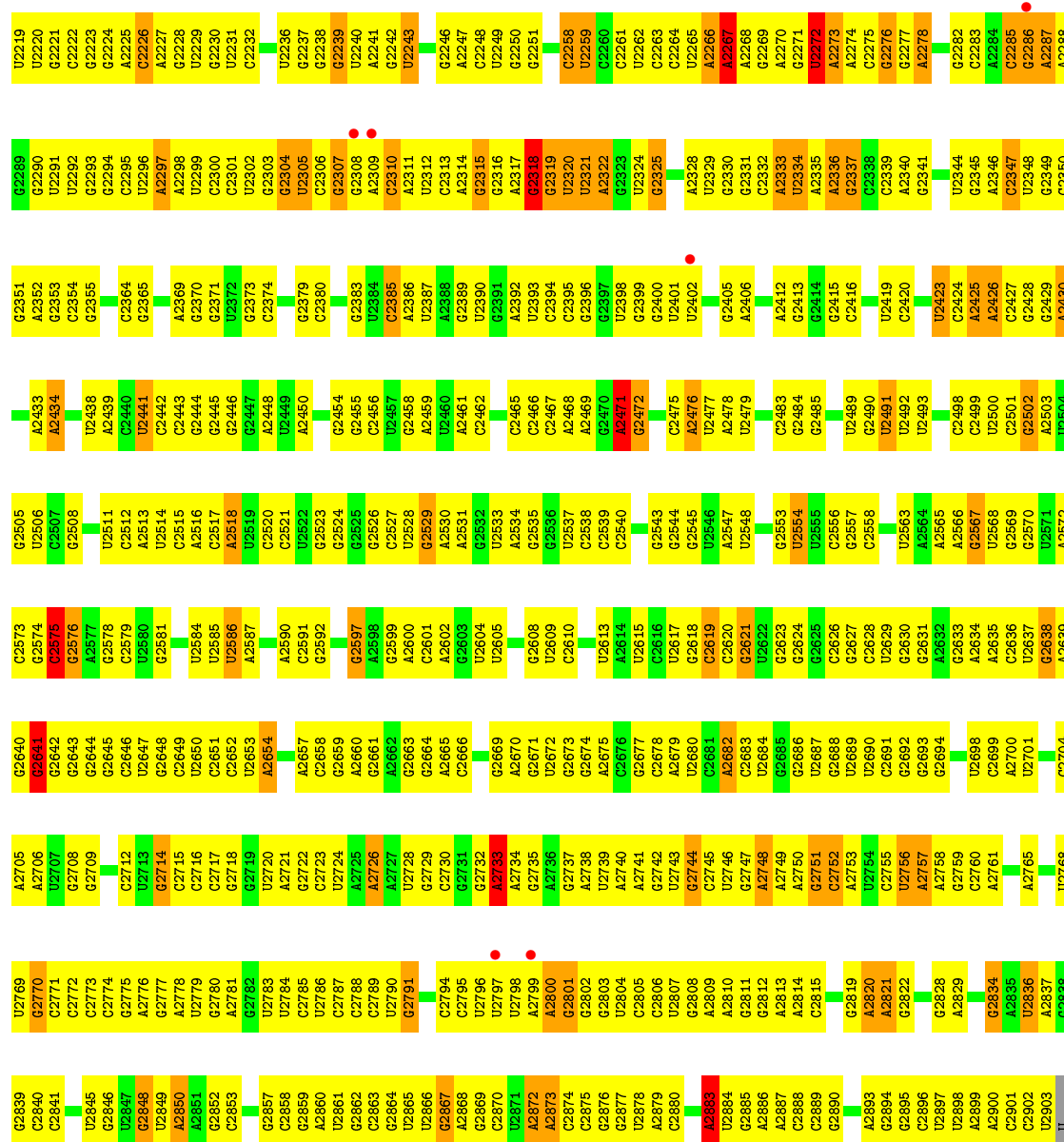
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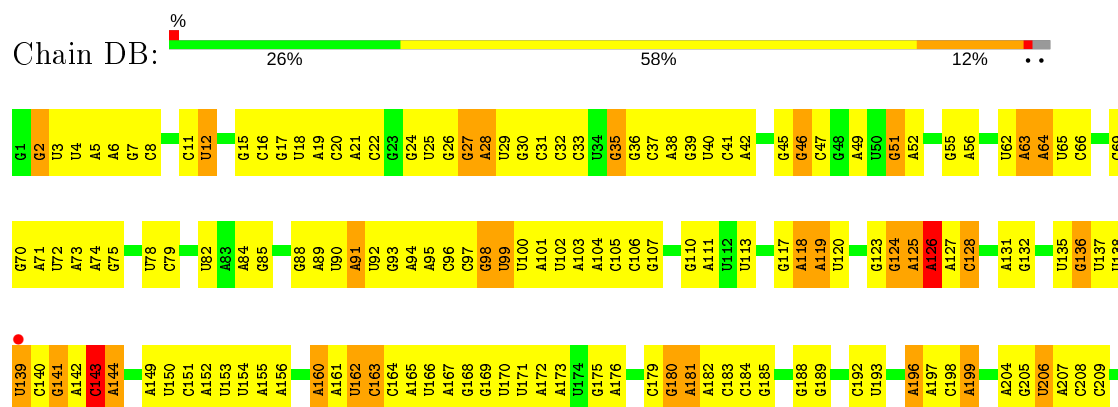
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G1216	A1020	A959	U831	U754	G673	A608	C540	A478	G406	A340	G273
G1217	A1021	A960	U832	U755	G674	U608	A541	A479	G407	C341	C274
G1218	G1022	C961	A833	G757	C679	C610	C542	A479	G408	A342	U275
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G1221	G1025	G964	U839	G760	G684	G613	U545	A482	G411	A278	A278
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	G1031	U971	A900		A690			A492	C353	U284	U284
	A1032	G971	A905		C691			G493	A354	G285	G285
	U1033	A972	U845		C692			G494	U355	U286	U286
	G1034	A973	U847		C693			G495	G356	G287	G287
	U1035	G974	C848		C694			G496	C357	U288	U288
		A975	A849		A699			A497	U358	G289	G289
	G1038	G976	U850		G700	A627		G498	C360	G295	G295
	A1039	U977	C851		G701			G499	U361	U296	U296
	A1040	G978	U852		U702			G500	A362	G297	G297
	G1041	A979	C853		U703			A428	G363	G298	G298
	G1042	U980	C854		G704			A429	C364	A299	A299
		A981	G855		A705			A502	U365	A300	A300
	A1046	C982	G856		A782			A503	G366	G301	G301
	G1047	A983	G857		G708			A504	C370	A302	A302
	A1048	U984	G858		U709			A505	G371	G303	G303
	C1049	C985	G859		U710			G506	U372	U304	U304
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	G1062	U998	G875		U653			A521	G389	U321	U321
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G1136	G1007	C1007	G		C660			A530	U395	U328	U328
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• Molecule 23: 23S ribosomal RNA

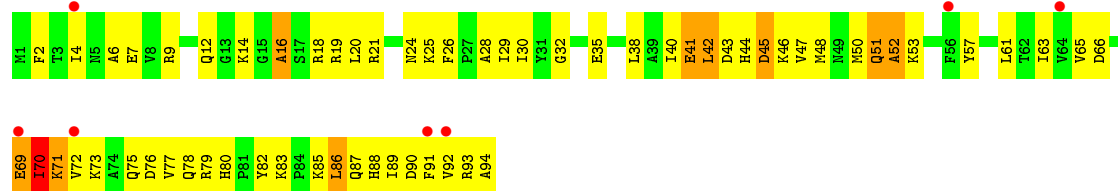


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G	U2075	U2007	C1934	U1865	U1796	U1729	U1663	G1587	G1524	G1455	A1387	C1319	C1265
U	U2076	C2008	G1935	A1867	G1797	C1730	G1666	U1588	U1525	U1456	G1388	C1320	U1268
A	A2077	C2009	A1936	G1867	U1798	G1731	G1667	U1589	A1526	U1457	U1394	A1321	G1269
G	C2078	A2010	U1937	C1868	G1799	C1732	G1667	U1590	G1527	U1458	A1395	A1322	A1260
U	C2079	U2011	A1938	G1869	C1800	G1733	A1668	A1591	G1527	G1459	A1396	C1323	C1261
A	A2080	G2012	U1939	A1870	A1801	G1734	A1669	A1592	A1528	U1460	U1396	G1324	A1262
G	U2081	U2013	U1940	A1871	A1802	G1735	C1670	C1592	G1529	C1461	U1387	U1325	U1263
C	A2082	U2016	U1941	A1872	A1803	U1736	U1671	A1593	G1530	C1462	C1388	U1326	A1264
G	U2083	U2017	U1942	G1873	C1804	U1737	A1672	U1594	C1531	C1463	U1389	A1327	A1265
U	C2145	C2018	U1943	C1874	A1805	G1738	A1673	C1595	A1532	G1464	U1400	A1328	G1266
A	C2146	A2019	G1945	U1875	G1806	A1739	G1674	U1599	C1533	G1465	U1401	U1329	U1267
G	A2147	A2020	U1946	A1876	G1807	G1740	C1675	U1599	U1534	U1462	U1402	C1330	A1268
U	C2148	C2021	C1947	A1877	A1810	U1742	A1676	C1600	A1535	A1469	A1403	A1269	A1270
G	U2149	U2022	G1948	C1878	G1811	G1743	A1677	G1601	C1536	A1470	C1404	G1332	C1271
A	C2150	C2023	U1949	U1879	A1812	A1744	G1681	U1602	U1538	U1471	U1405	G1333	A1272
U	U2151	G1950	U1950	C1880	G1813	A1745	U1682	C1603	G1539	U1474	G1407	G1334	U1273
C	C2152	C2025	U1951	U1881	A1814	A1746	U1683	C1606	G1540	U1475	G1408	A1336	A1274
A	C2153	G2026	A1952	U1882	A1815	U1747	G1684	C1607	C1541	U1476	U1409	G1337	U1275
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U	U2155	U2028	G1954	U1884	G1817	A1749	C1686	A1609	G1543	G1478	U1411	G1341	G1277
A	C2096	G2029	U1955	A1885	U1818	G1750	G1687	A1610	A1544	G1479	U1412	A1342	C1278
G	A2097	U2030	U1956	U1888	A1819	U1751	U1688	C1611	A1545	U1480	C1414	G1345	G1279
C	U2098	A2031	C1957	A1889	U1820	C1752	A1689	C1612	G1546	U1481	U1415	G1346	G1281
C	G2100	A2033	G1959	A1890	A1821	G1753	A1690	G1613	A1547	G1482	G1416	A1347	U1282
C	A2101	U2034	U1963	C1891	G1822	A1754	C1691	U1616	A1548	U1484	A1419	C1348	G1283
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C	G	A	A1981	A1912	G1842	C1774	U1709	C1639	U1563	C1499	A1434	G1364	C1297
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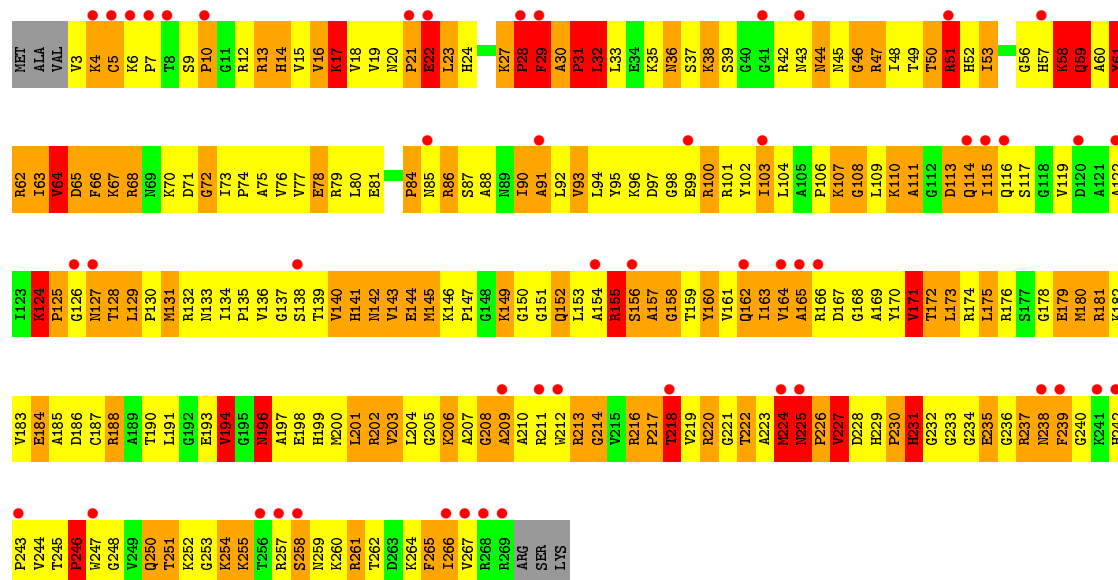


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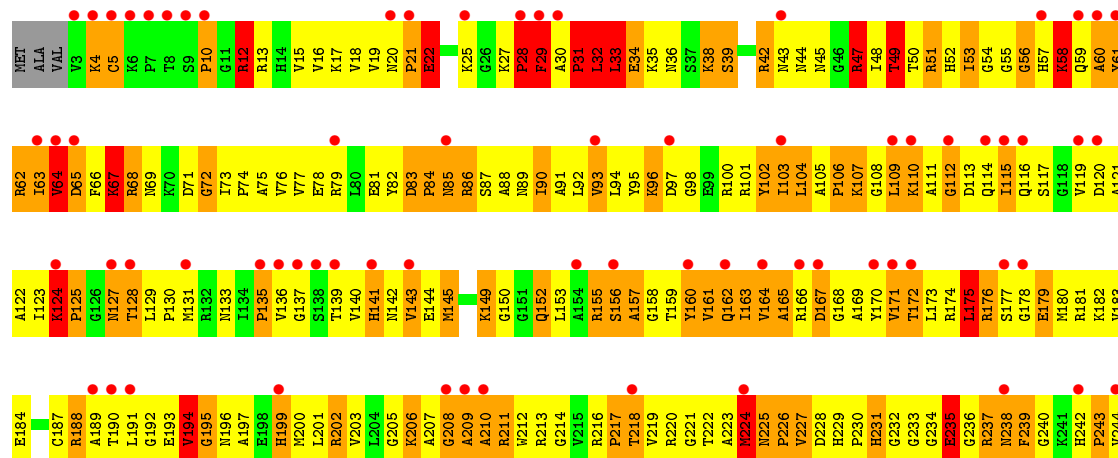
• Molecule 25: 50S ribosomal protein L2

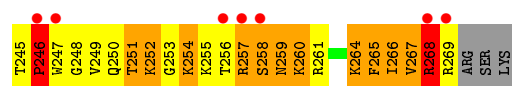
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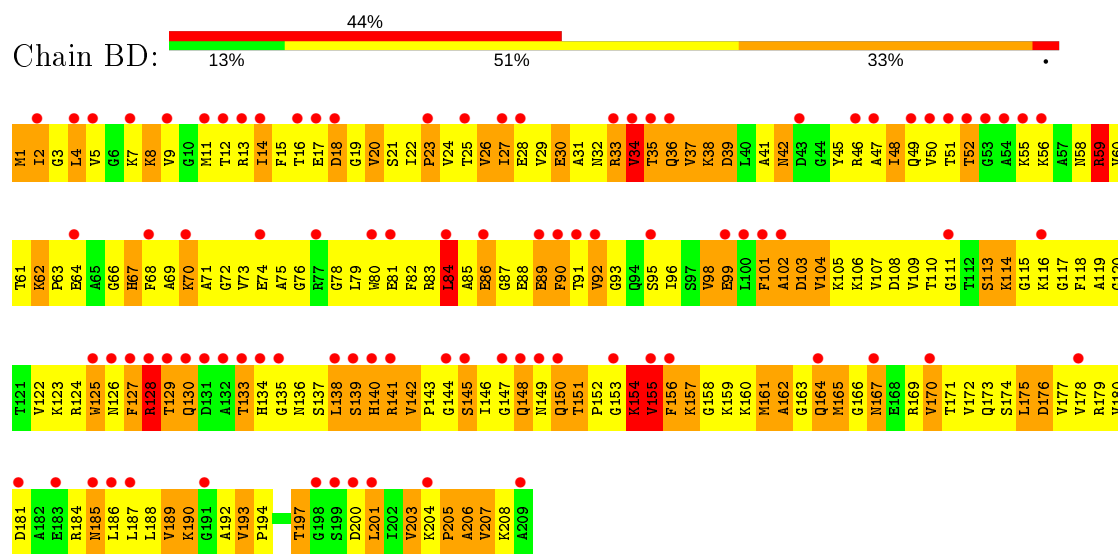
• Molecule 25: 50S ribosomal protein L2

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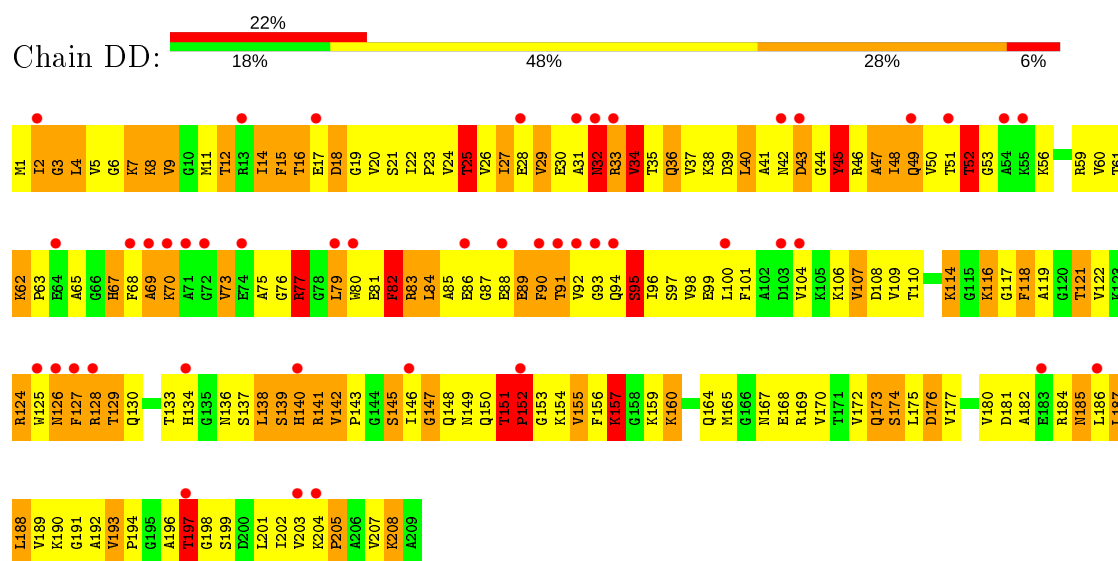




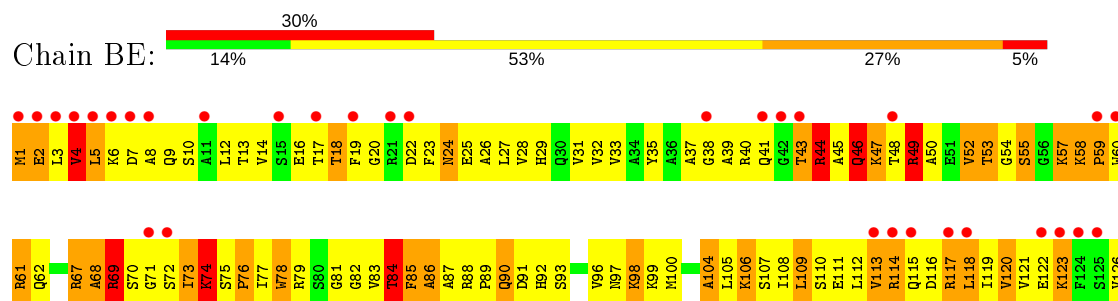
• Molecule 26: 50S ribosomal protein L3

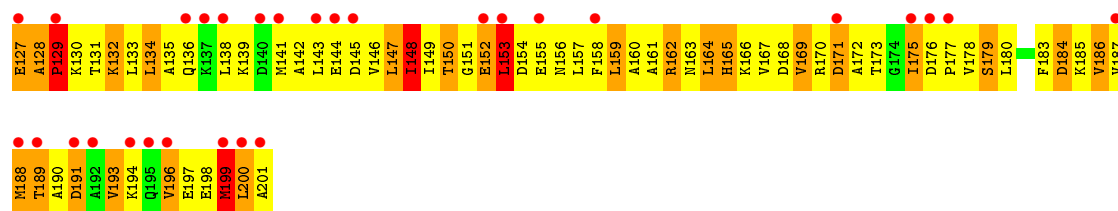


• Molecule 26: 50S ribosomal protein L3

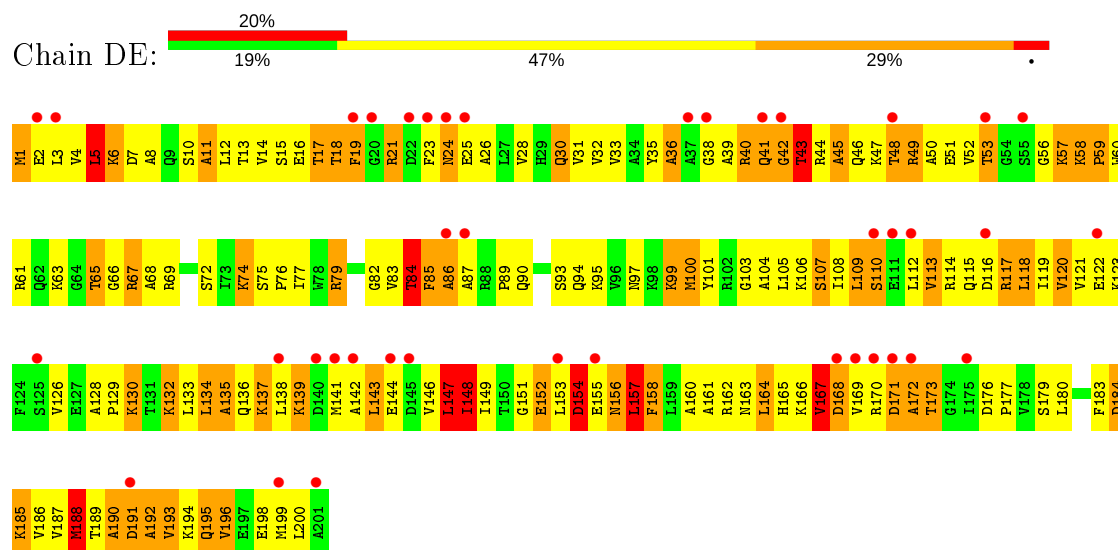


• Molecule 27: 50S ribosomal protein L4

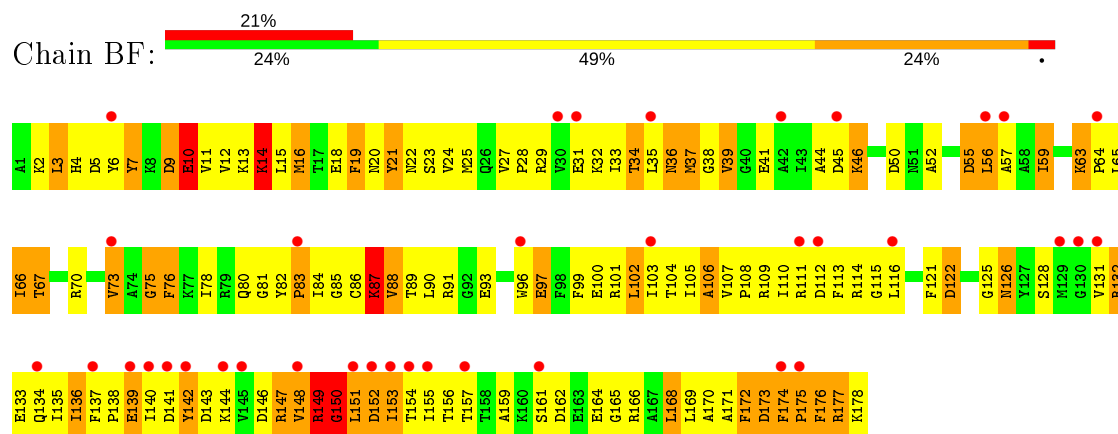




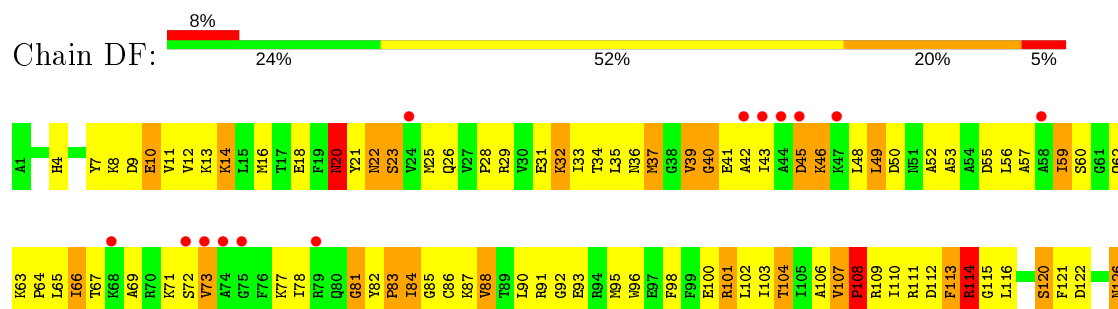
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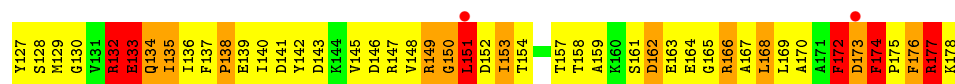


• Molecule 28: 50S ribosomal protein L5

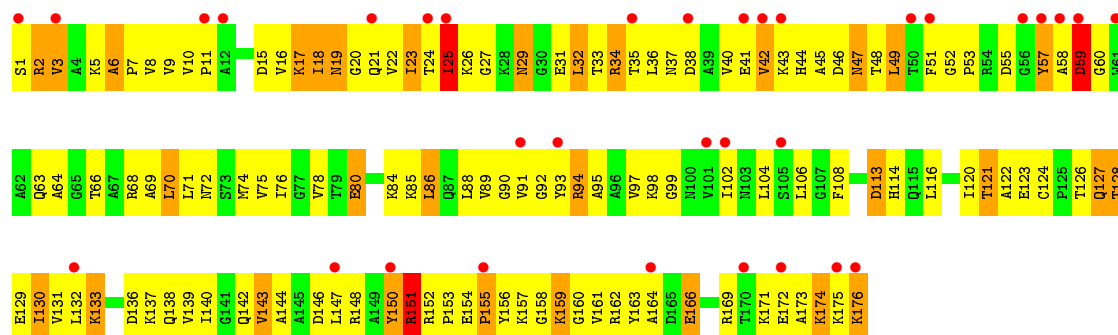


• Molecule 28: 50S ribosomal protein L5

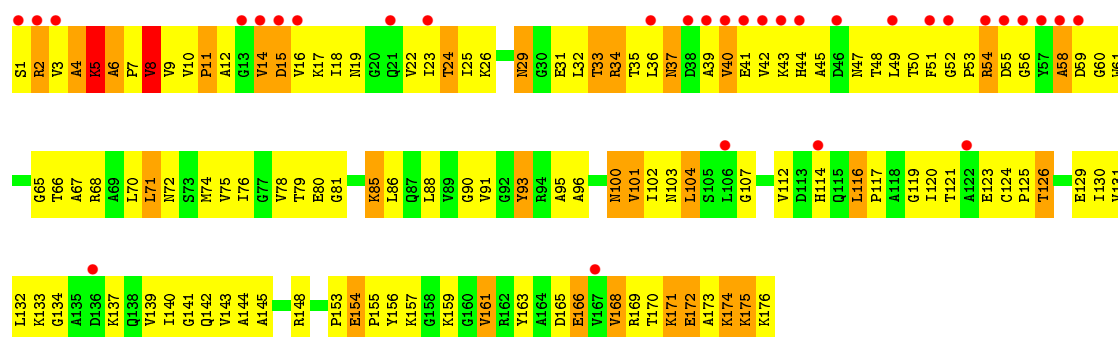




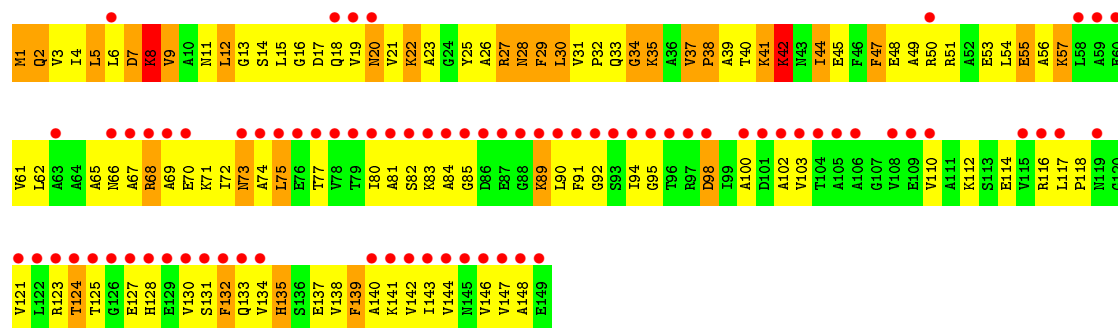
• Molecule 29: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L6

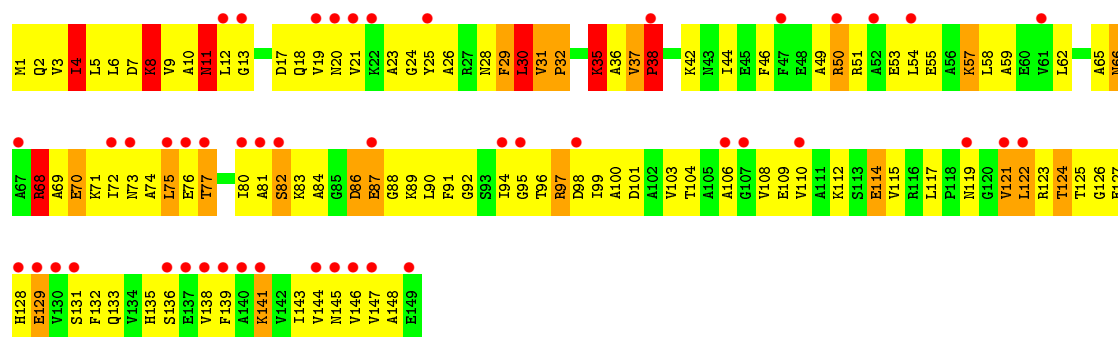


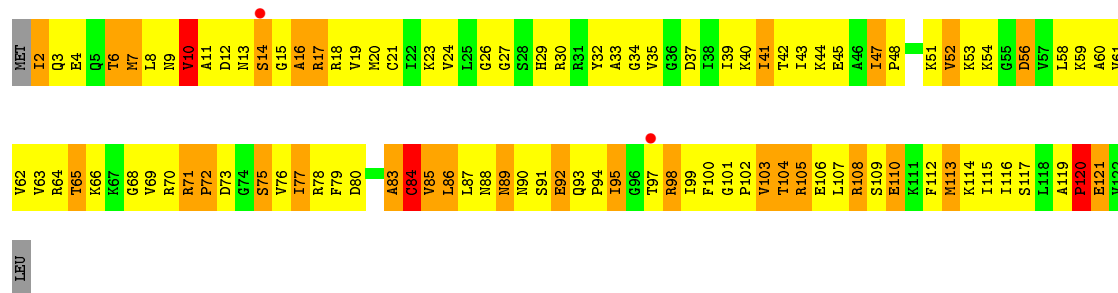
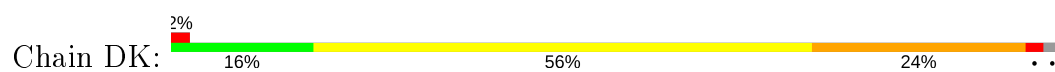
• Molecule 30: 50S ribosomal protein L9



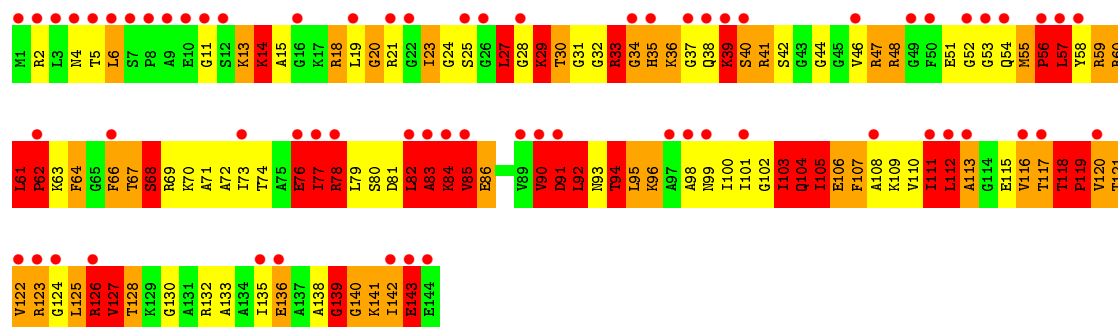
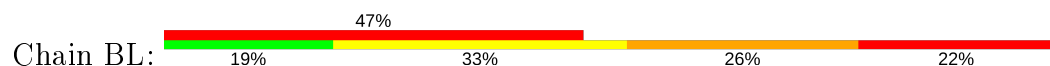
• Molecule 30: 50S ribosomal protein L9



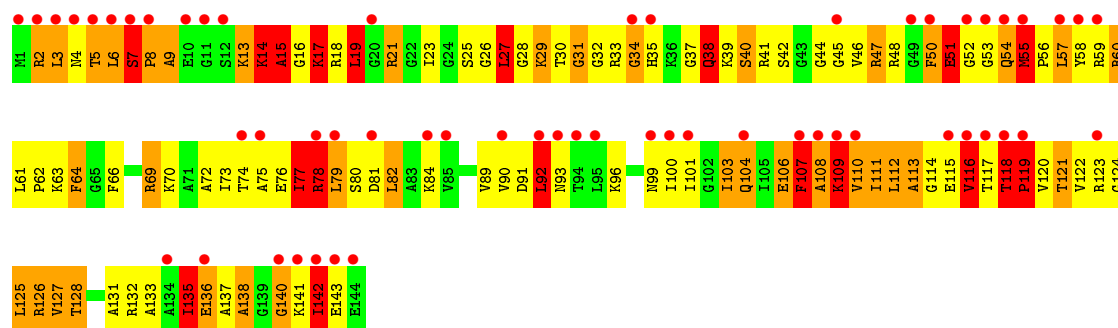
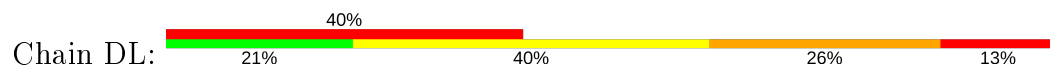




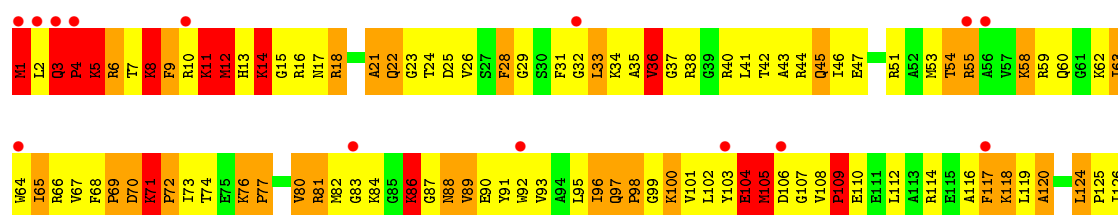
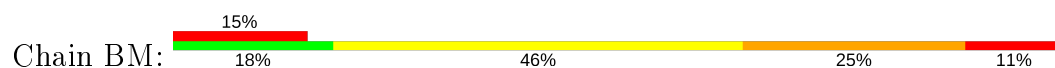
• Molecule 33: 50S ribosomal protein L15

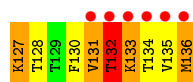


• Molecule 33: 50S ribosomal protein L15

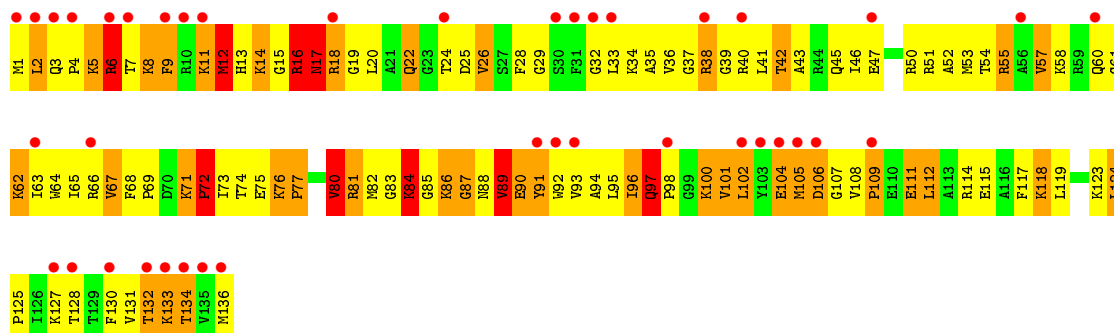
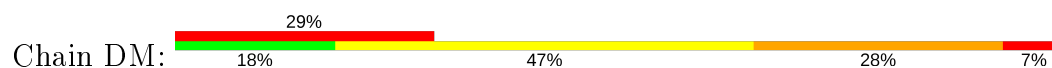


• Molecule 34: 50S ribosomal protein L16

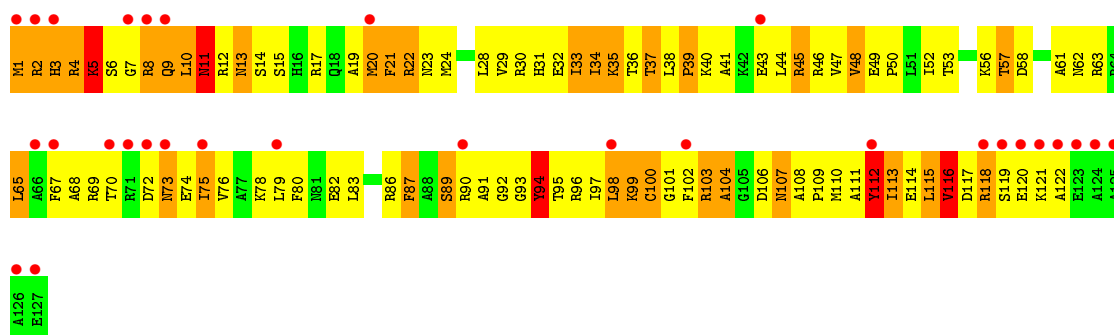




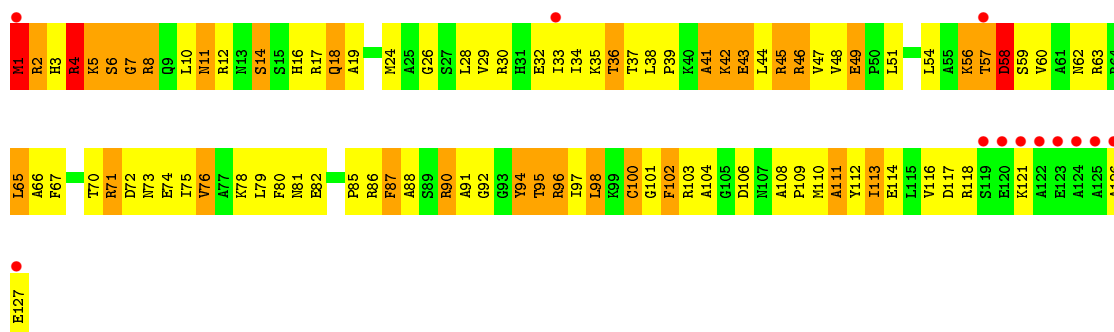
• Molecule 34: 50S ribosomal protein L16



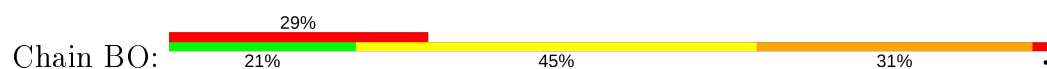
• Molecule 35: 50S ribosomal protein L17

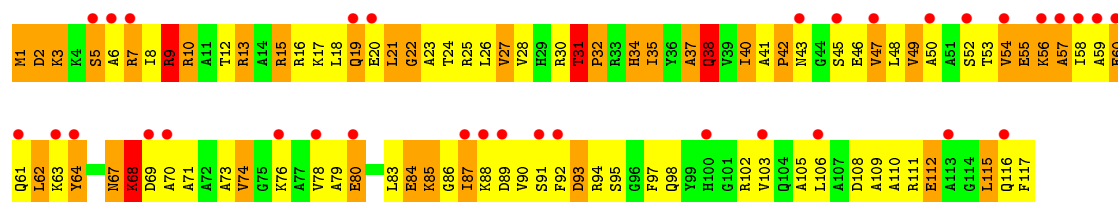


• Molecule 35: 50S ribosomal protein L17

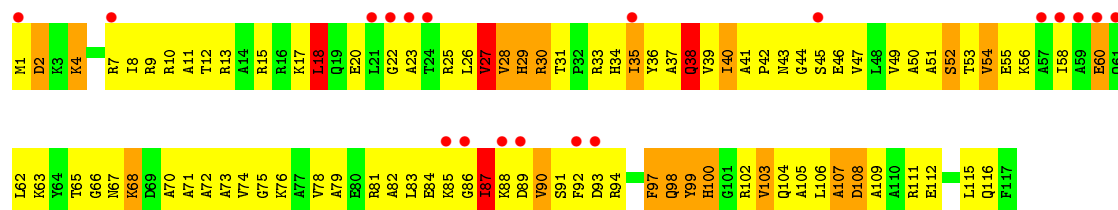


• Molecule 36: 50S ribosomal protein L18

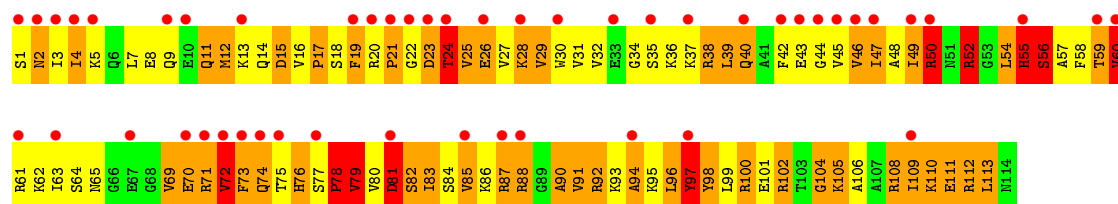
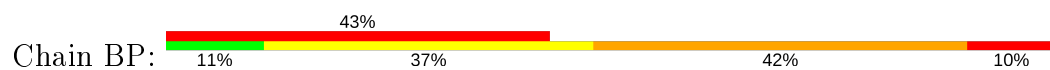




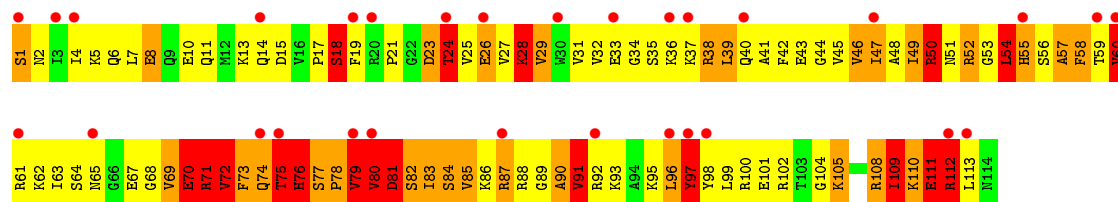
• Molecule 36: 50S ribosomal protein L18



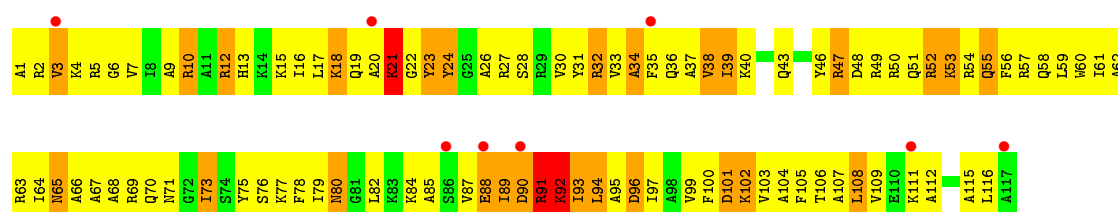
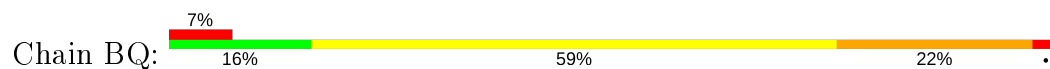
• Molecule 37: 50S ribosomal protein L19



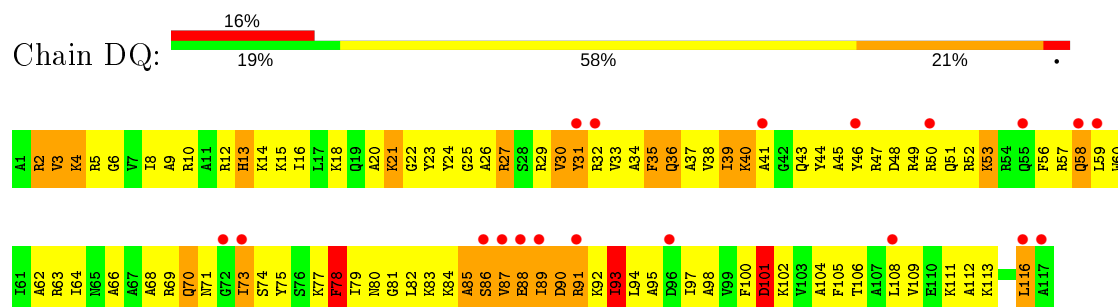
• Molecule 37: 50S ribosomal protein L19



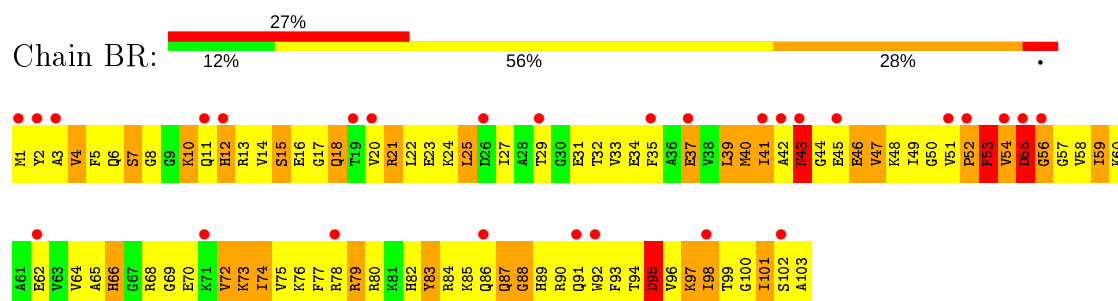
• Molecule 38: 50S ribosomal protein L20



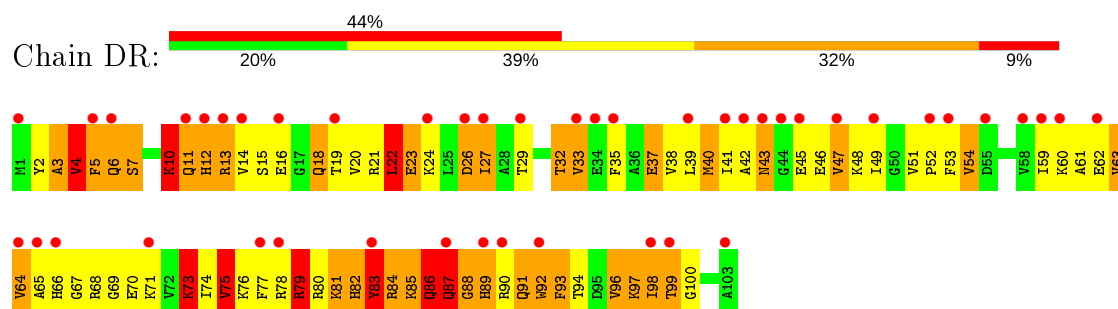
- Molecule 38: 50S ribosomal protein L20



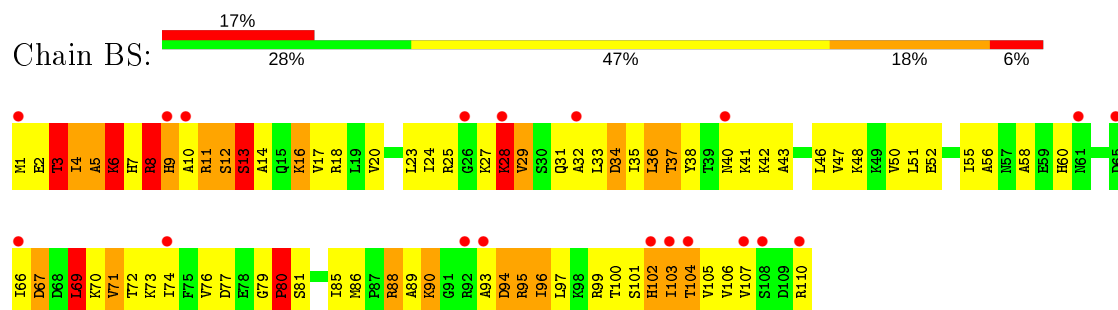
- Molecule 39: 50S ribosomal protein L21



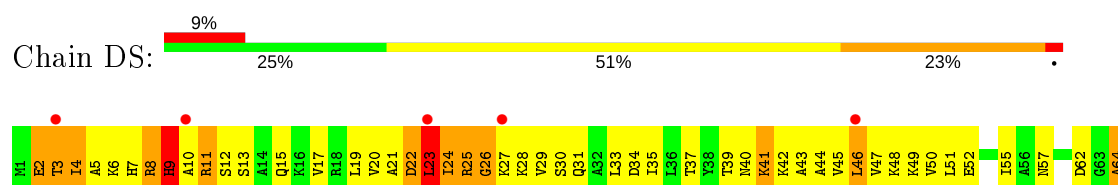
- Molecule 39: 50S ribosomal protein L21

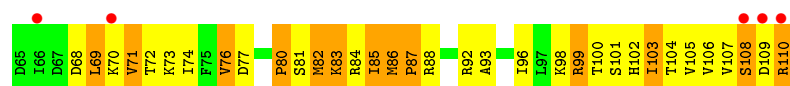


- Molecule 40: 50S ribosomal protein L22

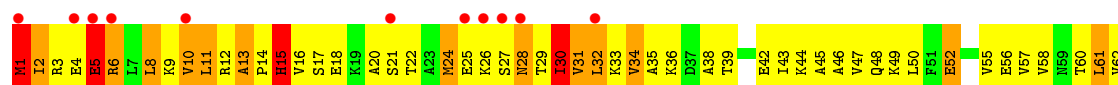
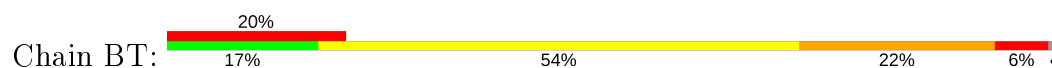


- Molecule 40: 50S ribosomal protein L22

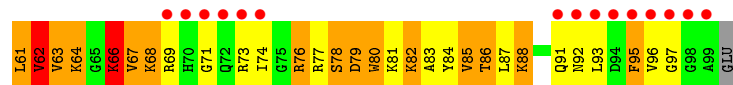
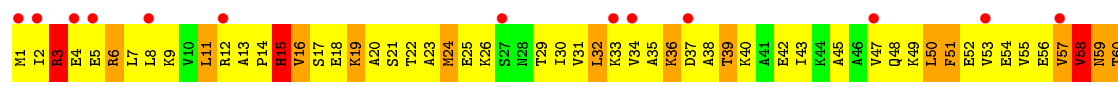
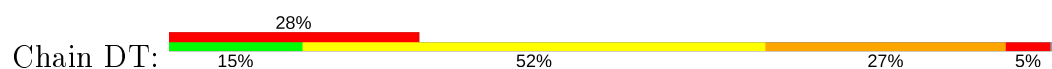




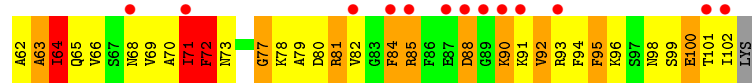
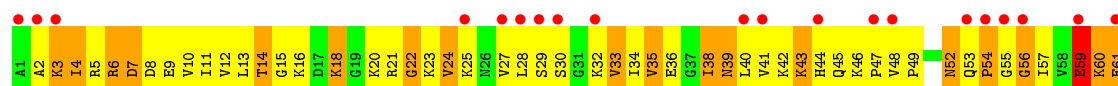
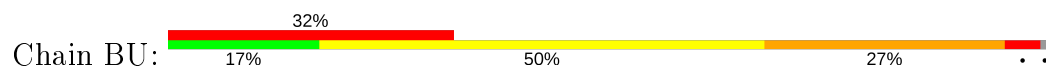
- Molecule 41: 50S ribosomal protein L23



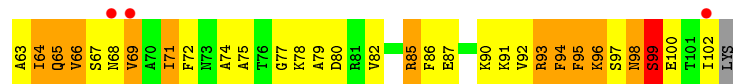
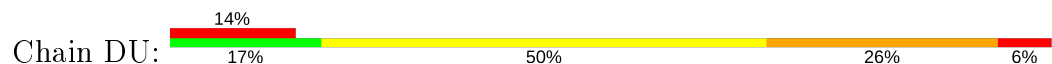
- Molecule 41: 50S ribosomal protein L23



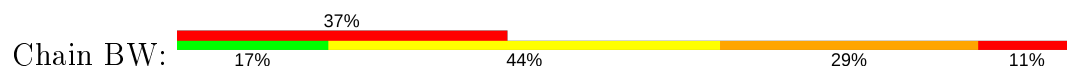
- Molecule 42: 50S ribosomal protein L24

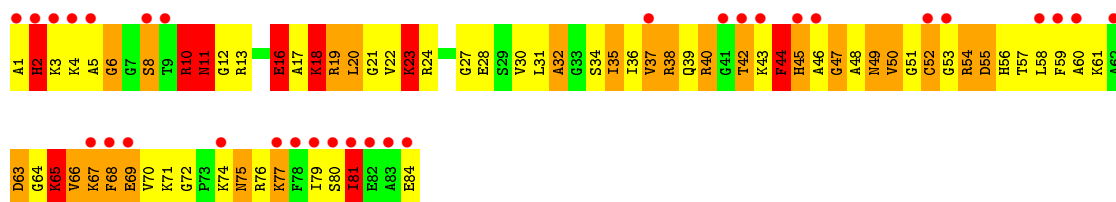


- Molecule 42: 50S ribosomal protein L24

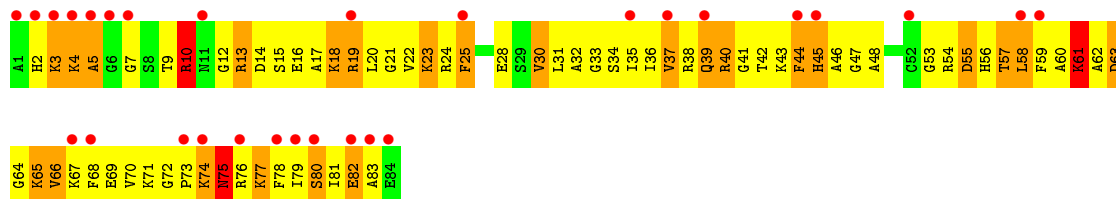
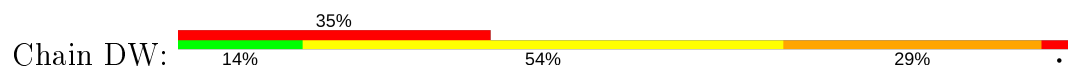


- Molecule 43: 50S ribosomal protein L27

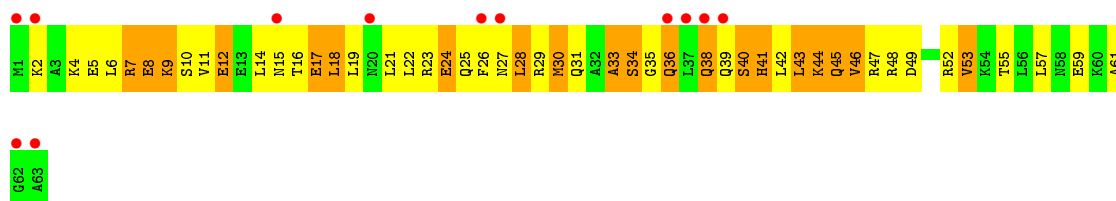




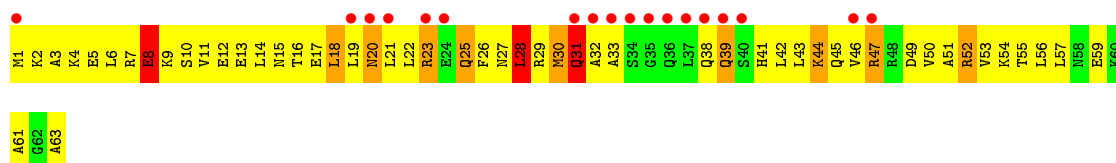
- Molecule 43: 50S ribosomal protein L27



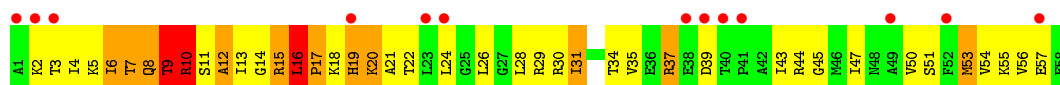
- Molecule 44: 50S ribosomal protein L29



- Molecule 44: 50S ribosomal protein L29

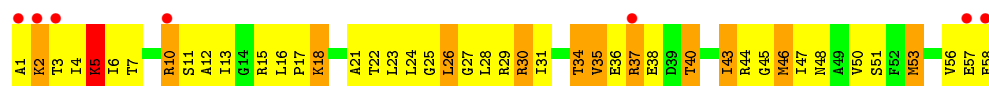


- Molecule 45: 50S ribosomal protein L30

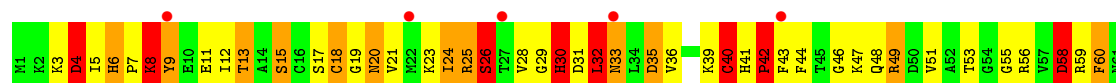
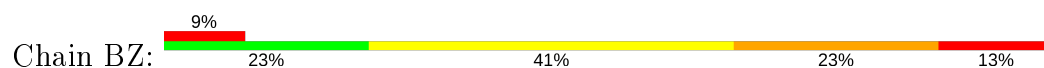


- Molecule 45: 50S ribosomal protein L30

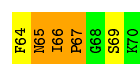




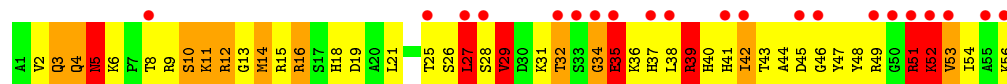
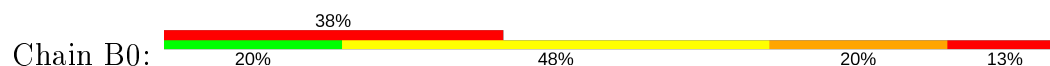
- Molecule 46: 50S ribosomal protein L31



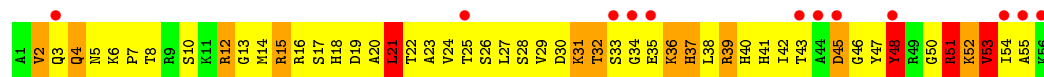
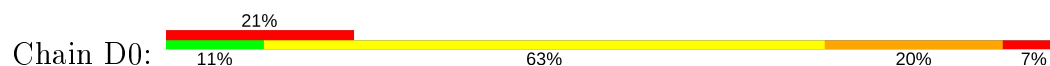
- Molecule 46: 50S ribosomal protein L31



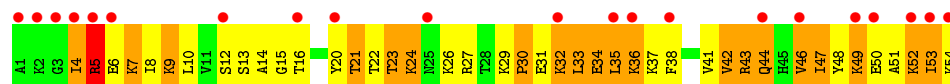
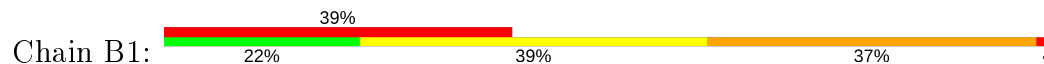
- Molecule 47: 50S ribosomal protein L32



- Molecule 47: 50S ribosomal protein L32

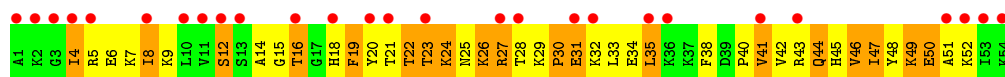


- Molecule 48: 50S ribosomal protein L33



- Molecule 48: 50S ribosomal protein L33

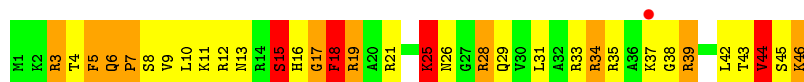




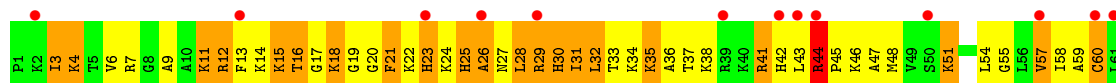
- Molecule 49: 50S ribosomal protein L34



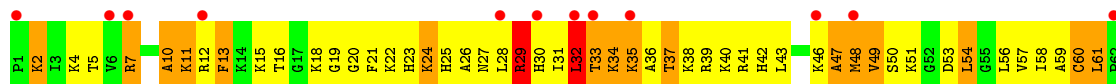
- Molecule 49: 50S ribosomal protein L34



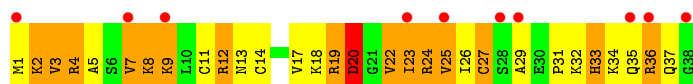
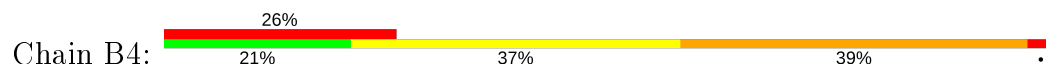
- Molecule 50: 50S ribosomal protein L35



- Molecule 50: 50S ribosomal protein L35

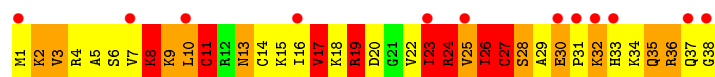


- Molecule 51: 50S ribosomal protein L36

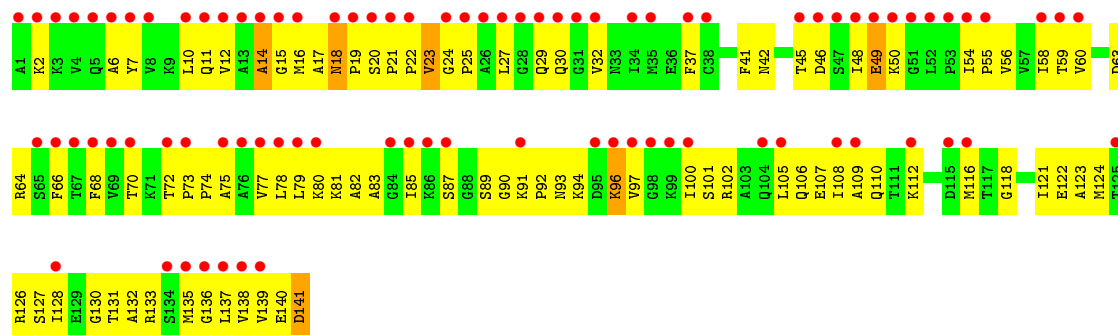


- Molecule 51: 50S ribosomal protein L36

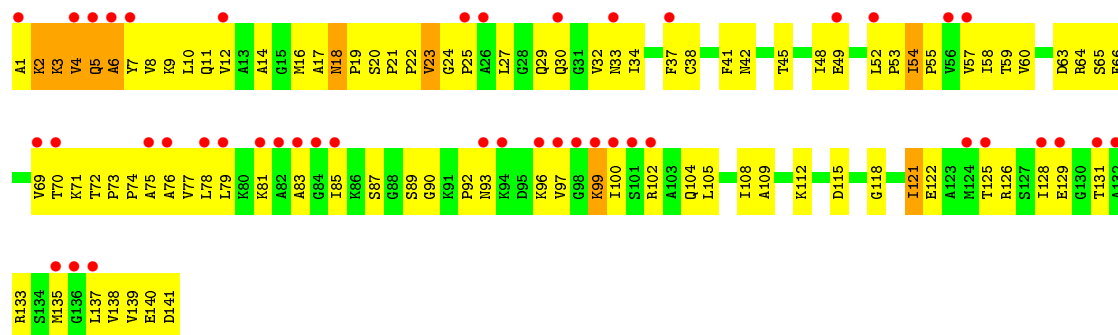
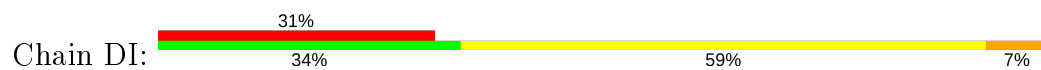




● Molecule 52: 50S ribosomal protein L11



● Molecule 52: 50S ribosomal protein L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 163.96 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 91.6 (163.96-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.331 0.260 , 0.306	Depositor DCC
R_{free} test set	35586 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	284107	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.26	1/36762 (0.0%)	0.75	7/57350 (0.0%)
1	CA	0.26	2/36762 (0.0%)	0.75	11/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.47	0/2225
3	AD	0.23	0/1665	0.46	0/2227
3	CD	0.23	0/1665	0.45	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.24	0/1118	0.45	0/1504
5	AF	0.25	0/835	0.47	0/1128
5	CF	0.24	0/835	0.49	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.46	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.23	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.47	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.48	0/1193
12	CM	0.21	0/884	0.46	0/1181
13	AN	0.24	0/785	0.46	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/724	0.45	0/966
14	CO	0.23	0/724	0.44	0/966
15	AP	0.26	0/659	0.44	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.46	0/881
16	CQ	0.24	0/665	0.47	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.47	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.24	0/671	0.42	0/888
20	AB	0.25	0/1735	0.47	0/2338
20	CB	0.25	0/1735	0.47	0/2338
21	AU	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
21	CU	0.98	3/430 (0.7%)	0.82	3/570 (0.5%)
22	BA	0.27	0/2803	0.74	0/4371
22	DA	0.28	0/2803	0.77	0/4371
23	BB	0.33	15/68314 (0.0%)	0.79	63/106569 (0.1%)
23	DB	0.34	18/68314 (0.0%)	0.79	75/106569 (0.1%)
24	BV	0.30	0/766	0.53	0/1025
24	DV	0.25	0/766	0.46	0/1025
25	BC	0.40	0/2092	0.88	7/2813 (0.2%)
25	DC	0.40	0/2092	0.90	8/2813 (0.3%)
26	BD	0.40	0/1586	0.80	2/2134 (0.1%)
26	DD	0.37	0/1586	0.82	4/2134 (0.2%)
27	BE	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
27	DE	0.70	4/1571 (0.3%)	0.83	5/2113 (0.2%)
28	BF	0.33	0/1444	0.87	5/1937 (0.3%)
28	DF	0.41	1/1444 (0.1%)	1.00	10/1937 (0.5%)
29	BG	0.31	0/1343	0.69	0/1816
29	DG	0.30	0/1343	0.67	1/1816 (0.1%)
30	BH	0.28	0/1122	0.60	0/1515
30	DH	0.34	0/1122	0.71	1/1515 (0.1%)
31	BJ	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
31	DJ	0.32	0/1135	0.76	3/1529 (0.2%)
32	BK	0.35	0/939	1.00	2/1258 (0.2%)
32	DK	0.35	0/939	0.99	4/1258 (0.3%)
33	BL	0.69	0/1062	1.60	31/1413 (2.2%)
33	DL	0.74	1/1062 (0.1%)	1.58	25/1413 (1.8%)
34	BM	0.48	0/1093	1.03	8/1460 (0.5%)
34	DM	0.39	0/1093	0.85	5/1460 (0.3%)
35	BN	0.37	0/1021	0.92	7/1364 (0.5%)
35	DN	0.37	0/1021	0.80	3/1364 (0.2%)
36	BO	0.30	0/910	0.67	0/1219
36	DO	0.31	0/910	0.64	0/1219
37	BP	0.55	0/929	1.40	16/1242 (1.3%)
37	DP	0.58	0/929	1.40	16/1242 (1.3%)
38	BQ	0.41	0/960	0.86	3/1278 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.36	0/960	0.75	0/1278
39	BR	1.06	6/829 (0.7%)	1.42	13/1107 (1.2%)
39	DR	0.38	0/829	0.82	3/1107 (0.3%)
40	BS	0.27	0/864	0.68	1/1156 (0.1%)
40	DS	0.26	0/864	0.60	0/1156
41	BT	0.39	0/784	0.78	4/1048 (0.4%)
41	DT	0.45	1/784 (0.1%)	0.80	1/1048 (0.1%)
42	BU	0.33	0/787	0.74	0/1051
42	DU	0.37	0/787	0.94	7/1051 (0.7%)
43	BW	0.36	0/642	0.96	5/848 (0.6%)
43	DW	0.39	0/642	0.80	2/848 (0.2%)
44	BX	0.29	0/510	0.80	1/677 (0.1%)
44	DX	0.29	0/510	0.66	0/677
45	BY	0.31	0/453	0.64	0/605
45	DY	0.31	0/453	0.69	1/605 (0.2%)
46	BZ	0.48	0/559	1.04	5/745 (0.7%)
46	DZ	0.52	0/559	0.91	1/745 (0.1%)
47	B0	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
47	D0	0.41	0/450	0.97	3/599 (0.5%)
48	B1	0.36	0/448	0.71	0/594
48	D1	0.32	0/448	0.69	0/594
49	B2	0.33	0/380	0.64	0/498
49	D2	0.30	0/380	0.60	0/498
50	B3	0.47	0/513	0.95	1/676 (0.1%)
50	D3	0.39	0/513	0.80	1/676 (0.1%)
51	B4	0.40	0/303	0.73	0/397
51	D4	0.32	0/303	0.77	0/397
52	BI	0.26	0/1046	0.58	0/1410
52	DI	0.60	4/1046 (0.4%)	0.76	4/1410 (0.3%)
All	All	0.33	63/306469 (0.0%)	0.77	396/458101 (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
1	CA	0	20
21	AU	0	1
22	DA	0	1
23	BB	0	60

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	1	65
25	BC	0	3
25	DC	0	2
31	BJ	0	2
33	BL	0	1
37	BP	0	1
37	DP	0	1
38	BQ	0	1
39	BR	0	1
39	DR	0	1
46	DZ	0	1
47	D0	0	1
All	All	1	178

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	DE	79	ARG	CD-NE	18.29	1.77	1.46
39	BR	53	PHE	CB-CG	17.86	1.81	1.51
23	DB	1086	A	C5-C6	-17.70	1.25	1.41
23	BB	1086	A	C5-C6	-17.70	1.25	1.41
21	CU	25	ALA	C-N	15.34	1.60	1.33

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-28.71	76.25	110.70
23	DB	2791	G	O5'-P-OP2	-27.77	77.38	110.70
23	DB	2791	G	O5'-P-OP1	18.50	132.90	110.70
23	BB	2791	G	O5'-P-OP2	18.20	132.54	110.70
23	DB	448	U	N1-C1'-C2'	17.52	136.78	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	DB	2076	U	C3'

5 of 178 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	58	C	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1157	0
1	CA	32831	0	16521	1198	0
2	AC	1624	0	1699	159	0
2	CC	1624	0	1699	148	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	167	0
4	AE	1105	0	1148	109	0
4	CE	1105	0	1148	143	0
5	AF	817	0	808	78	0
5	CF	817	0	808	93	0
6	AG	1174	0	1230	100	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	78	0
7	CH	979	0	1034	86	0
8	AI	1022	0	1070	144	0
8	CI	1022	0	1070	127	0
9	AJ	786	0	828	92	0
9	CJ	786	0	828	106	0
10	AK	877	0	887	111	0
10	CK	877	0	887	108	0
11	AL	955	0	1019	103	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	88	0
12	CM	876	0	937	95	0
13	AN	774	0	827	93	0
13	CN	774	0	827	114	0
14	AO	716	0	742	53	0
14	CO	716	0	742	50	0
15	AP	649	0	666	77	0
15	CP	638	0	656	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AQ	648	0	691	80	0
16	CQ	656	0	702	85	0
17	AR	455	0	478	39	0
17	CR	455	0	478	41	0
18	AS	637	0	665	75	0
18	CS	644	0	675	87	0
19	AT	665	0	714	52	0
19	CT	665	0	714	64	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	152	0
21	AU	425	0	447	104	0
21	CU	425	0	449	84	0
22	BA	2507	0	1270	87	0
22	DA	2507	0	1270	97	0
23	BB	60995	0	30678	2393	0
23	DB	60995	0	30677	2365	0
24	BV	753	0	780	107	0
24	DV	753	0	780	69	0
25	BC	2053	0	2122	436	0
25	DC	2053	0	2122	433	0
26	BD	1565	0	1616	372	0
26	DD	1565	0	1616	316	0
27	BE	1552	0	1619	261	0
27	DE	1552	0	1619	266	0
28	BF	1420	0	1460	169	0
28	DF	1420	0	1460	181	0
29	BG	1323	0	1374	175	0
29	DG	1323	0	1374	162	0
30	BH	1111	0	1148	160	0
30	DH	1111	0	1148	145	0
31	BJ	1112	0	1147	219	0
31	DJ	1112	0	1147	231	0
32	BK	930	0	1000	121	0
32	DK	930	0	1000	126	0
33	BL	1053	0	1129	284	0
33	DL	1053	0	1129	227	0
34	BM	1074	0	1157	237	0
34	DM	1074	0	1157	189	0
35	BN	1008	0	1045	157	0
35	DN	1008	0	1045	133	0
36	BO	900	0	935	128	0
36	DO	900	0	935	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	BP	917	0	965	206	0
37	DP	917	0	965	209	0
38	BQ	947	0	1022	178	0
38	DQ	947	0	1022	161	0
39	BR	816	0	838	165	0
39	DR	816	0	839	180	0
40	BS	857	0	922	122	0
40	DS	857	0	922	111	0
41	BT	777	0	840	139	0
41	DT	777	0	840	129	0
42	BU	779	0	834	152	0
42	DU	779	0	834	134	0
43	BW	634	0	656	155	0
43	DW	634	0	656	156	0
44	BX	509	0	543	73	0
44	DX	509	0	543	90	0
45	BY	449	0	491	57	0
45	DY	449	0	491	64	0
46	BZ	549	0	552	114	0
46	DZ	549	0	552	101	0
47	B0	444	0	461	75	0
47	D0	444	0	461	80	0
48	B1	441	0	485	63	0
48	D1	441	0	485	69	0
49	B2	377	0	418	55	0
49	D2	377	0	418	66	0
50	B3	504	0	574	111	0
50	D3	504	0	574	113	0
51	B4	302	0	343	44	0
51	D4	302	0	343	80	0
52	BI	1032	0	1088	129	0
52	DI	1032	0	1088	214	0
53	AA	59	0	0	0	0
53	AP	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	62	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	290	0	0	0	0
54	AE	3	0	0	0	0
54	AK	2	0	0	0	0
54	AN	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AP	1	0	0	0	0
54	BB	497	0	0	12	0
54	BC	1	0	0	0	0
54	BE	5	0	0	0	0
54	BH	1	0	0	0	0
54	BL	2	0	0	0	0
54	BN	1	0	0	0	0
54	CA	295	0	0	1	0
54	CE	3	0	0	0	0
54	CK	1	0	0	0	0
54	CL	4	0	0	0	0
54	CN	2	0	0	0	0
54	CP	1	0	0	0	0
54	CT	2	0	0	0	0
54	D2	2	0	0	0	0
54	DB	499	0	0	7	0
54	DC	1	0	0	0	0
54	DD	1	0	0	0	0
54	DE	3	0	0	0	0
54	DJ	2	0	0	1	0
54	DL	1	0	0	0	0
54	DN	2	0	0	0	0
54	DQ	1	0	0	0	0
All	All	284107	0	190766	18478	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 18478 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)
52:DI:3:LYS:CE	52:DI:3:LYS:CD	1.74	1.64
39:BR:53:PHE:CG	39:BR:53:PHE:CB	1.81	1.61
39:BR:54:VAL:CA	39:BR:54:VAL:CB	1.78	1.57
27:DE:79:ARG:CG	27:DE:79:ARG:CD	1.78	1.57
52:DI:3:LYS:CG	52:DI:3:LYS:CD	1.81	1.56

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/232 (88%)	135 (66%)	49 (24%)	20 (10%)	0	6
2	CC	204/232 (88%)	139 (68%)	45 (22%)	20 (10%)	0	6
3	AD	203/205 (99%)	131 (64%)	54 (27%)	18 (9%)	1	7
3	CD	203/205 (99%)	137 (68%)	49 (24%)	17 (8%)	1	8
4	AE	148/166 (89%)	107 (72%)	34 (23%)	7 (5%)	2	19
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	1	13
5	AF	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	1	13
5	CF	98/135 (73%)	65 (66%)	23 (24%)	10 (10%)	0	6
6	AG	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	2	16
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	1	8
7	AH	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	6	34
7	CH	127/129 (98%)	90 (71%)	31 (24%)	6 (5%)	2	19
8	AI	125/129 (97%)	87 (70%)	27 (22%)	11 (9%)	1	7
8	CI	125/129 (97%)	82 (66%)	33 (26%)	10 (8%)	1	9
9	AJ	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	0	4
9	CJ	96/103 (93%)	58 (60%)	21 (22%)	17 (18%)	0	1
10	AK	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	0	5
10	CK	115/128 (90%)	78 (68%)	27 (24%)	10 (9%)	1	8
11	AL	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	3
11	CL	121/123 (98%)	75 (62%)	28 (23%)	18 (15%)	0	2
12	AM	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	0	6
12	CM	111/117 (95%)	79 (71%)	17 (15%)	15 (14%)	0	3
13	AN	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	0	6
13	CN	92/100 (92%)	53 (58%)	24 (26%)	15 (16%)	0	2
14	AO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	26
15	AP	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	2	18
15	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	7
16	AQ	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	2	17
16	CQ	79/83 (95%)	61 (77%)	13 (16%)	5 (6%)	1	13
17	AR	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	3
17	CR	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	1	15
18	AS	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	9
18	CS	78/91 (86%)	48 (62%)	17 (22%)	13 (17%)	0	2
19	AT	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	1	10
19	CT	83/86 (96%)	61 (74%)	16 (19%)	6 (7%)	1	10
20	AB	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	8
20	CB	216/240 (90%)	150 (69%)	36 (17%)	30 (14%)	0	3
21	AU	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
21	CU	49/71 (69%)	28 (57%)	15 (31%)	6 (12%)	0	4
24	BV	92/94 (98%)	62 (67%)	21 (23%)	9 (10%)	0	6
24	DV	92/94 (98%)	59 (64%)	27 (29%)	6 (6%)	1	12
25	BC	265/273 (97%)	103 (39%)	83 (31%)	79 (30%)	0	0
25	DC	265/273 (97%)	97 (37%)	93 (35%)	75 (28%)	0	0
26	BD	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	1
26	DD	207/209 (99%)	96 (46%)	67 (32%)	44 (21%)	0	1
27	BE	199/201 (99%)	98 (49%)	60 (30%)	41 (21%)	0	1
27	DE	199/201 (99%)	87 (44%)	63 (32%)	49 (25%)	0	0
28	BF	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	1
28	DF	176/178 (99%)	91 (52%)	53 (30%)	32 (18%)	0	1
29	BG	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	0	6
29	DG	174/176 (99%)	117 (67%)	39 (22%)	18 (10%)	0	6
30	BH	147/149 (99%)	87 (59%)	45 (31%)	15 (10%)	0	6
30	DH	147/149 (99%)	84 (57%)	44 (30%)	19 (13%)	0	3
31	BJ	138/142 (97%)	67 (49%)	42 (30%)	29 (21%)	0	1
31	DJ	138/142 (97%)	70 (51%)	36 (26%)	32 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	119/123 (97%)	71 (60%)	32 (27%)	16 (13%)	0	3
32	DK	119/123 (97%)	72 (60%)	25 (21%)	22 (18%)	0	1
33	BL	142/144 (99%)	60 (42%)	40 (28%)	42 (30%)	0	0
33	DL	142/144 (99%)	66 (46%)	37 (26%)	39 (28%)	0	0
34	BM	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	1
34	DM	134/136 (98%)	79 (59%)	31 (23%)	24 (18%)	0	1
35	BN	125/127 (98%)	73 (58%)	35 (28%)	17 (14%)	0	3
35	DN	125/127 (98%)	82 (66%)	32 (26%)	11 (9%)	1	7
36	BO	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	1
36	DO	115/117 (98%)	63 (55%)	33 (29%)	19 (16%)	0	2
37	BP	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
37	DP	112/114 (98%)	42 (38%)	38 (34%)	32 (29%)	0	0
38	BQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	6
38	DQ	115/117 (98%)	79 (69%)	22 (19%)	14 (12%)	0	4
39	BR	101/103 (98%)	44 (44%)	31 (31%)	26 (26%)	0	0
39	DR	101/103 (98%)	42 (42%)	31 (31%)	28 (28%)	0	0
40	BS	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	2
40	DS	108/110 (98%)	67 (62%)	20 (18%)	21 (19%)	0	1
41	BT	97/100 (97%)	42 (43%)	40 (41%)	15 (16%)	0	2
41	DT	97/100 (97%)	42 (43%)	32 (33%)	23 (24%)	0	1
42	BU	100/103 (97%)	33 (33%)	46 (46%)	21 (21%)	0	1
42	DU	100/103 (97%)	46 (46%)	41 (41%)	13 (13%)	0	3
43	BW	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
43	DW	82/84 (98%)	31 (38%)	30 (37%)	21 (26%)	0	0
44	BX	61/63 (97%)	28 (46%)	21 (34%)	12 (20%)	0	1
44	DX	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	3
45	BY	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	1
45	DY	56/58 (97%)	35 (62%)	17 (30%)	4 (7%)	1	11
46	BZ	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	1
46	DZ	68/70 (97%)	37 (54%)	22 (32%)	9 (13%)	0	3
47	B0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	D0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	2
48	B1	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	1
48	D1	52/54 (96%)	21 (40%)	22 (42%)	9 (17%)	0	2
49	B2	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	2
49	D2	44/46 (96%)	24 (54%)	12 (27%)	8 (18%)	0	1
50	B3	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	0	5
50	D3	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	2
51	B4	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	0
51	D4	36/38 (95%)	13 (36%)	11 (31%)	12 (33%)	0	0
52	BI	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	4	30
52	DI	139/141 (99%)	123 (88%)	11 (8%)	5 (4%)	3	25
All	All	11263/11902 (95%)	6645 (59%)	2936 (26%)	1682 (15%)	0	2

5 of 1682 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	2	GLN
2	AC	91	ALA
2	AC	153	SER
3	AD	18	LEU
3	AD	31	CYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	142 (84%)	28 (16%)	2	12
2	CC	170/189 (90%)	146 (86%)	24 (14%)	3	17
3	AD	172/172 (100%)	140 (81%)	32 (19%)	1	7
3	CD	172/172 (100%)	137 (80%)	35 (20%)	1	5
4	AE	113/125 (90%)	92 (81%)	21 (19%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CE	113/125 (90%)	92 (81%)	21 (19%)	1	7
5	AF	87/116 (75%)	68 (78%)	19 (22%)	1	4
5	CF	87/116 (75%)	74 (85%)	13 (15%)	3	16
6	AG	123/146 (84%)	102 (83%)	21 (17%)	2	10
6	CG	125/146 (86%)	106 (85%)	19 (15%)	3	15
7	AH	104/104 (100%)	87 (84%)	17 (16%)	2	12
7	CH	104/104 (100%)	85 (82%)	19 (18%)	1	7
8	AI	105/106 (99%)	83 (79%)	22 (21%)	1	4
8	CI	105/106 (99%)	89 (85%)	16 (15%)	3	15
9	AJ	86/90 (96%)	66 (77%)	20 (23%)	1	3
9	CJ	86/90 (96%)	78 (91%)	8 (9%)	9	34
10	AK	90/98 (92%)	70 (78%)	20 (22%)	1	4
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	8
11	AL	103/103 (100%)	88 (85%)	15 (15%)	3	16
11	CL	103/103 (100%)	79 (77%)	24 (23%)	1	3
12	AM	92/95 (97%)	70 (76%)	22 (24%)	0	3
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2	9
13	AN	79/83 (95%)	67 (85%)	12 (15%)	3	15
13	CN	79/83 (95%)	68 (86%)	11 (14%)	3	18
14	AO	76/77 (99%)	69 (91%)	7 (9%)	9	34
14	CO	76/77 (99%)	63 (83%)	13 (17%)	2	10
15	AP	65/65 (100%)	56 (86%)	9 (14%)	3	18
15	CP	65/65 (100%)	54 (83%)	11 (17%)	2	11
16	AQ	74/77 (96%)	60 (81%)	14 (19%)	1	6
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	5	23
17	AR	48/64 (75%)	45 (94%)	3 (6%)	18	50
17	CR	48/64 (75%)	41 (85%)	7 (15%)	3	16
18	AS	70/78 (90%)	60 (86%)	10 (14%)	3	17
18	CS	71/78 (91%)	53 (75%)	18 (25%)	0	2
19	AT	65/65 (100%)	56 (86%)	9 (14%)	3	18
19	CT	65/65 (100%)	51 (78%)	14 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AB	180/198 (91%)	142 (79%)	38 (21%)	1	4
20	CB	180/198 (91%)	153 (85%)	27 (15%)	3	15
21	AU	44/61 (72%)	36 (82%)	8 (18%)	1	8
21	CU	44/61 (72%)	30 (68%)	14 (32%)	0	2
24	BV	78/78 (100%)	66 (85%)	12 (15%)	2	14
24	DV	78/78 (100%)	69 (88%)	9 (12%)	5	24
25	BC	213/218 (98%)	145 (68%)	68 (32%)	0	2
25	DC	213/218 (98%)	150 (70%)	63 (30%)	0	2
26	BD	164/164 (100%)	112 (68%)	52 (32%)	0	2
26	DD	164/164 (100%)	113 (69%)	51 (31%)	0	2
27	BE	165/165 (100%)	115 (70%)	50 (30%)	0	2
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	3
28	BF	149/149 (100%)	119 (80%)	30 (20%)	1	5
28	DF	149/149 (100%)	122 (82%)	27 (18%)	1	8
29	BG	137/137 (100%)	105 (77%)	32 (23%)	1	3
29	DG	137/137 (100%)	111 (81%)	26 (19%)	1	7
30	BH	114/114 (100%)	85 (75%)	29 (25%)	0	2
30	DH	114/114 (100%)	90 (79%)	24 (21%)	1	4
31	BJ	114/116 (98%)	84 (74%)	30 (26%)	0	2
31	DJ	114/116 (98%)	85 (75%)	29 (25%)	0	2
32	BK	102/104 (98%)	78 (76%)	24 (24%)	1	3
32	DK	102/104 (98%)	81 (79%)	21 (21%)	1	5
33	BL	103/103 (100%)	62 (60%)	41 (40%)	0	1
33	DL	103/103 (100%)	68 (66%)	35 (34%)	0	1
34	BM	109/109 (100%)	77 (71%)	32 (29%)	0	2
34	DM	109/109 (100%)	75 (69%)	34 (31%)	0	2
35	BN	103/103 (100%)	78 (76%)	25 (24%)	0	3
35	DN	103/103 (100%)	76 (74%)	27 (26%)	0	2
36	BO	87/87 (100%)	58 (67%)	29 (33%)	0	1
36	DO	87/87 (100%)	69 (79%)	18 (21%)	1	5
37	BP	99/99 (100%)	77 (78%)	22 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DP	99/99 (100%)	67 (68%)	32 (32%)	0	1
38	BQ	89/89 (100%)	66 (74%)	23 (26%)	0	2
38	DQ	89/89 (100%)	71 (80%)	18 (20%)	1	5
39	BR	84/84 (100%)	68 (81%)	16 (19%)	1	7
39	DR	84/84 (100%)	58 (69%)	26 (31%)	0	2
40	BS	93/93 (100%)	72 (77%)	21 (23%)	1	3
40	DS	93/93 (100%)	77 (83%)	16 (17%)	2	10
41	BT	83/84 (99%)	60 (72%)	23 (28%)	0	2
41	DT	83/84 (99%)	60 (72%)	23 (28%)	0	2
42	BU	83/84 (99%)	62 (75%)	21 (25%)	0	3
42	DU	83/84 (99%)	60 (72%)	23 (28%)	0	2
43	BW	62/62 (100%)	46 (74%)	16 (26%)	0	2
43	DW	62/62 (100%)	45 (73%)	17 (27%)	0	2
44	BX	55/55 (100%)	40 (73%)	15 (27%)	0	2
44	DX	55/55 (100%)	43 (78%)	12 (22%)	1	4
45	BY	48/48 (100%)	36 (75%)	12 (25%)	0	3
45	DY	48/48 (100%)	33 (69%)	15 (31%)	0	2
46	BZ	62/62 (100%)	43 (69%)	19 (31%)	0	2
46	DZ	62/62 (100%)	46 (74%)	16 (26%)	0	2
47	B0	47/47 (100%)	31 (66%)	16 (34%)	0	1
47	D0	47/47 (100%)	33 (70%)	14 (30%)	0	2
48	B1	48/48 (100%)	33 (69%)	15 (31%)	0	2
48	D1	48/48 (100%)	33 (69%)	15 (31%)	0	2
49	B2	38/38 (100%)	27 (71%)	11 (29%)	0	2
49	D2	38/38 (100%)	27 (71%)	11 (29%)	0	2
50	B3	51/51 (100%)	33 (65%)	18 (35%)	0	1
50	D3	51/51 (100%)	40 (78%)	11 (22%)	1	4
51	B4	34/34 (100%)	21 (62%)	13 (38%)	0	1
51	D4	34/34 (100%)	17 (50%)	17 (50%)	0	0
52	BI	109/109 (100%)	106 (97%)	3 (3%)	43	72
52	DI	109/109 (100%)	104 (95%)	5 (5%)	27	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9341/9692 (96%)	7268 (78%)	2073 (22%)	1 4

5 of 2073 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BW	54	ARG
6	CG	10	LYS
41	DT	82	LYS
45	BY	19	HIS
51	B4	9	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
40	BS	9	HIS
3	CD	53	GLN
39	DR	6	GLN
42	BU	65	GLN
46	BZ	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	277 (18%)	25 (1%)
1	CA	1529/1542 (99%)	249 (16%)	26 (1%)
22	BA	116/120 (96%)	23 (19%)	0
22	DA	116/120 (96%)	20 (17%)	1 (0%)
23	BB	2837/2904 (97%)	451 (15%)	18 (0%)
23	DB	2837/2904 (97%)	482 (16%)	22 (0%)
All	All	8964/9132 (98%)	1502 (16%)	92 (1%)

5 of 1502 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	429	U
23	DB	2198	A
23	BB	2756	U
1	CA	279	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 343 ligands modelled in this entry, 343 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	AU	2
21	CU	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CU	25:ALA	C	26:GLY	N	1.60
1	AU	25:ALA	C	26:GLY	N	1.16
1	AU	15:LEU	C	16:ARG	N	0.99

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%)	-0.28	11 (0%) 87 85	16, 66, 135, 180	0
1	CA	1530/1542 (99%)	-0.36	7 (0%) 91 89	11, 49, 119, 180	0
2	AC	206/232 (88%)	0.32	6 (2%) 51 49	8, 56, 116, 163	0
2	CC	206/232 (88%)	0.20	7 (3%) 45 43	13, 68, 122, 154	0
3	AD	205/205 (100%)	0.76	24 (11%) 4 6	16, 65, 125, 180	0
3	CD	205/205 (100%)	0.77	12 (5%) 22 23	5, 49, 103, 156	0
4	AE	150/166 (90%)	0.48	5 (3%) 46 44	5, 56, 104, 151	0
4	CE	150/166 (90%)	0.60	9 (6%) 21 22	5, 49, 101, 167	0
5	AF	100/135 (74%)	1.22	19 (19%) 1 1	19, 64, 113, 150	0
5	CF	100/135 (74%)	1.15	16 (16%) 1 3	10, 65, 113, 147	0
6	AG	150/178 (84%)	0.26	9 (6%) 21 22	23, 86, 133, 180	0
6	CG	152/178 (85%)	-0.07	4 (2%) 56 53	22, 83, 132, 166	0
7	AH	129/129 (100%)	0.81	17 (13%) 3 5	8, 63, 113, 155	0
7	CH	129/129 (100%)	0.73	15 (11%) 4 6	5, 49, 104, 154	0
8	AI	127/129 (98%)	0.25	10 (7%) 12 15	5, 83, 126, 169	0
8	CI	127/129 (98%)	-0.19	1 (0%) 86 82	23, 81, 135, 161	0
9	AJ	98/103 (95%)	0.36	5 (5%) 28 27	14, 76, 141, 160	0
9	CJ	98/103 (95%)	0.09	2 (2%) 65 63	27, 78, 122, 143	0
10	AK	117/128 (91%)	0.69	6 (5%) 28 27	6, 56, 99, 164	0
10	CK	117/128 (91%)	0.37	7 (5%) 21 22	5, 44, 95, 117	0
11	AL	123/123 (100%)	0.75	12 (9%) 7 9	18, 59, 115, 162	0
11	CL	123/123 (100%)	0.51	6 (4%) 29 29	5, 34, 109, 141	0
12	AM	114/117 (97%)	0.37	7 (6%) 21 22	37, 96, 137, 155	0
12	CM	113/117 (96%)	0.08	3 (2%) 54 52	19, 92, 143, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.11	5 (5%) 27 27	11, 76, 133, 147	0
13	CN	96/100 (96%)	0.06	5 (5%) 27 27	32, 73, 130, 160	0
14	AO	88/89 (98%)	0.69	8 (9%) 9 11	15, 62, 104, 177	0
14	CO	88/89 (98%)	0.79	7 (7%) 12 14	5, 46, 113, 136	0
15	AP	82/82 (100%)	0.54	8 (9%) 7 9	20, 72, 132, 171	0
15	CP	80/82 (97%)	0.34	4 (5%) 28 28	5, 42, 126, 137	0
16	AQ	80/83 (96%)	1.28	23 (28%) 0 0	34, 77, 119, 158	0
16	CQ	81/83 (97%)	0.85	9 (11%) 5 7	11, 52, 113, 155	0
17	AR	55/74 (74%)	0.88	9 (16%) 1 2	16, 60, 124, 148	0
17	CR	55/74 (74%)	0.75	7 (12%) 3 5	17, 45, 118, 139	0
18	AS	79/91 (86%)	0.53	9 (11%) 5 7	44, 110, 140, 169	0
18	CS	80/91 (87%)	0.38	5 (6%) 20 20	47, 99, 151, 161	0
19	AT	85/86 (98%)	0.08	1 (1%) 79 75	37, 83, 123, 155	0
19	CT	85/86 (98%)	0.18	1 (1%) 79 75	9, 49, 103, 139	0
20	AB	218/240 (90%)	0.93	38 (17%) 1 2	17, 82, 131, 156	0
20	CB	218/240 (90%)	1.27	54 (24%) 0 0	13, 90, 135, 162	0
21	AU	51/71 (71%)	0.66	5 (9%) 7 9	29, 80, 131, 158	0
21	CU	51/71 (71%)	0.62	4 (7%) 13 15	34, 73, 112, 140	0
22	BA	117/120 (97%)	-0.24	2 (1%) 70 67	36, 62, 94, 157	0
22	DA	117/120 (97%)	-0.22	2 (1%) 70 67	27, 62, 113, 180	0
23	BB	2841/2904 (97%)	-0.09	29 (1%) 82 79	10, 49, 134, 180	0
23	DB	2841/2904 (97%)	-0.17	24 (0%) 86 82	5, 39, 133, 180	0
24	BV	94/94 (100%)	0.74	13 (13%) 2 4	20, 75, 130, 149	0
24	DV	94/94 (100%)	0.83	7 (7%) 14 17	17, 71, 119, 130	0
25	BC	267/273 (97%)	1.22	51 (19%) 1 1	5, 51, 136, 180	0
25	DC	267/273 (97%)	1.58	77 (28%) 0 0	5, 46, 139, 180	0
26	BD	209/209 (100%)	2.25	91 (43%) 0 0	21, 82, 174, 180	0
26	DD	209/209 (100%)	1.21	45 (21%) 0 1	5, 60, 139, 180	0
27	BE	201/201 (100%)	1.58	61 (30%) 0 0	8, 78, 147, 180	0
27	DE	201/201 (100%)	1.30	40 (19%) 1 1	5, 76, 164, 180	0
28	BF	178/178 (100%)	1.18	37 (20%) 1 1	43, 98, 152, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
28	DF	178/178 (100%)	0.39	15 (8%) 11 13	29, 89, 138, 180	0
29	BG	176/176 (100%)	1.19	33 (18%) 1 2	23, 94, 154, 180	0
29	DG	176/176 (100%)	1.02	32 (18%) 1 2	20, 86, 154, 172	0
30	BH	149/149 (100%)	2.78	78 (52%) 0 0	23, 120, 170, 180	0
30	DH	149/149 (100%)	1.57	47 (31%) 0 0	31, 100, 153, 180	0
31	BJ	140/142 (98%)	1.03	24 (17%) 1 2	14, 79, 160, 180	0
31	DJ	140/142 (98%)	0.93	22 (15%) 2 3	14, 61, 136, 162	0
32	BK	121/123 (98%)	1.44	30 (24%) 0 0	13, 57, 106, 147	0
32	DK	121/123 (98%)	0.52	2 (1%) 70 67	5, 37, 84, 143	0
33	BL	144/144 (100%)	2.79	67 (46%) 0 0	19, 93, 160, 180	0
33	DL	144/144 (100%)	2.02	57 (39%) 0 0	7, 74, 150, 179	0
34	BM	136/136 (100%)	0.83	20 (14%) 2 3	16, 71, 168, 180	0
34	DM	136/136 (100%)	1.64	40 (29%) 0 0	10, 66, 152, 180	0
35	BN	127/127 (100%)	1.64	30 (23%) 0 0	19, 67, 149, 180	0
35	DN	127/127 (100%)	0.88	12 (9%) 8 10	5, 45, 143, 180	0
36	BO	117/117 (100%)	2.03	34 (29%) 0 0	20, 82, 150, 180	0
36	DO	117/117 (100%)	1.22	19 (16%) 1 2	20, 77, 150, 169	0
37	BP	114/114 (100%)	1.85	49 (42%) 0 0	21, 84, 177, 180	0
37	DP	114/114 (100%)	1.40	30 (26%) 0 0	8, 69, 148, 180	0
38	BQ	117/117 (100%)	0.46	8 (6%) 17 19	8, 63, 125, 174	0
38	DQ	117/117 (100%)	1.12	19 (16%) 1 2	11, 57, 127, 180	0
39	BR	103/103 (100%)	1.50	28 (27%) 0 0	33, 100, 153, 180	0
39	DR	103/103 (100%)	2.34	45 (43%) 0 0	26, 92, 154, 180	0
40	BS	110/110 (100%)	1.12	19 (17%) 1 2	14, 57, 132, 180	0
40	DS	110/110 (100%)	0.69	10 (9%) 9 11	5, 45, 137, 175	0
41	BT	99/100 (99%)	1.12	20 (20%) 1 1	25, 73, 150, 170	0
41	DT	99/100 (99%)	1.54	28 (28%) 0 0	16, 84, 160, 180	0
42	BU	102/103 (99%)	1.64	33 (32%) 0 0	18, 92, 158, 178	0
42	DU	102/103 (99%)	0.60	14 (13%) 3 4	11, 103, 161, 180	0
43	BW	84/84 (100%)	2.26	31 (36%) 0 0	22, 87, 153, 180	0
43	DW	84/84 (100%)	1.58	29 (34%) 0 0	20, 81, 149, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	1.45	12 (19%) 1 1	28, 92, 148, 170	0
44	DX	63/63 (100%)	1.48	18 (28%) 0 0	47, 96, 162, 171	0
45	BY	58/58 (100%)	1.62	13 (22%) 0 0	29, 72, 150, 180	0
45	DY	58/58 (100%)	1.16	7 (12%) 4 6	5, 60, 129, 177	0
46	BZ	70/70 (100%)	0.69	6 (8%) 10 13	20, 68, 134, 168	0
46	DZ	70/70 (100%)	0.89	7 (10%) 7 9	16, 59, 132, 180	0
47	B0	56/56 (100%)	2.15	21 (37%) 0 0	23, 89, 163, 180	0
47	D0	56/56 (100%)	1.55	12 (21%) 0 1	12, 61, 148, 180	0
48	B1	54/54 (100%)	2.30	21 (38%) 0 0	18, 89, 142, 179	0
48	D1	54/54 (100%)	2.78	27 (50%) 0 0	22, 77, 153, 173	0
49	B2	46/46 (100%)	0.74	7 (15%) 2 3	11, 47, 152, 180	0
49	D2	46/46 (100%)	0.58	1 (2%) 62 59	13, 48, 112, 129	0
50	B3	64/64 (100%)	1.48	16 (25%) 0 0	15, 61, 149, 180	0
50	D3	64/64 (100%)	1.33	14 (21%) 0 1	8, 55, 125, 169	0
51	B4	38/38 (100%)	1.62	10 (26%) 0 0	36, 85, 161, 180	0
51	D4	38/38 (100%)	1.62	12 (31%) 0 0	20, 80, 168, 180	0
52	BI	141/141 (100%)	2.90	87 (61%) 0 0	61, 151, 180, 180	0
52	DI	141/141 (100%)	1.55	44 (31%) 0 0	84, 157, 180, 180	0
All	All	20439/21034 (97%)	0.51	2161 (10%) 6 8	5, 61, 145, 180	0

The worst 5 of 2161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BO	57	ALA	23.4
36	BO	58	ILE	21.6
33	BL	98	ALA	18.3
45	BY	3	THR	17.6
36	BO	59	ALA	16.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
53	MG	AP	101	1/1	0.41	0.37	53,53,53,53	1
53	MG	BB	3042	1/1	0.48	0.09	95,95,95,95	0
53	MG	CA	1623	1/1	0.53	0.16	151,151,151,151	0
53	MG	AA	1612	1/1	0.58	0.16	104,104,104,104	0
53	MG	AA	1655	1/1	0.66	0.18	75,75,75,75	0
53	MG	BB	3082	1/1	0.68	0.16	19,19,19,19	0
53	MG	DB	3082	1/1	0.69	0.16	73,73,73,73	0
53	MG	AA	1644	1/1	0.70	0.10	96,96,96,96	0
53	MG	AA	1614	1/1	0.71	0.11	62,62,62,62	0
53	MG	DB	3059	1/1	0.72	0.09	127,127,127,127	0
53	MG	AA	1619	1/1	0.73	0.13	100,100,100,100	0
53	MG	BB	3090	1/1	0.75	0.08	74,74,74,74	0
53	MG	AA	1622	1/1	0.75	0.21	116,116,116,116	0
53	MG	AA	1636	1/1	0.77	0.61	127,127,127,127	0
53	MG	AA	1649	1/1	0.77	0.18	114,114,114,114	0
53	MG	BB	3033	1/1	0.78	0.29	93,93,93,93	0
53	MG	DB	3058	1/1	0.78	0.31	30,30,30,30	1
53	MG	DB	3060	1/1	0.79	0.11	77,77,77,77	0
53	MG	DB	3030	1/1	0.80	0.15	23,23,23,23	0
53	MG	AA	1625	1/1	0.80	0.19	5,5,5,5	1
53	MG	DB	3024	1/1	0.80	0.11	36,36,36,36	0
53	MG	DB	3057	1/1	0.80	0.09	28,28,28,28	0
53	MG	AA	1654	1/1	0.81	0.10	59,59,59,59	0
53	MG	CA	1660	1/1	0.81	0.15	65,65,65,65	0
53	MG	AA	1608	1/1	0.81	0.08	121,121,121,121	0
53	MG	BB	3017	1/1	0.82	0.10	72,72,72,72	0
53	MG	BB	3094	1/1	0.82	0.08	35,35,35,35	0
53	MG	AA	1638	1/1	0.82	0.21	98,98,98,98	0
53	MG	AA	1623	1/1	0.82	0.17	32,32,32,32	1
53	MG	CA	1636	1/1	0.83	0.10	51,51,51,51	0
53	MG	BB	3054	1/1	0.83	0.13	72,72,72,72	0
53	MG	BB	3088	1/1	0.83	0.15	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3081	1/1	0.83	0.16	46,46,46,46	0
53	MG	BB	3028	1/1	0.84	0.20	40,40,40,40	0
53	MG	DB	3050	1/1	0.84	0.11	74,74,74,74	0
53	MG	BB	3051	1/1	0.84	0.09	71,71,71,71	0
53	MG	AA	1629	1/1	0.84	0.14	138,138,138,138	0
53	MG	DB	3065	1/1	0.84	0.16	47,47,47,47	1
53	MG	DB	3034	1/1	0.84	0.16	66,66,66,66	0
53	MG	DB	3013	1/1	0.84	0.15	34,34,34,34	0
53	MG	AA	1653	1/1	0.85	0.10	65,65,65,65	0
53	MG	BB	3049	1/1	0.85	0.10	11,11,11,11	0
53	MG	BB	3010	1/1	0.85	0.11	39,39,39,39	0
53	MG	AA	1659	1/1	0.85	0.12	105,105,105,105	0
53	MG	CA	1662	1/1	0.85	0.14	26,26,26,26	0
53	MG	DB	3104	1/1	0.85	0.12	50,50,50,50	0
53	MG	BB	3021	1/1	0.86	0.14	55,55,55,55	0
53	MG	AA	1607	1/1	0.86	0.09	27,27,27,27	0
53	MG	BB	3110	1/1	0.86	0.13	60,60,60,60	0
53	MG	AA	1615	1/1	0.86	0.12	43,43,43,43	0
53	MG	BB	3034	1/1	0.86	0.12	25,25,25,25	0
53	MG	AA	1641	1/1	0.86	0.11	49,49,49,49	0
53	MG	BB	3067	1/1	0.87	0.18	78,78,78,78	0
53	MG	BB	3007	1/1	0.87	0.15	28,28,28,28	0
53	MG	CA	1630	1/1	0.87	0.09	5,5,5,5	1
53	MG	BB	3074	1/1	0.87	0.11	13,13,13,13	0
53	MG	DB	3054	1/1	0.87	0.07	15,15,15,15	0
53	MG	BB	3018	1/1	0.87	0.09	27,27,27,27	0
53	MG	BB	3100	1/1	0.87	0.20	11,11,11,11	1
53	MG	CA	1627	1/1	0.88	0.14	29,29,29,29	1
53	MG	DB	3053	1/1	0.88	0.12	27,27,27,27	0
53	MG	BB	3046	1/1	0.88	0.07	51,51,51,51	0
53	MG	DB	3014	1/1	0.88	0.07	5,5,5,5	0
53	MG	CA	1645	1/1	0.89	0.12	82,82,82,82	0
53	MG	AA	1639	1/1	0.89	0.06	47,47,47,47	0
53	MG	CA	1639	1/1	0.89	0.08	117,117,117,117	0
53	MG	DB	3052	1/1	0.89	0.17	60,60,60,60	0
53	MG	BB	3104	1/1	0.89	0.12	18,18,18,18	0
53	MG	DB	3094	1/1	0.90	0.24	5,5,5,5	1
53	MG	DB	3110	1/1	0.90	0.18	54,54,54,54	0
53	MG	BB	3105	1/1	0.90	0.22	64,64,64,64	0
53	MG	BB	3057	1/1	0.90	0.17	27,27,27,27	0
53	MG	BB	3005	1/1	0.90	0.12	5,5,5,5	0
53	MG	BB	3043	1/1	0.90	0.09	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	CA	1624	1/1	0.90	0.13	48,48,48,48	0
53	MG	CA	1643	1/1	0.90	0.08	41,41,41,41	0
53	MG	CA	1637	1/1	0.90	0.09	68,68,68,68	0
53	MG	CA	1649	1/1	0.90	0.18	88,88,88,88	0
53	MG	AA	1650	1/1	0.90	0.05	72,72,72,72	0
53	MG	CA	1608	1/1	0.90	0.06	110,110,110,110	0
53	MG	AA	1631	1/1	0.90	0.08	61,61,61,61	0
53	MG	AA	1620	1/1	0.90	0.12	62,62,62,62	0
53	MG	BB	3059	1/1	0.91	0.08	10,10,10,10	0
53	MG	DB	3061	1/1	0.91	0.07	78,78,78,78	0
53	MG	AA	1602	1/1	0.91	0.08	62,62,62,62	0
53	MG	AA	1657	1/1	0.91	0.06	81,81,81,81	0
53	MG	DB	3023	1/1	0.91	0.06	34,34,34,34	0
53	MG	CA	1611	1/1	0.91	0.12	71,71,71,71	0
53	MG	CA	1616	1/1	0.91	0.08	68,68,68,68	0
53	MG	DB	3016	1/1	0.91	0.11	23,23,23,23	0
53	MG	CA	1614	1/1	0.91	0.09	47,47,47,47	0
53	MG	CA	1631	1/1	0.91	0.08	36,36,36,36	0
53	MG	CA	1626	1/1	0.91	0.10	73,73,73,73	0
53	MG	CA	1657	1/1	0.91	0.07	37,37,37,37	0
53	MG	CA	1609	1/1	0.91	0.18	45,45,45,45	0
53	MG	DB	3007	1/1	0.91	0.10	12,12,12,12	0
53	MG	AA	1617	1/1	0.91	0.12	78,78,78,78	0
53	MG	BB	3096	1/1	0.91	0.14	43,43,43,43	0
53	MG	CA	1635	1/1	0.91	0.11	20,20,20,20	0
53	MG	BB	3079	1/1	0.91	0.10	38,38,38,38	0
53	MG	DB	3063	1/1	0.91	0.08	13,13,13,13	0
53	MG	BB	3060	1/1	0.91	0.08	69,69,69,69	0
53	MG	DB	3029	1/1	0.91	0.29	41,41,41,41	0
53	MG	BB	3097	1/1	0.92	0.16	74,74,74,74	0
53	MG	AA	1635	1/1	0.92	0.06	85,85,85,85	0
53	MG	CA	1650	1/1	0.92	0.12	82,82,82,82	0
53	MG	BB	3089	1/1	0.92	0.09	45,45,45,45	0
53	MG	BB	3009	1/1	0.92	0.07	35,35,35,35	0
53	MG	DB	3025	1/1	0.92	0.15	21,21,21,21	0
53	MG	BB	3109	1/1	0.92	0.14	15,15,15,15	0
53	MG	CA	1632	1/1	0.92	0.12	61,61,61,61	0
53	MG	DB	3067	1/1	0.92	0.11	17,17,17,17	0
53	MG	CA	1628	1/1	0.92	0.06	55,55,55,55	1
53	MG	BB	3080	1/1	0.92	0.08	31,31,31,31	0
53	MG	CA	1607	1/1	0.92	0.06	18,18,18,18	0
53	MG	CA	1629	1/1	0.92	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3091	1/1	0.92	0.07	19,19,19,19	0
53	MG	DB	3031	1/1	0.92	0.12	18,18,18,18	0
53	MG	DB	3045	1/1	0.92	0.07	61,61,61,61	0
53	MG	BB	3040	1/1	0.92	0.10	21,21,21,21	0
53	MG	AA	1618	1/1	0.92	0.06	46,46,46,46	0
53	MG	CA	1646	1/1	0.92	0.08	42,42,42,42	0
53	MG	DB	3021	1/1	0.92	0.10	16,16,16,16	0
53	MG	AA	1624	1/1	0.92	0.16	79,79,79,79	0
53	MG	CA	1622	1/1	0.92	0.09	67,67,67,67	0
53	MG	DN	201	1/1	0.92	0.19	49,49,49,49	0
53	MG	BB	3053	1/1	0.93	0.07	6,6,6,6	0
53	MG	AA	1643	1/1	0.93	0.09	73,73,73,73	0
53	MG	BB	3098	1/1	0.93	0.16	45,45,45,45	0
53	MG	AA	1604	1/1	0.93	0.14	45,45,45,45	0
53	MG	DB	3083	1/1	0.93	0.17	27,27,27,27	0
53	MG	CA	1653	1/1	0.93	0.26	45,45,45,45	0
53	MG	CA	1613	1/1	0.93	0.14	78,78,78,78	0
53	MG	CA	1638	1/1	0.93	0.04	37,37,37,37	0
53	MG	DB	3017	1/1	0.93	0.12	5,5,5,5	0
53	MG	AA	1606	1/1	0.93	0.06	59,59,59,59	0
53	MG	AA	1656	1/1	0.93	0.26	66,66,66,66	0
53	MG	AA	1637	1/1	0.93	0.11	81,81,81,81	0
53	MG	CA	1634	1/1	0.93	0.15	61,61,61,61	0
53	MG	DB	3018	1/1	0.93	0.09	29,29,29,29	0
53	MG	AA	1634	1/1	0.93	0.10	85,85,85,85	0
53	MG	AA	1647	1/1	0.93	0.10	23,23,23,23	0
53	MG	AA	1605	1/1	0.93	0.09	48,48,48,48	0
53	MG	DB	3108	1/1	0.93	0.07	5,5,5,5	0
53	MG	BB	3084	1/1	0.93	0.11	5,5,5,5	0
53	MG	BB	3065	1/1	0.93	0.13	47,47,47,47	0
53	MG	DB	3055	1/1	0.93	0.09	19,19,19,19	0
53	MG	AA	1632	1/1	0.93	0.05	53,53,53,53	0
53	MG	BB	3035	1/1	0.93	0.08	12,12,12,12	0
53	MG	BB	3052	1/1	0.93	0.10	19,19,19,19	0
53	MG	BB	3071	1/1	0.93	0.11	24,24,24,24	0
53	MG	DB	3062	1/1	0.93	0.13	43,43,43,43	0
53	MG	DB	3071	1/1	0.93	0.08	39,39,39,39	0
53	MG	BB	3093	1/1	0.94	0.23	5,5,5,5	1
53	MG	BB	3031	1/1	0.94	0.19	45,45,45,45	0
53	MG	DB	3032	1/1	0.94	0.10	46,46,46,46	0
53	MG	AA	1658	1/1	0.94	0.21	167,167,167,167	0
53	MG	CA	1652	1/1	0.94	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3072	1/1	0.94	0.07	30,30,30,30	0
53	MG	AA	1630	1/1	0.94	0.08	30,30,30,30	0
53	MG	DB	3096	1/1	0.94	0.08	20,20,20,20	0
53	MG	DB	3001	1/1	0.94	0.16	7,7,7,7	0
53	MG	CA	1656	1/1	0.94	0.11	48,48,48,48	0
53	MG	AA	1613	1/1	0.94	0.06	42,42,42,42	0
53	MG	DB	3107	1/1	0.94	0.09	19,19,19,19	0
53	MG	BB	3083	1/1	0.94	0.09	20,20,20,20	0
53	MG	AA	1642	1/1	0.94	0.08	70,70,70,70	0
53	MG	BB	3087	1/1	0.94	0.13	45,45,45,45	0
53	MG	BB	3072	1/1	0.94	0.09	24,24,24,24	0
53	MG	DB	3043	1/1	0.94	0.14	9,9,9,9	0
53	MG	CA	1654	1/1	0.94	0.05	40,40,40,40	0
53	MG	BB	3075	1/1	0.94	0.18	31,31,31,31	0
53	MG	CA	1640	1/1	0.94	0.07	11,11,11,11	0
53	MG	DB	3102	1/1	0.94	0.10	26,26,26,26	0
53	MG	AA	1645	1/1	0.94	0.11	27,27,27,27	0
53	MG	CA	1642	1/1	0.94	0.09	45,45,45,45	0
53	MG	BB	3099	1/1	0.94	0.11	30,30,30,30	0
53	MG	AA	1611	1/1	0.94	0.06	40,40,40,40	0
53	MG	DB	3077	1/1	0.94	0.17	57,57,57,57	0
53	MG	DB	3089	1/1	0.94	0.06	65,65,65,65	0
53	MG	AA	1603	1/1	0.94	0.11	43,43,43,43	0
53	MG	DB	3076	1/1	0.94	0.07	17,17,17,17	0
53	MG	DB	3027	1/1	0.95	0.08	10,10,10,10	0
53	MG	DB	3105	1/1	0.95	0.11	23,23,23,23	0
53	MG	CA	1605	1/1	0.95	0.07	18,18,18,18	0
53	MG	BB	3078	1/1	0.95	0.19	25,25,25,25	0
53	MG	DB	3040	1/1	0.95	0.12	5,5,5,5	0
53	MG	AA	1633	1/1	0.95	0.05	75,75,75,75	0
53	MG	BB	3064	1/1	0.95	0.06	39,39,39,39	0
53	MG	BB	3016	1/1	0.95	0.13	15,15,15,15	0
53	MG	DB	3002	1/1	0.95	0.12	37,37,37,37	0
53	MG	CA	1625	1/1	0.95	0.09	26,26,26,26	0
53	MG	BB	3019	1/1	0.95	0.08	27,27,27,27	0
53	MG	AA	1616	1/1	0.95	0.07	46,46,46,46	0
53	MG	BB	3041	1/1	0.95	0.05	30,30,30,30	0
53	MG	DB	3088	1/1	0.95	0.14	35,35,35,35	0
53	MG	AA	1652	1/1	0.95	0.08	25,25,25,25	0
53	MG	DB	3004	1/1	0.95	0.13	19,19,19,19	0
53	MG	BB	3101	1/1	0.95	0.05	12,12,12,12	0
53	MG	DB	3099	1/1	0.95	0.07	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3027	1/1	0.95	0.09	23,23,23,23	0
53	MG	DB	3015	1/1	0.95	0.09	49,49,49,49	0
53	MG	CA	1606	1/1	0.95	0.09	74,74,74,74	0
53	MG	DB	3098	1/1	0.95	0.12	18,18,18,18	0
53	MG	DB	3106	1/1	0.95	0.06	21,21,21,21	0
53	MG	CA	1620	1/1	0.95	0.07	35,35,35,35	0
53	MG	AA	1648	1/1	0.95	0.05	94,94,94,94	0
53	MG	BB	3039	1/1	0.95	0.18	45,45,45,45	0
53	MG	DB	3026	1/1	0.95	0.14	18,18,18,18	0
53	MG	CA	1648	1/1	0.95	0.08	56,56,56,56	0
53	MG	DB	3066	1/1	0.95	0.08	5,5,5,5	0
53	MG	DB	3020	1/1	0.95	0.12	20,20,20,20	0
53	MG	BB	3030	1/1	0.95	0.05	53,53,53,53	0
53	MG	BB	3036	1/1	0.95	0.14	37,37,37,37	0
53	MG	AA	1646	1/1	0.95	0.30	60,60,60,60	0
53	MG	AA	1627	1/1	0.95	0.14	72,72,72,72	0
53	MG	BB	3058	1/1	0.95	0.10	28,28,28,28	0
53	MG	AA	1601	1/1	0.95	0.06	26,26,26,26	0
53	MG	CA	1612	1/1	0.95	0.08	29,29,29,29	0
53	MG	AA	1628	1/1	0.95	0.10	26,26,26,26	0
53	MG	CA	1603	1/1	0.95	0.13	69,69,69,69	0
53	MG	BB	3077	1/1	0.96	0.08	44,44,44,44	0
53	MG	BB	3004	1/1	0.96	0.04	21,21,21,21	0
53	MG	DB	3070	1/1	0.96	0.07	46,46,46,46	0
53	MG	DB	3033	1/1	0.96	0.09	11,11,11,11	0
53	MG	DB	3051	1/1	0.96	0.13	53,53,53,53	0
53	MG	BB	3055	1/1	0.96	0.13	27,27,27,27	0
53	MG	CA	1621	1/1	0.96	0.24	113,113,113,113	0
53	MG	DB	3046	1/1	0.96	0.08	33,33,33,33	0
53	MG	DB	3039	1/1	0.96	0.07	19,19,19,19	0
53	MG	AA	1626	1/1	0.96	0.06	35,35,35,35	0
53	MG	DB	3090	1/1	0.96	0.15	28,28,28,28	0
53	MG	BB	3047	1/1	0.96	0.06	114,114,114,114	0
53	MG	DB	3042	1/1	0.96	0.10	27,27,27,27	0
53	MG	DB	3022	1/1	0.96	0.08	15,15,15,15	0
53	MG	DB	3036	1/1	0.96	0.09	16,16,16,16	0
53	MG	BB	3048	1/1	0.96	0.06	20,20,20,20	0
53	MG	CA	1615	1/1	0.96	0.09	101,101,101,101	0
53	MG	CA	1644	1/1	0.96	0.06	29,29,29,29	0
53	MG	CA	1618	1/1	0.96	0.10	5,5,5,5	0
53	MG	BB	3038	1/1	0.96	0.04	58,58,58,58	0
53	MG	BB	3037	1/1	0.96	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	DB	3073	1/1	0.96	0.11	16,16,16,16	0
53	MG	CA	1659	1/1	0.96	0.17	48,48,48,48	0
53	MG	BB	3063	1/1	0.96	0.14	27,27,27,27	0
53	MG	AA	1610	1/1	0.96	0.09	34,34,34,34	0
53	MG	BB	3076	1/1	0.96	0.05	24,24,24,24	0
53	MG	DB	3091	1/1	0.96	0.08	96,96,96,96	0
53	MG	AA	1621	1/1	0.96	0.09	23,23,23,23	0
53	MG	DB	3008	1/1	0.96	0.13	24,24,24,24	0
53	MG	DB	3103	1/1	0.96	0.12	50,50,50,50	0
53	MG	DB	3005	1/1	0.96	0.07	9,9,9,9	0
53	MG	BB	3013	1/1	0.96	0.09	31,31,31,31	0
53	MG	BB	3108	1/1	0.96	0.08	19,19,19,19	0
53	MG	BB	3032	1/1	0.96	0.12	9,9,9,9	0
53	MG	CA	1633	1/1	0.97	0.09	47,47,47,47	0
53	MG	BB	3011	1/1	0.97	0.13	7,7,7,7	0
53	MG	CA	1641	1/1	0.97	0.11	92,92,92,92	0
53	MG	BB	3029	1/1	0.97	0.08	13,13,13,13	0
53	MG	DB	3109	1/1	0.97	0.07	24,24,24,24	0
53	MG	BB	3026	1/1	0.97	0.10	5,5,5,5	0
53	MG	BB	3045	1/1	0.97	0.05	31,31,31,31	0
53	MG	BB	3073	1/1	0.97	0.09	28,28,28,28	0
53	MG	DB	3085	1/1	0.97	0.09	17,17,17,17	0
53	MG	BB	3025	1/1	0.97	0.16	53,53,53,53	0
53	MG	CA	1655	1/1	0.97	0.14	48,48,48,48	0
53	MG	BB	3008	1/1	0.97	0.06	58,58,58,58	0
53	MG	BB	3020	1/1	0.97	0.06	23,23,23,23	0
53	MG	CA	1619	1/1	0.97	0.09	26,26,26,26	0
53	MG	DB	3010	1/1	0.97	0.09	12,12,12,12	0
53	MG	DB	3086	1/1	0.97	0.14	69,69,69,69	0
53	MG	BB	3014	1/1	0.97	0.04	29,29,29,29	0
53	MG	BB	3001	1/1	0.97	0.06	10,10,10,10	0
53	MG	BB	3107	1/1	0.97	0.07	27,27,27,27	0
53	MG	DB	3041	1/1	0.97	0.07	18,18,18,18	0
53	MG	CA	1658	1/1	0.97	0.07	38,38,38,38	0
53	MG	BB	3022	1/1	0.97	0.08	38,38,38,38	0
53	MG	DB	3035	1/1	0.97	0.10	30,30,30,30	0
53	MG	DB	3044	1/1	0.97	0.07	7,7,7,7	0
53	MG	BB	3102	1/1	0.97	0.13	19,19,19,19	0
53	MG	AA	1640	1/1	0.97	0.08	44,44,44,44	0
53	MG	DB	3087	1/1	0.97	0.12	6,6,6,6	0
53	MG	BB	3061	1/1	0.97	0.06	42,42,42,42	0
53	MG	DB	3028	1/1	0.97	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	BB	3066	1/1	0.97	0.09	59,59,59,59	0
53	MG	DB	3095	1/1	0.97	0.16	55,55,55,55	0
53	MG	BB	3069	1/1	0.97	0.07	9,9,9,9	0
53	MG	BB	3056	1/1	0.97	0.10	19,19,19,19	0
53	MG	AA	1651	1/1	0.97	0.07	84,84,84,84	0
53	MG	BB	3015	1/1	0.97	0.08	24,24,24,24	0
53	MG	CA	1651	1/1	0.97	0.09	14,14,14,14	0
53	MG	BB	3085	1/1	0.97	0.07	22,22,22,22	0
53	MG	DB	3100	1/1	0.97	0.09	11,11,11,11	0
53	MG	BB	3003	1/1	0.97	0.06	13,13,13,13	0
53	MG	CA	1602	1/1	0.98	0.15	32,32,32,32	0
53	MG	BB	3095	1/1	0.98	0.09	34,34,34,34	0
53	MG	DB	3037	1/1	0.98	0.09	13,13,13,13	0
53	MG	AA	1609	1/1	0.98	0.14	8,8,8,8	0
53	MG	BB	3103	1/1	0.98	0.07	7,7,7,7	0
53	MG	DB	3056	1/1	0.98	0.09	11,11,11,11	0
53	MG	BB	3002	1/1	0.98	0.10	10,10,10,10	0
53	MG	BB	3050	1/1	0.98	0.10	35,35,35,35	0
53	MG	DB	3068	1/1	0.98	0.12	14,14,14,14	0
53	MG	DB	3101	1/1	0.98	0.11	27,27,27,27	0
53	MG	DB	3006	1/1	0.98	0.07	5,5,5,5	0
53	MG	BB	3006	1/1	0.98	0.07	10,10,10,10	0
53	MG	DB	3012	1/1	0.98	0.12	6,6,6,6	0
53	MG	DB	3019	1/1	0.98	0.04	5,5,5,5	0
53	MG	DB	3064	1/1	0.98	0.07	28,28,28,28	0
53	MG	DB	3079	1/1	0.98	0.10	5,5,5,5	0
53	MG	BB	3068	1/1	0.98	0.09	24,24,24,24	0
53	MG	DB	3093	1/1	0.98	0.06	10,10,10,10	0
53	MG	BB	3024	1/1	0.98	0.09	22,22,22,22	0
53	MG	BB	3062	1/1	0.98	0.09	22,22,22,22	0
53	MG	DB	3038	1/1	0.98	0.09	16,16,16,16	0
53	MG	DB	3009	1/1	0.98	0.08	7,7,7,7	0
53	MG	BB	3106	1/1	0.98	0.11	46,46,46,46	0
53	MG	DB	3080	1/1	0.98	0.09	12,12,12,12	0
53	MG	DB	3003	1/1	0.98	0.07	14,14,14,14	0
53	MG	DB	3084	1/1	0.98	0.07	8,8,8,8	0
53	MG	BB	3092	1/1	0.98	0.07	11,11,11,11	0
53	MG	DB	3078	1/1	0.98	0.08	18,18,18,18	0
53	MG	DB	3074	1/1	0.98	0.09	25,25,25,25	0
53	MG	DB	3075	1/1	0.98	0.04	5,5,5,5	0
53	MG	DB	3092	1/1	0.98	0.08	23,23,23,23	0
53	MG	CA	1601	1/1	0.98	0.06	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	CA	1617	1/1	0.98	0.10	9,9,9,9	0
53	MG	CA	1610	1/1	0.98	0.03	34,34,34,34	0
53	MG	DB	3047	1/1	0.98	0.13	17,17,17,17	0
53	MG	BB	3023	1/1	0.98	0.07	22,22,22,22	0
53	MG	CA	1661	1/1	0.98	0.04	62,62,62,62	0
53	MG	CA	1604	1/1	0.98	0.09	18,18,18,18	0
53	MG	DB	3069	1/1	0.98	0.09	44,44,44,44	0
53	MG	DB	3049	1/1	0.98	0.06	5,5,5,5	0
53	MG	DB	3048	1/1	0.99	0.05	20,20,20,20	0
53	MG	BB	3070	1/1	0.99	0.09	32,32,32,32	0
53	MG	BB	3086	1/1	0.99	0.15	37,37,37,37	0
53	MG	DB	3011	1/1	0.99	0.09	8,8,8,8	0
53	MG	DB	3081	1/1	0.99	0.06	25,25,25,25	0
53	MG	BB	3012	1/1	0.99	0.08	41,41,41,41	0
53	MG	BB	3044	1/1	0.99	0.07	32,32,32,32	0
53	MG	DB	3097	1/1	0.99	0.11	15,15,15,15	0
53	MG	CA	1647	1/1	0.99	0.06	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.