



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2024 – 09:28 AM EDT

PDB ID : 4V6E  
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting  
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.  
Deposited on : 2009-06-28  
Resolution : 3.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

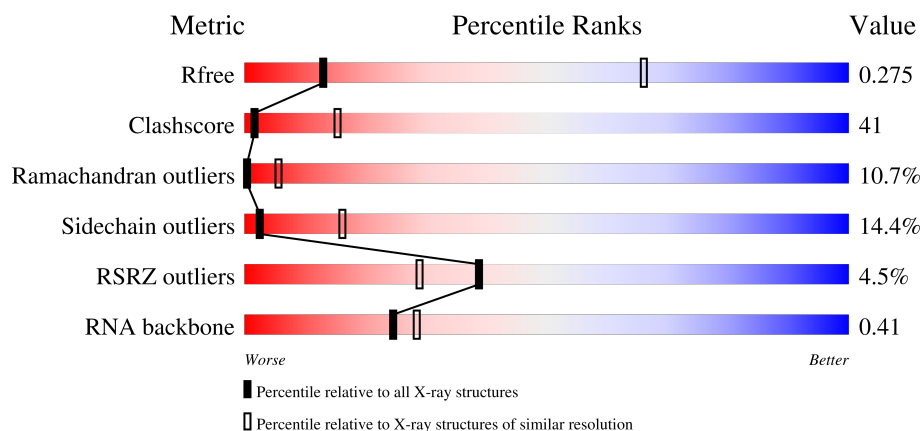
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1058 (3.84-3.60)
Clashscore	180529	1114 (3.84-3.60)
Ramachandran outliers	177936	1095 (3.84-3.60)
Sidechain outliers	177891	1091 (3.84-3.60)
RSRZ outliers	164620	1058 (3.84-3.60)
RNA backbone	3690	1122 (4.40-3.00)

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

Mol	Chain	Length	Quality of chain
1	AB	241	
1	CB	241	
2	AC	233	
2	CC	233	

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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	




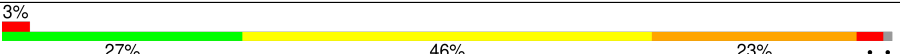
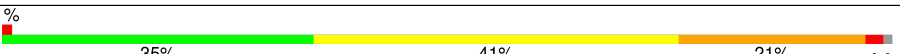
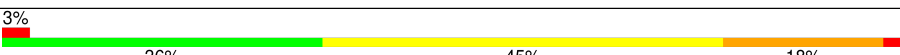
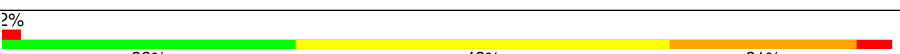
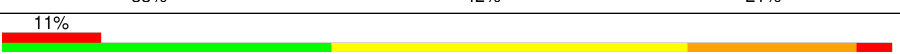
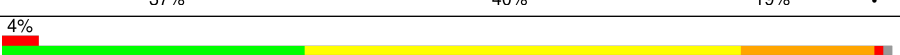
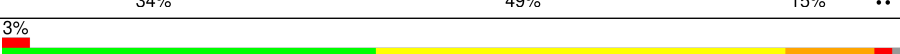
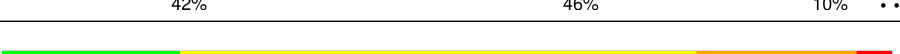
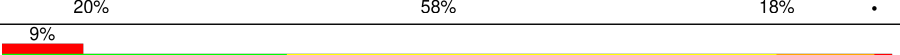
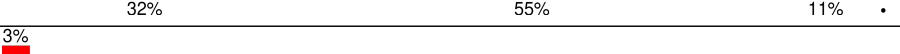
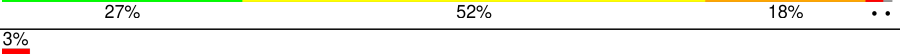
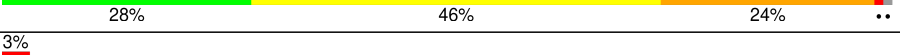
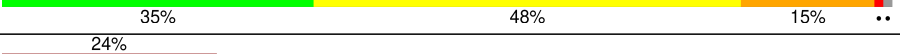
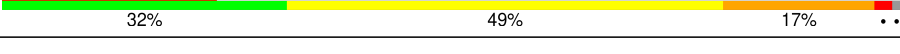
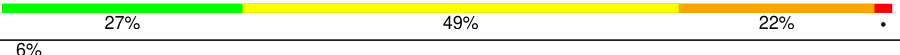
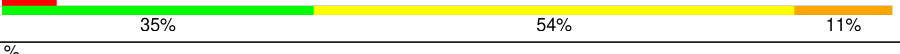
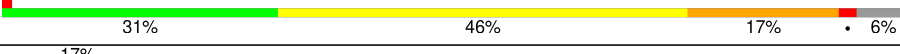
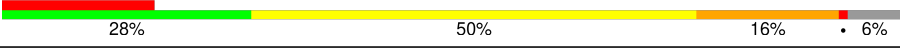
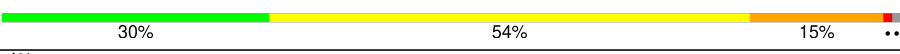

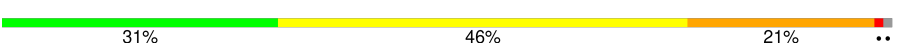

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	AV	17	
22	AX	17	
22	CV	17	
22	CX	17	
23	AW	6	
23	CW	6	
24	BA	2903	
24	DA	2903	
25	BB	118	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	

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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	




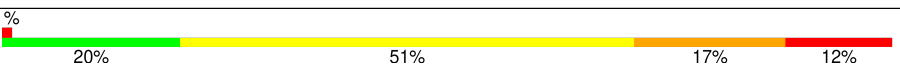
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Mol	Chain	Length	Quality of chain
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	

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Mol	Chain	Length	Quality of chain
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1627	-	-	-	X
57	MG	BA	3058	-	-	-	X
57	MG	BA	3062	-	-	-	X
57	MG	BA	3124	-	-	-	X
57	MG	BA	3131	-	-	-	X
57	MG	CA	1636	-	-	-	X
57	MG	DA	3058	-	-	-	X
57	MG	DA	3060	-	-	-	X
57	MG	DA	3063	-	-	-	X
57	MG	DA	3128	-	-	-	X
57	MG	DA	3129	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 286150 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 protein called 30S ribosomal protein S2.

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

- 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	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	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	95	Total	C	N	O	S	0	0	0
			769	480	159	127	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
			714	439	144	130	1			
14	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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	80	Total	C	N	O	S	0	0	0
			648	411	121	113	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	79	Total	C	N	O	S	0	0	0
			637	408	120	107	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 S21.

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

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	AX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
23	CW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
24	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called 16S rRNA.

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

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	43	Total	Mg	0	0
			43	43		
57	BA	136	Total	Mg	0	0
			136	136		
57	BB	4	Total	Mg	0	0
			4	4		
57	BD	1	Total	Mg	0	0
			1	1		
57	CA	42	Total	Mg	0	0
			42	42		
57	DA	132	Total	Mg	0	0
			132	132		
57	DB	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DC	2	Total	Mg	0	0
			2	2		
57	DJ	1	Total	Mg	0	0
			1	1		
57	D4	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AE	1	Total	O	0	0
			1	1		
59	AL	3	Total	O	0	0
			3	3		
59	AN	6	Total	O	0	0
			6	6		
59	AT	1	Total	O	0	0
			1	1		
59	AU	1	Total	O	0	0
			1	1		
59	AA	196	Total	O	0	0
			196	196		
59	BA	615	Total	O	0	0
			615	615		
59	BB	20	Total	O	0	0
			20	20		
59	BC	8	Total	O	0	0
			8	8		
59	BD	3	Total	O	0	0
			3	3		
59	BE	1	Total	O	0	0
			1	1		
59	BL	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BN	3	Total 3	O 3	0	0
59	BT	1	Total 1	O 1	0	0
59	B2	1	Total 1	O 1	0	0
59	B3	3	Total 3	O 3	0	0
59	B4	2	Total 2	O 2	0	0
59	CE	4	Total 4	O 4	0	0
59	CI	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0
59	CN	2	Total 2	O 2	0	0
59	CT	2	Total 2	O 2	0	0
59	CU	2	Total 2	O 2	0	0
59	CA	195	Total 195	O 195	0	0
59	DA	600	Total 600	O 600	0	0
59	DB	4	Total 4	O 4	0	0
59	DC	12	Total 12	O 12	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	3	Total 3	O 3	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	6	Total 6	O 6	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0

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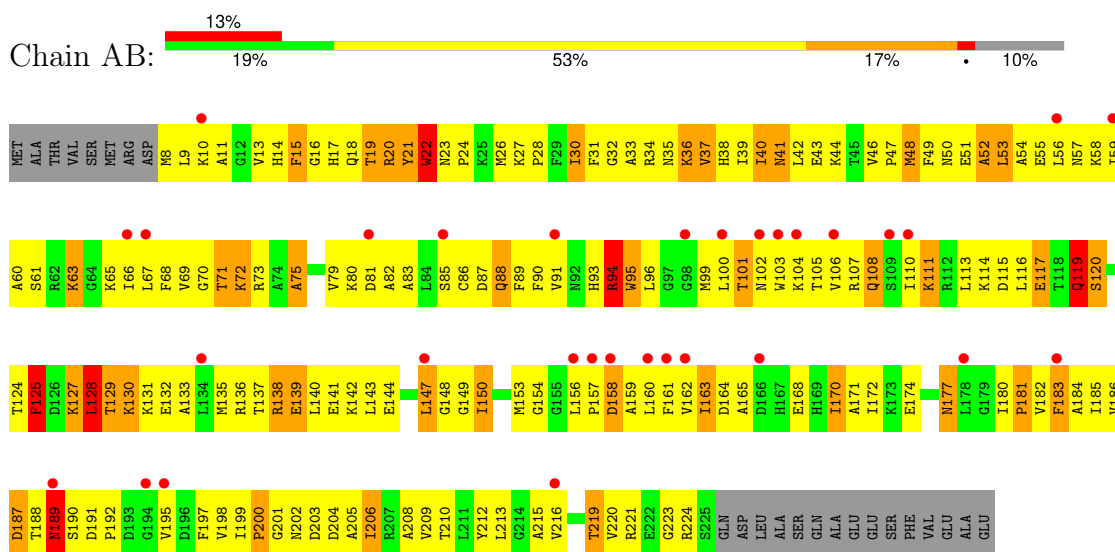
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D2	1	Total 1	O 1	0	0
59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0

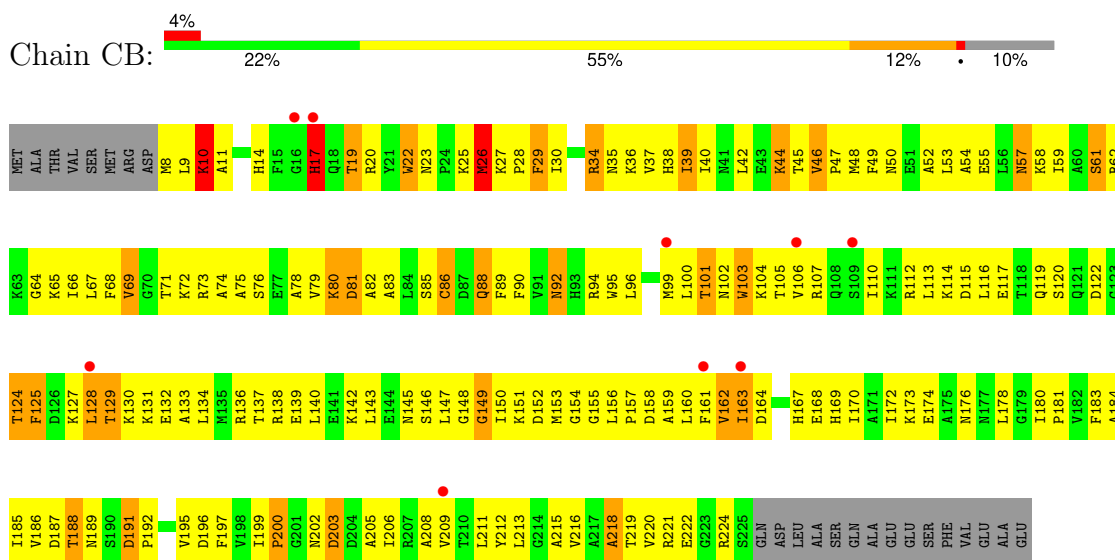
### 3 Residue-property plots

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

#### • Molecule 1: 30S ribosomal protein S2

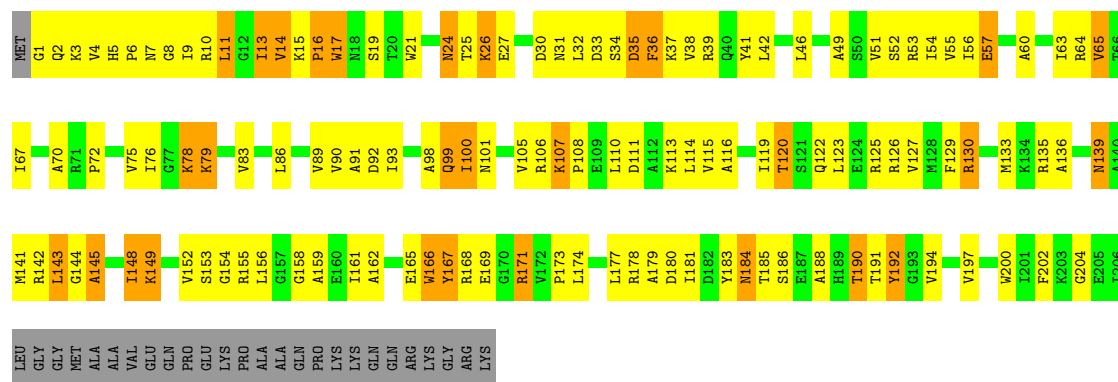


#### • Molecule 1: 30S ribosomal protein S2

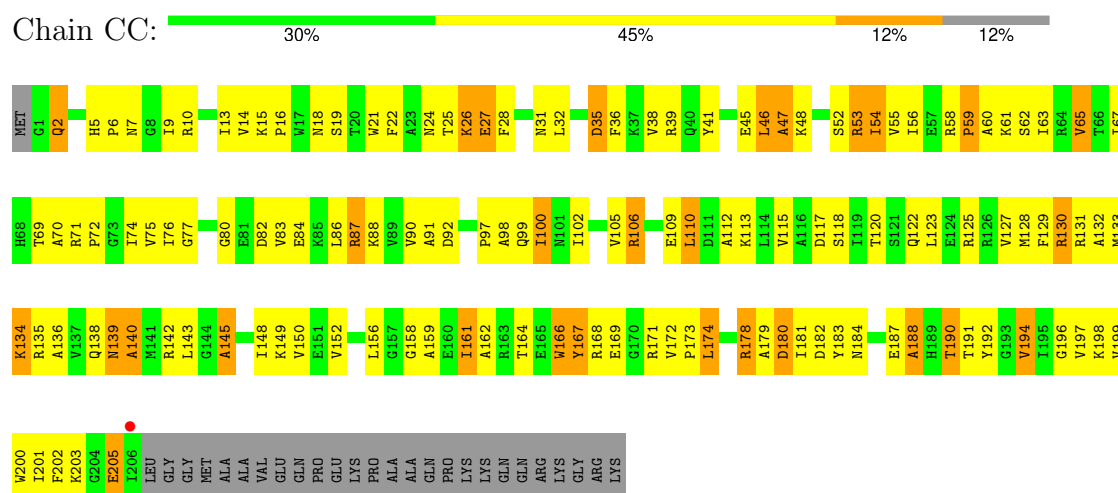


#### • Molecule 2: 30S ribosomal protein S3

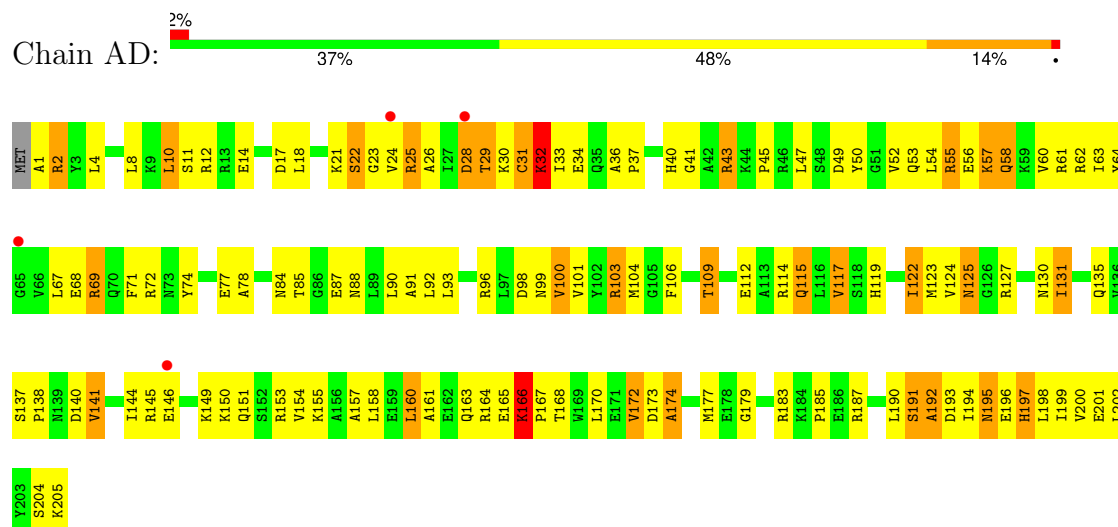




- Molecule 2: 30S ribosomal protein S3

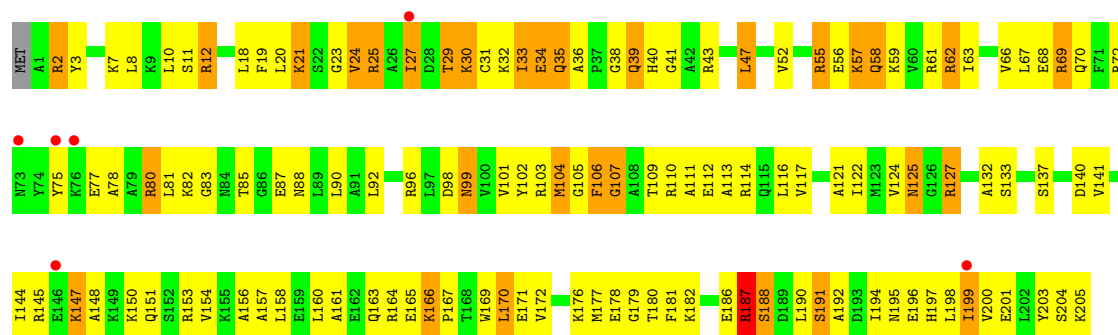


- Molecule 3: 30S ribosomal protein S4

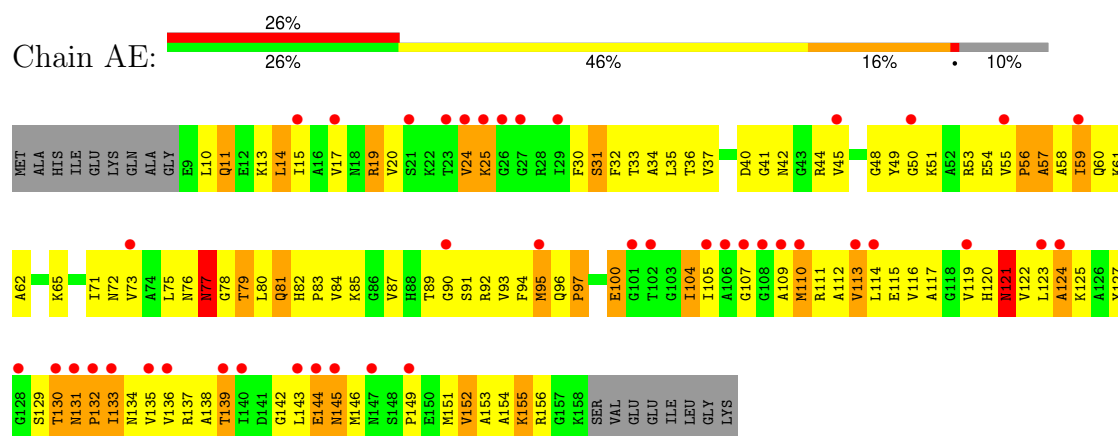


- Molecule 3: 30S ribosomal protein S4

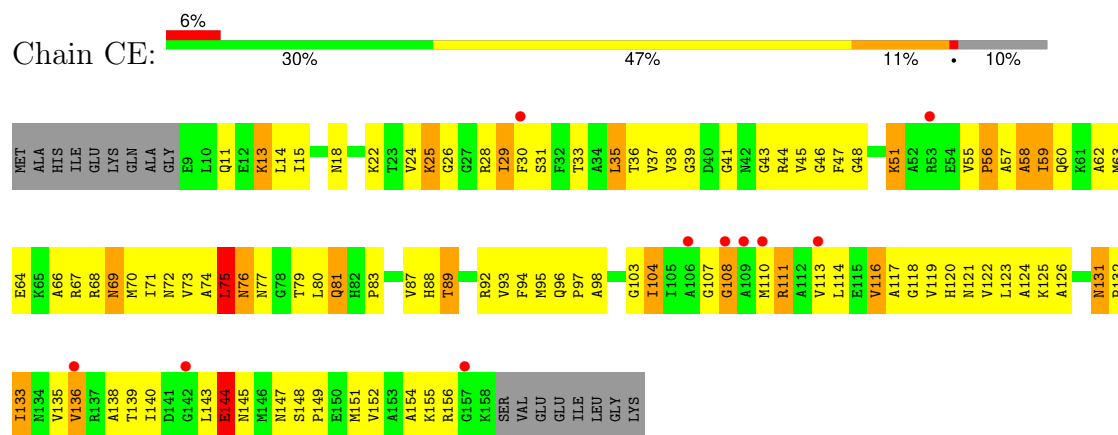




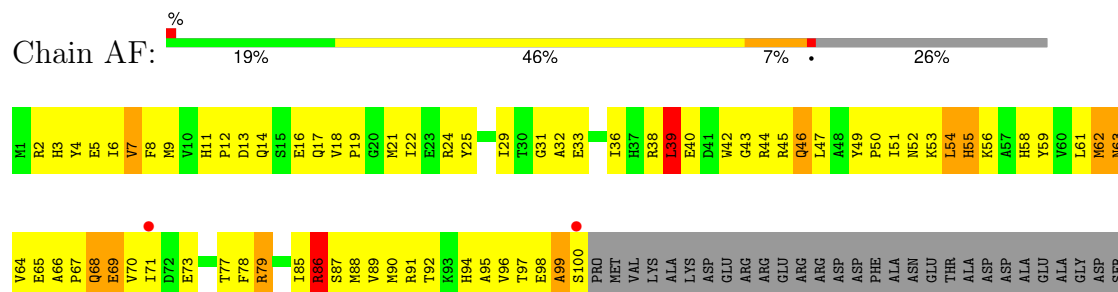
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5



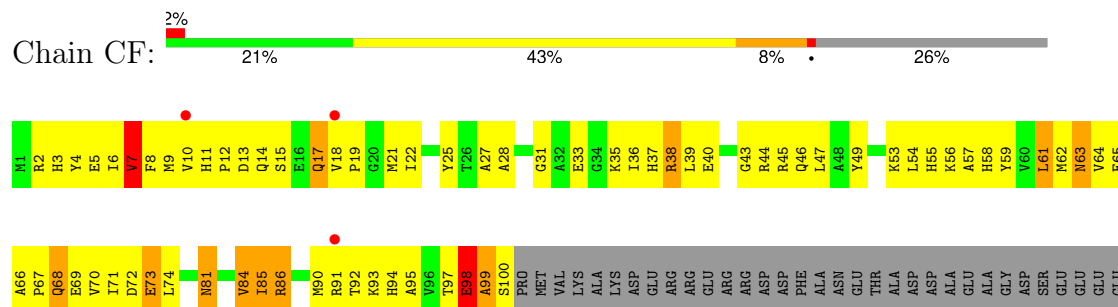
• Molecule 5: 30S ribosomal protein S6





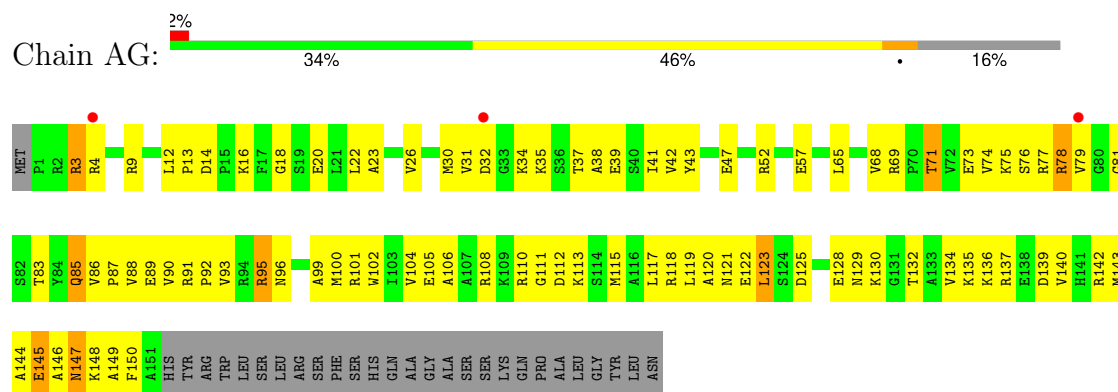
GLU  
GLU  
GLU  
GLU  
GLU

• Molecule 5: 30S ribosomal protein S6

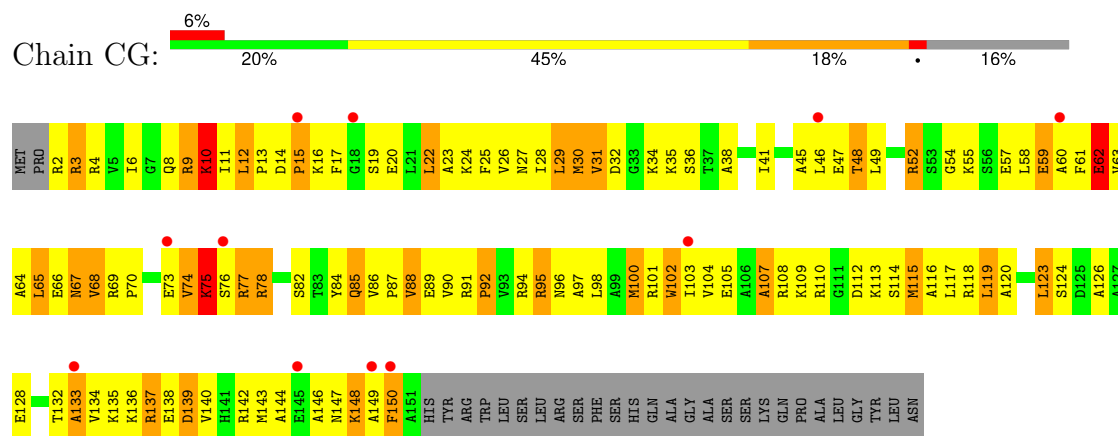


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GLU

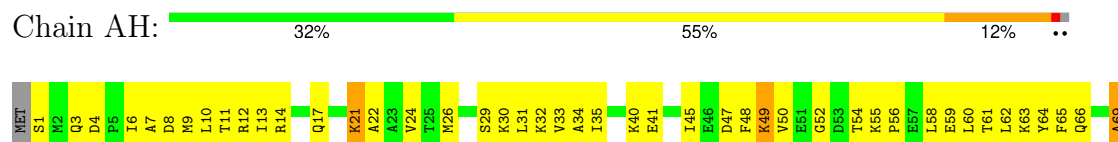
• Molecule 6: 30S ribosomal protein S7

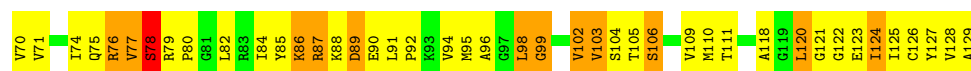


• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

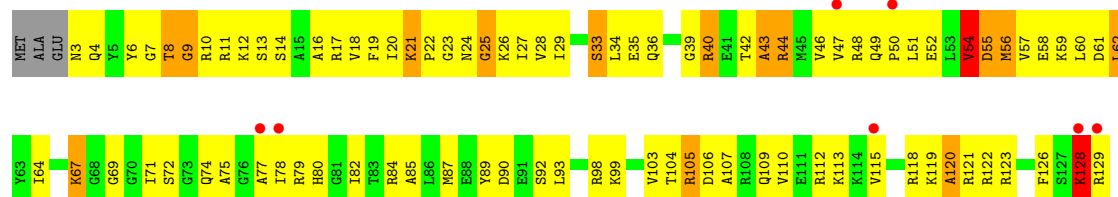




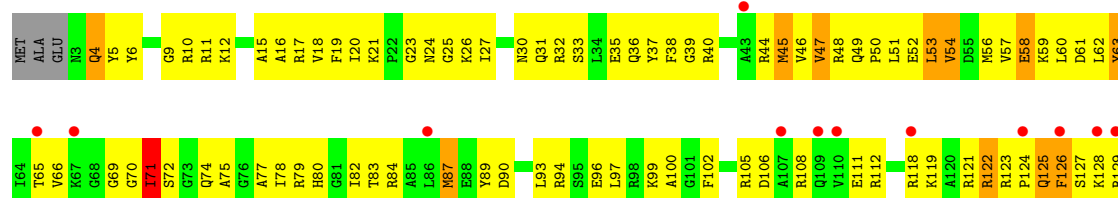
• Molecule 7: 30S ribosomal protein S8



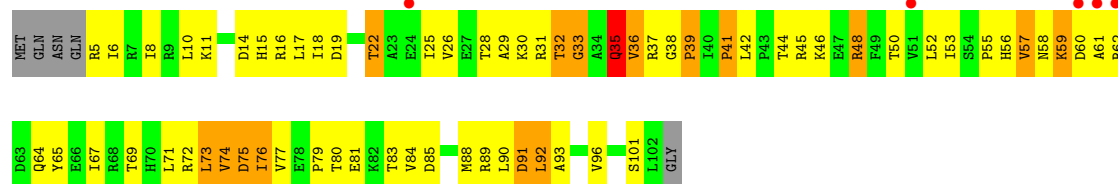
• Molecule 8: 30S ribosomal protein S9



• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10



• Molecule 9: 30S ribosomal protein S10

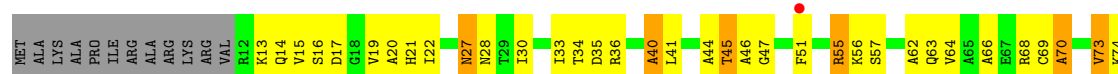
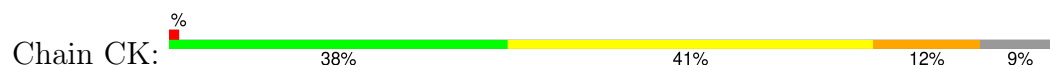




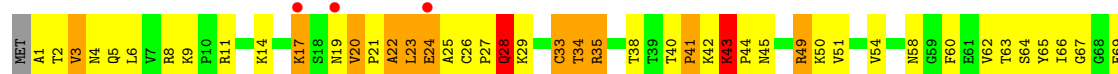
• Molecule 10: 30S ribosomal protein S11



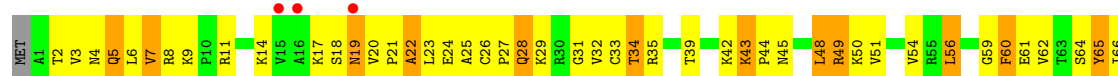
• Molecule 10: 30S ribosomal protein S11



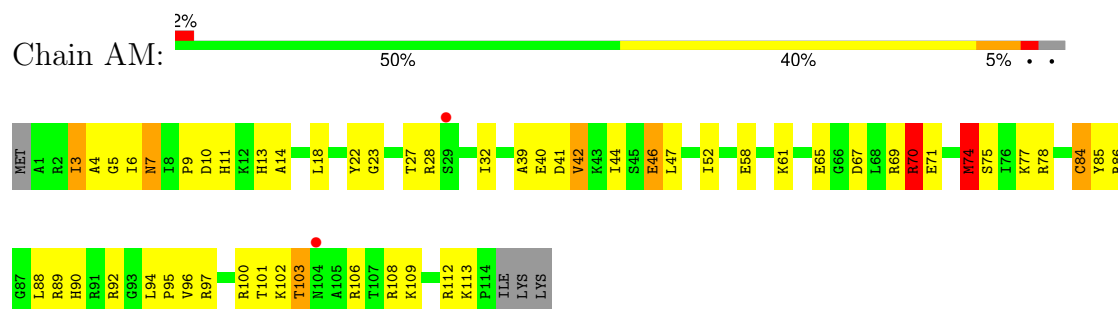
• Molecule 11: 30S ribosomal protein S12



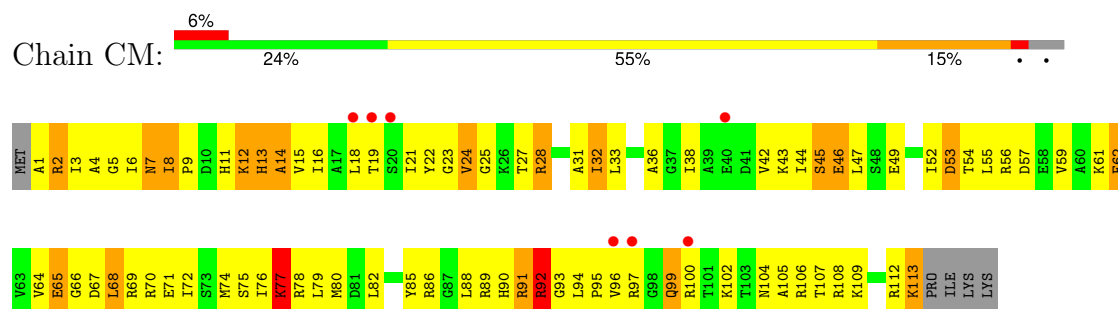
• Molecule 11: 30S ribosomal protein S12



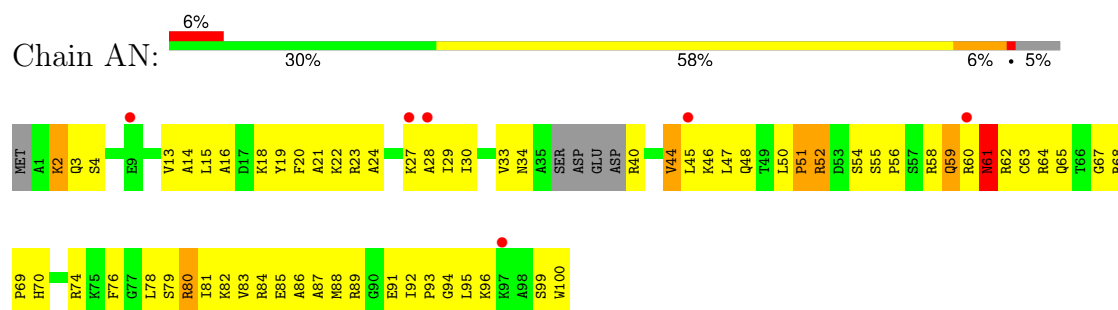
- Molecule 12: 30S ribosomal protein S13



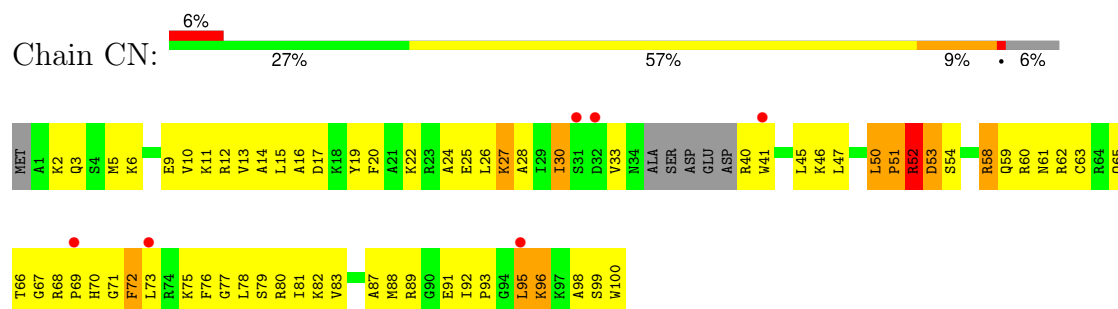
- Molecule 12: 30S ribosomal protein S13



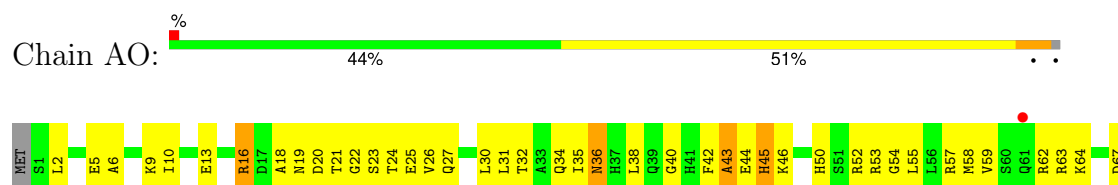
- Molecule 13: 30S ribosomal protein S14



- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15





- Molecule 14: 30S ribosomal protein S15



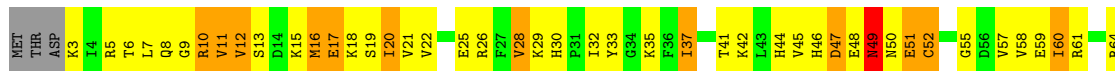
- Molecule 15: 30S ribosomal protein S16



- Molecule 15: 30S ribosomal protein S16

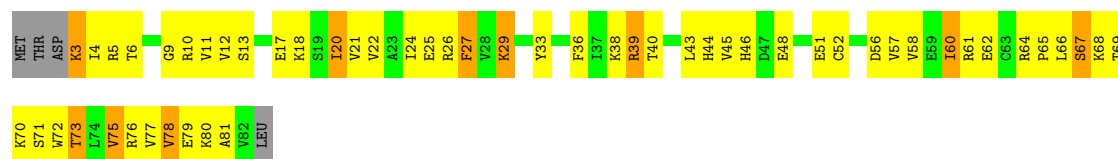


- Molecule 16: 30S ribosomal protein S17

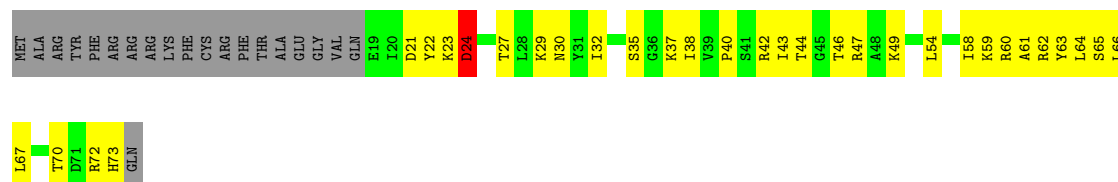


- Molecule 16: 30S ribosomal protein S17

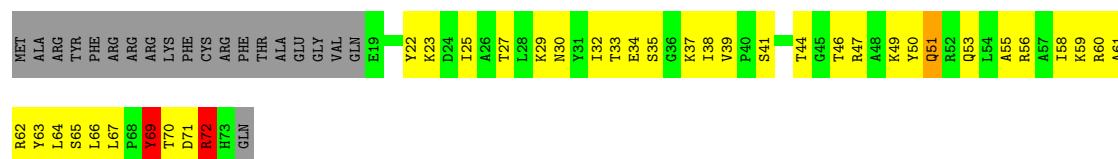




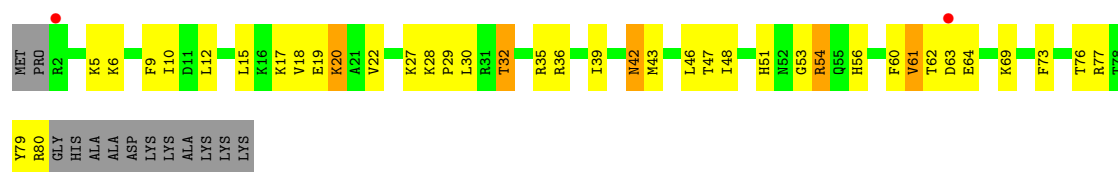
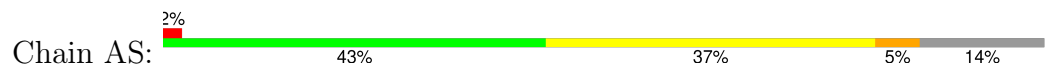
- Molecule 17: 30S ribosomal protein S18



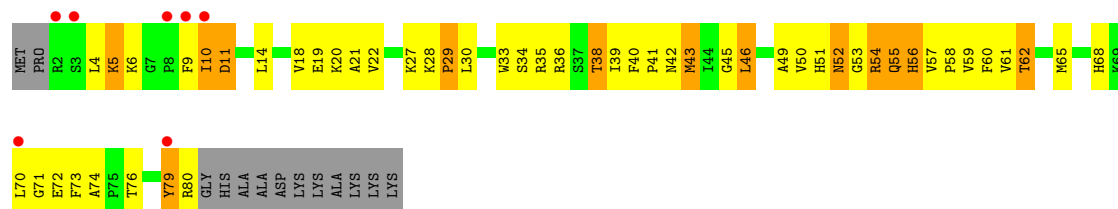
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

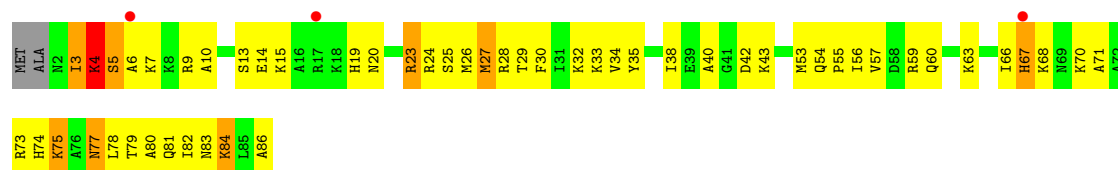


- Molecule 18: 30S ribosomal protein S19

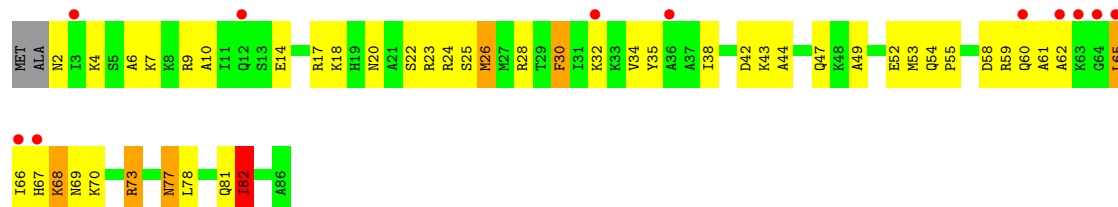


- Molecule 19: 30S ribosomal protein S20

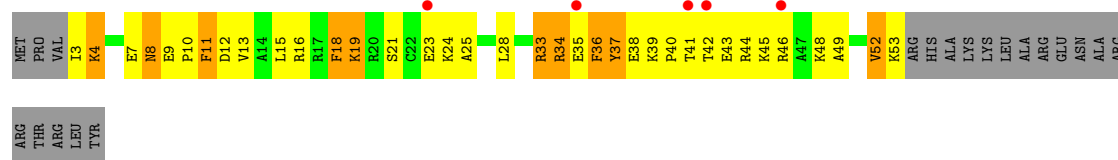
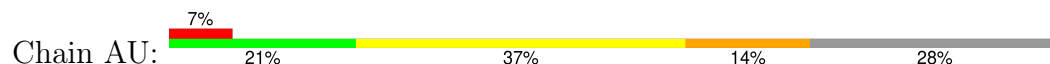




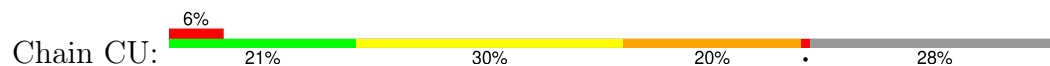
• Molecule 19: 30S ribosomal protein S20



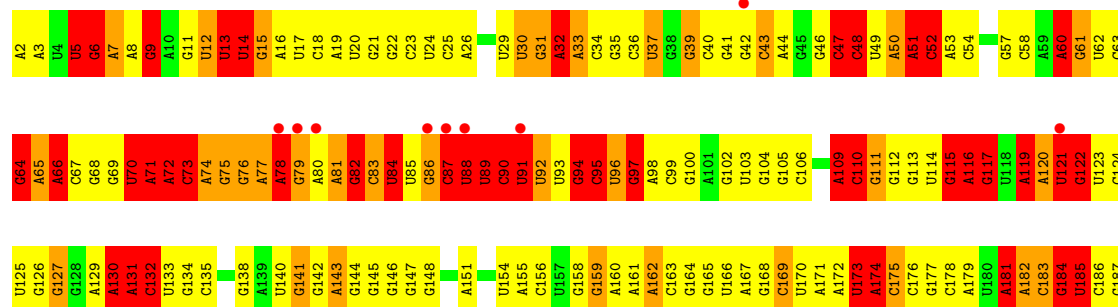
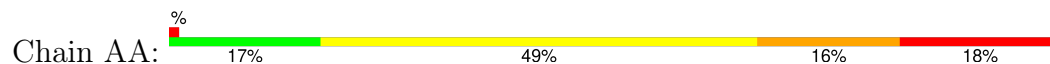
• Molecule 20: 30S ribosomal protein S21



• Molecule 20: 30S ribosomal protein S21

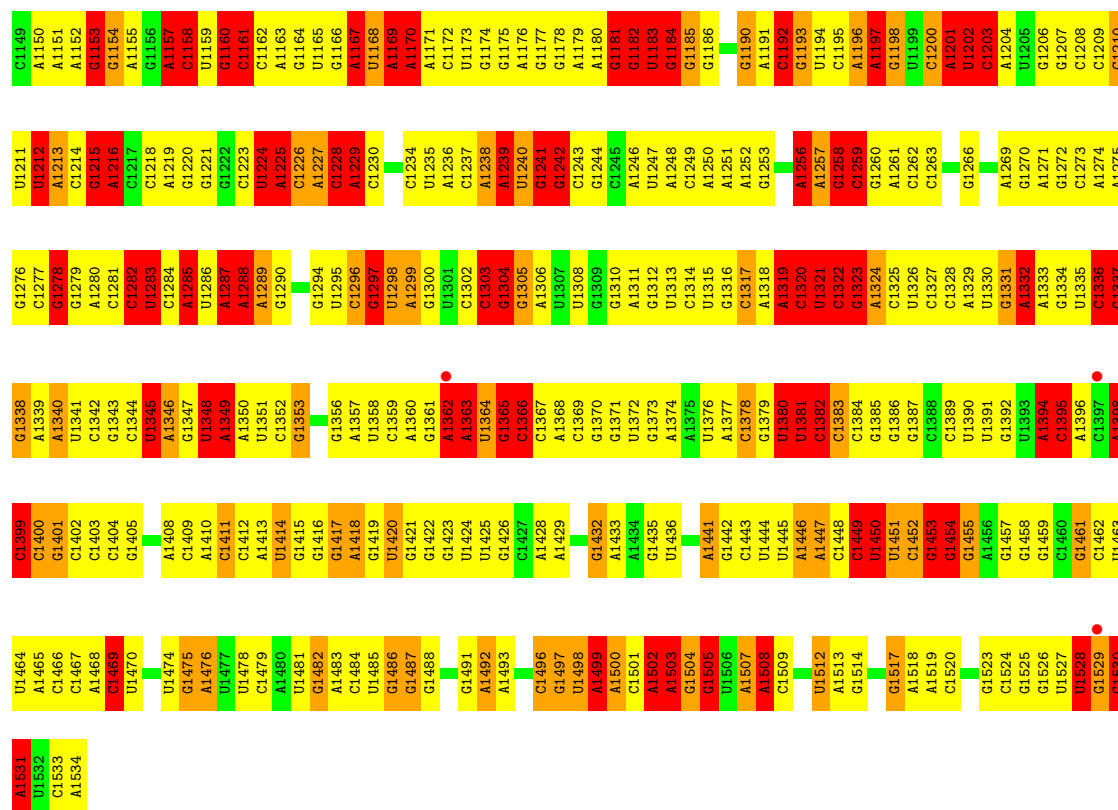


• Molecule 21: 16S rRNA

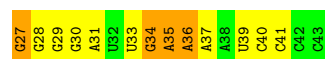


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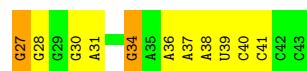
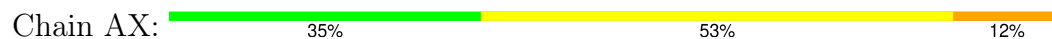




- Molecule 22: P-site tRNA ASL fragment



- Molecule 22: P-site tRNA ASL fragment



- Molecule 22: P-site tRNA ASL fragment



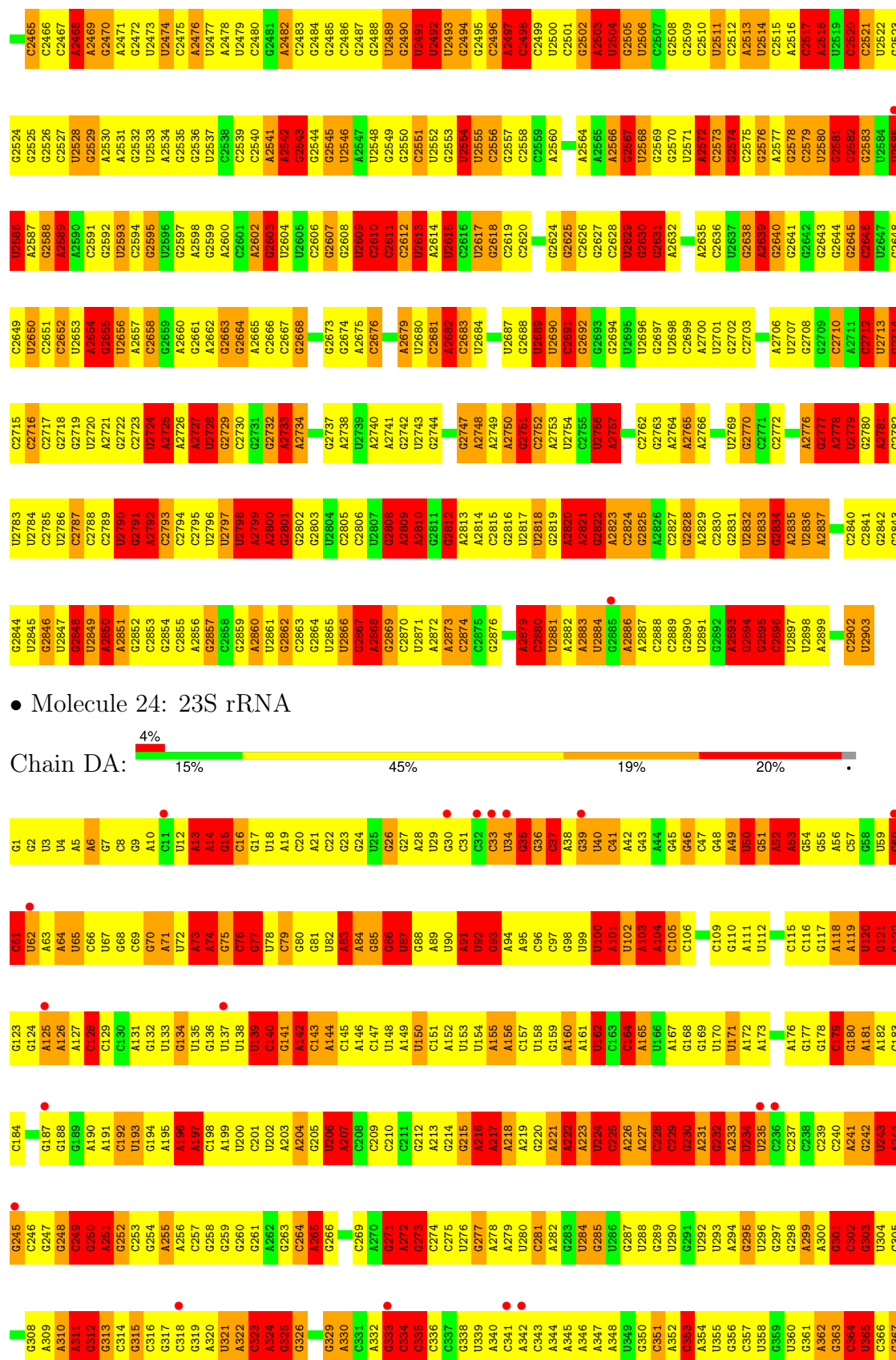
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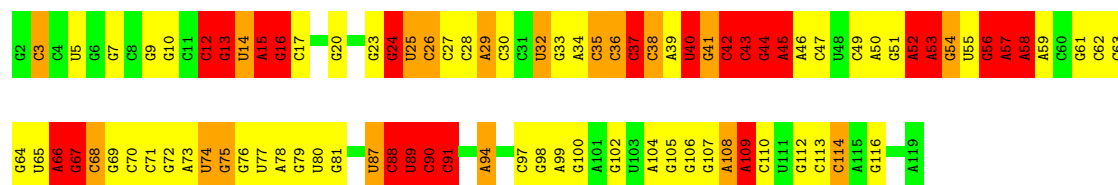




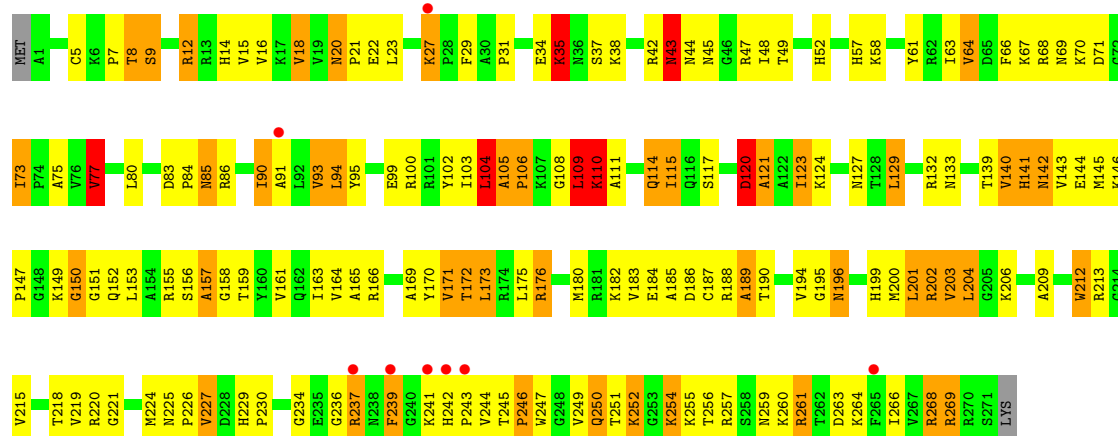
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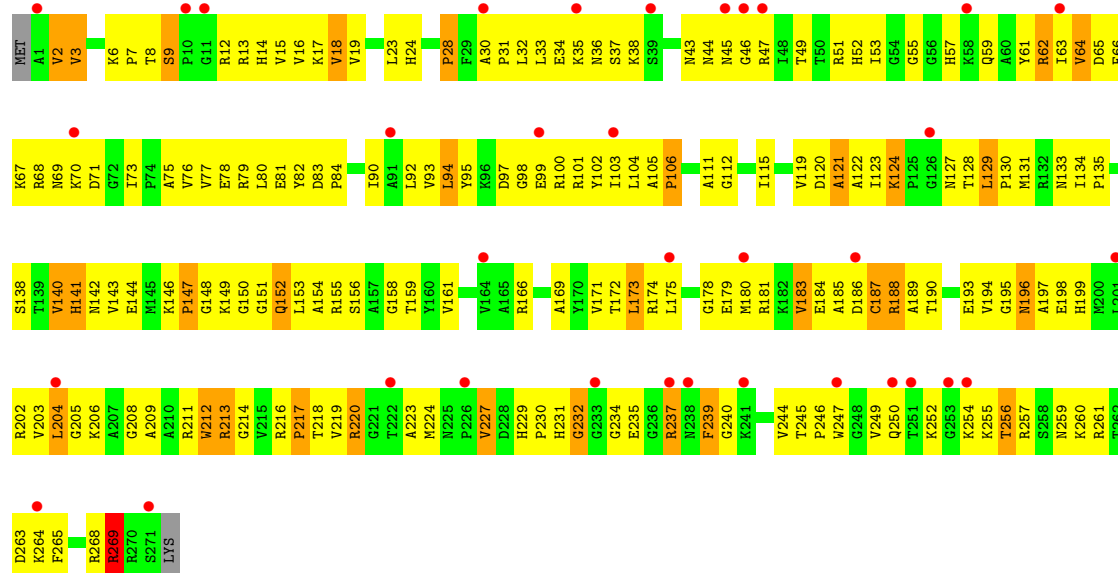




• Molecule 26: 50S ribosomal protein L2

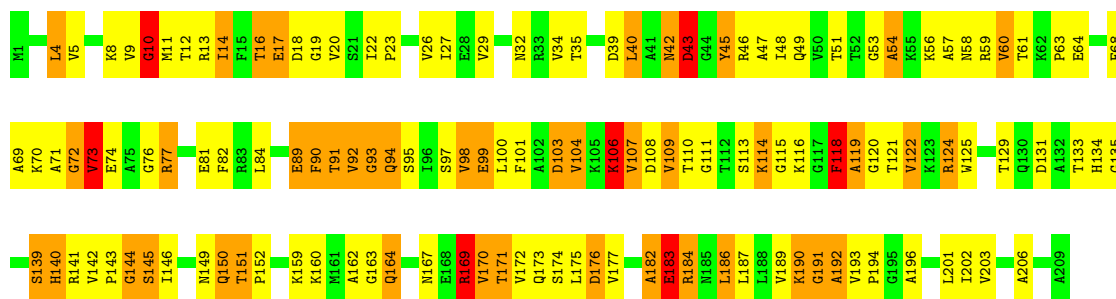


• Molecule 26: 50S ribosomal protein L2

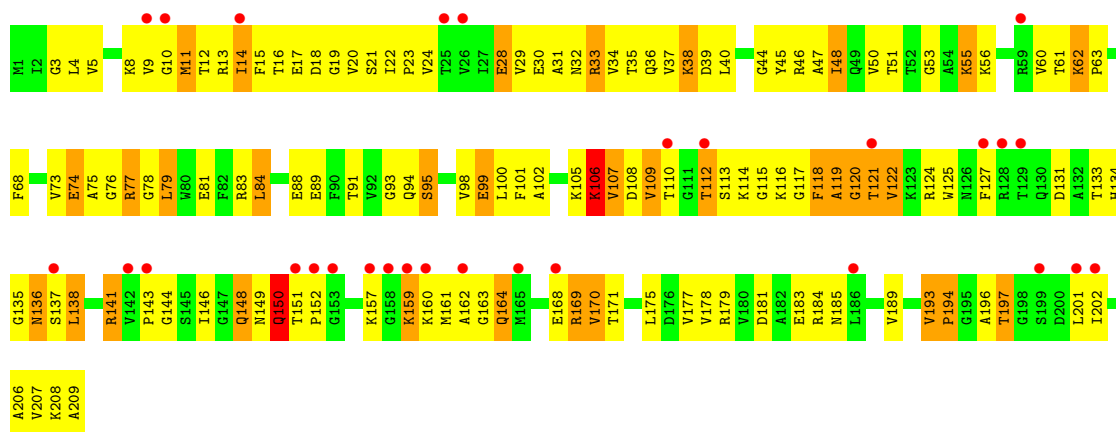


• Molecule 27: 50S ribosomal protein L3

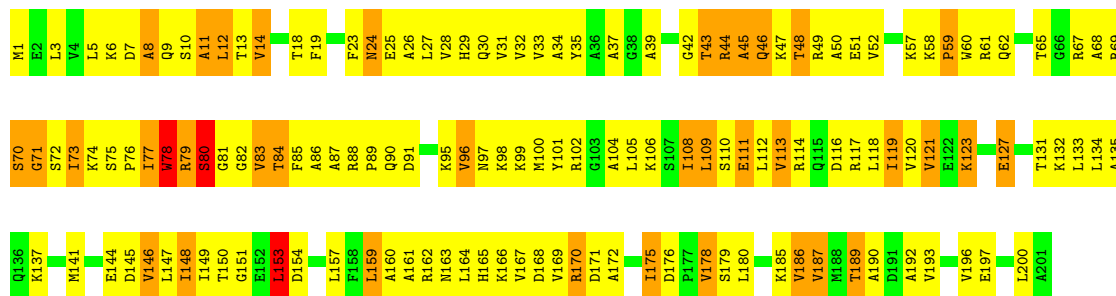
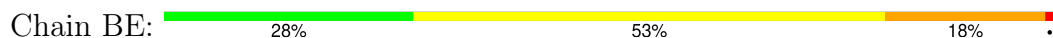




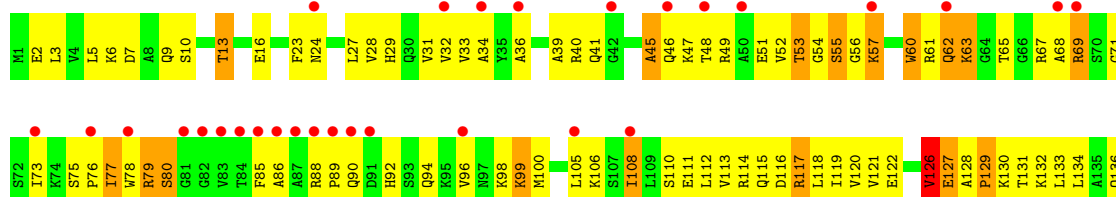
• Molecule 27: 50S ribosomal protein L3



• Molecule 28: 50S ribosomal protein L4

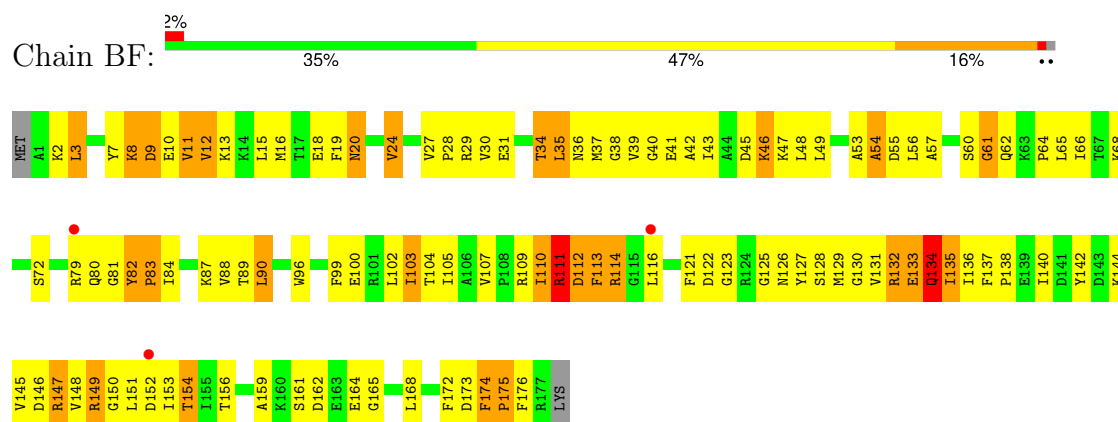


• Molecule 28: 50S ribosomal protein L4

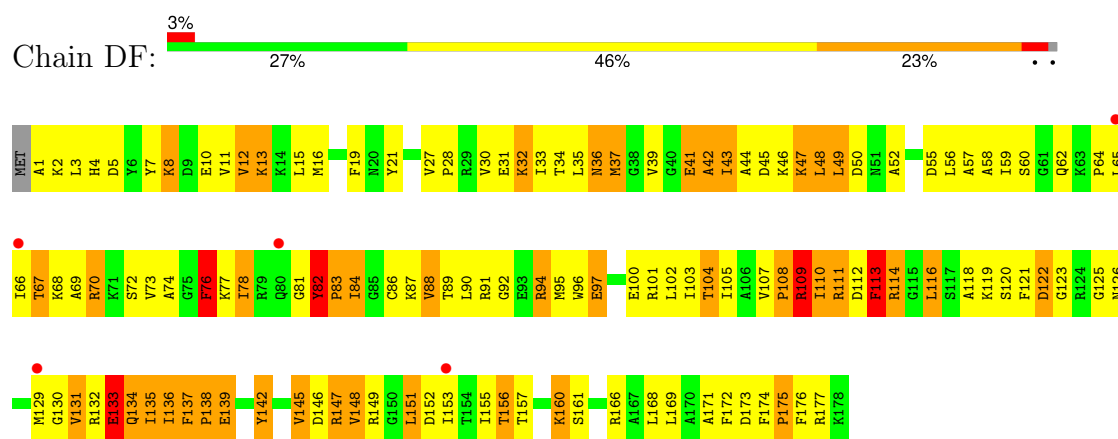




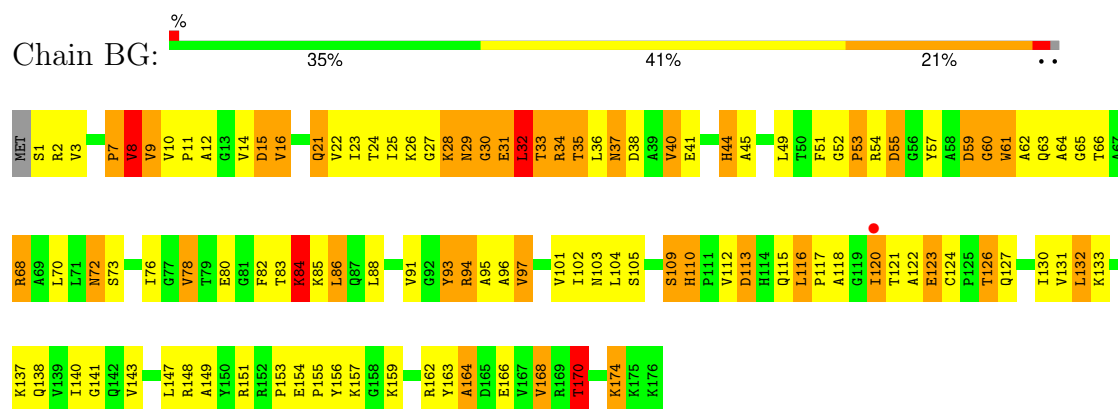
• Molecule 29: 50S ribosomal protein L5



• Molecule 29: 50S ribosomal protein L5

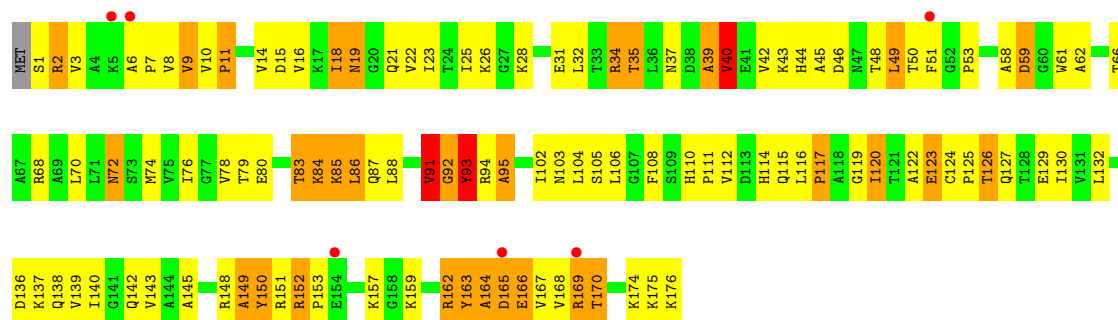


• Molecule 30: 50S ribosomal protein L6

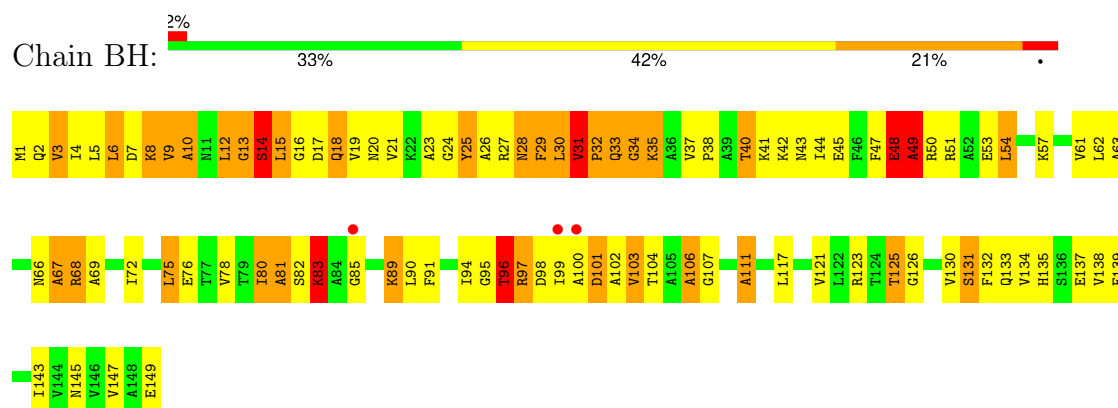


• Molecule 30: 50S ribosomal protein L6

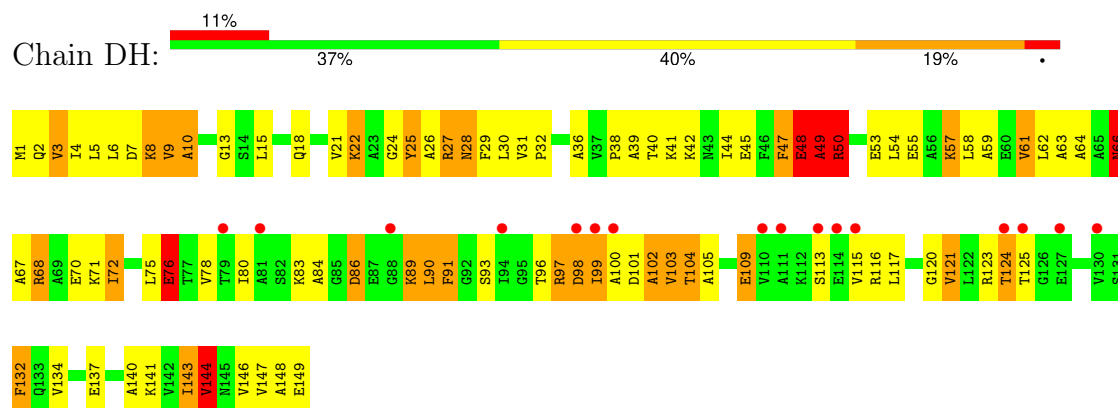




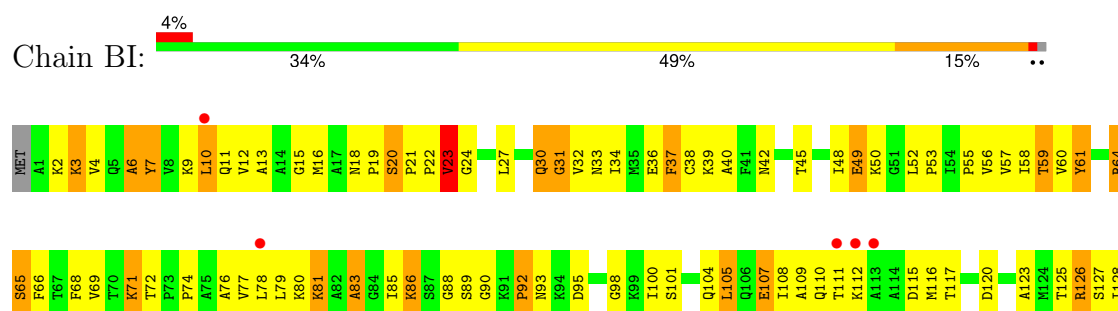
• Molecule 31: 50S ribosomal protein L9



• Molecule 31: 50S ribosomal protein L9

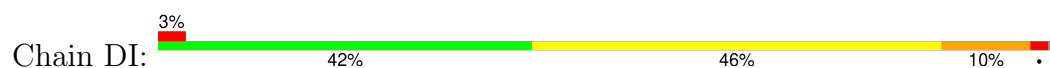


• Molecule 32: 50S ribosomal protein L11

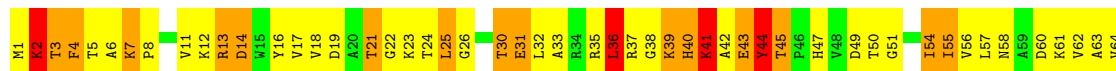
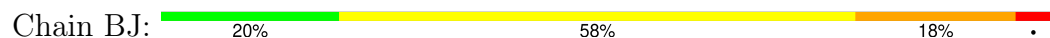




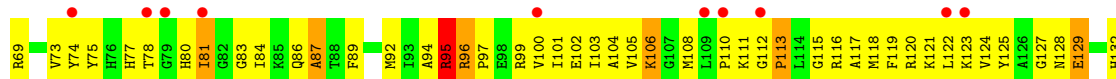
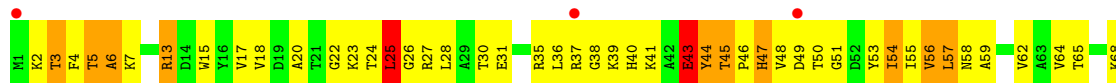
- Molecule 32: 50S ribosomal protein L11



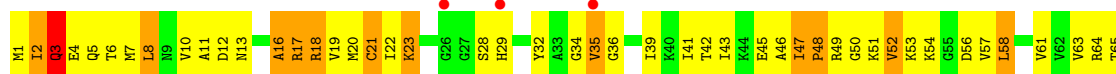
- Molecule 33: 50S ribosomal protein L13

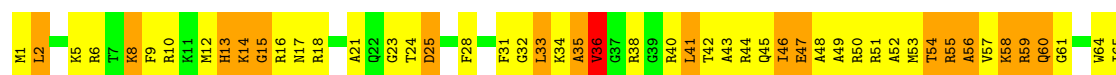


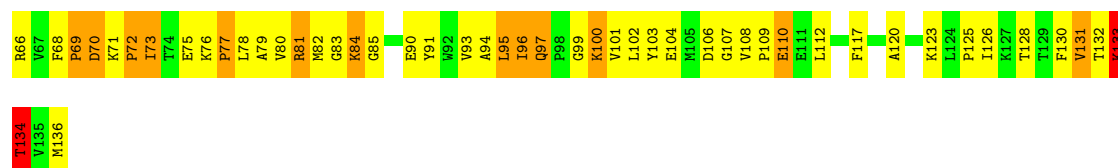
- Molecule 33: 50S ribosomal protein L13



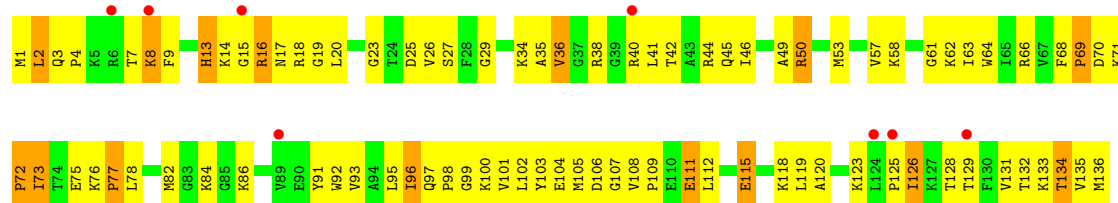
- Molecule 34: 50S ribosomal protein L14



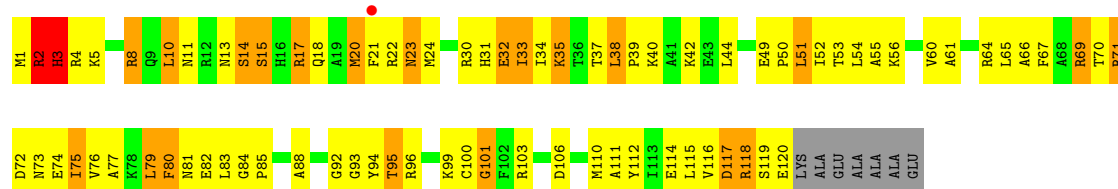




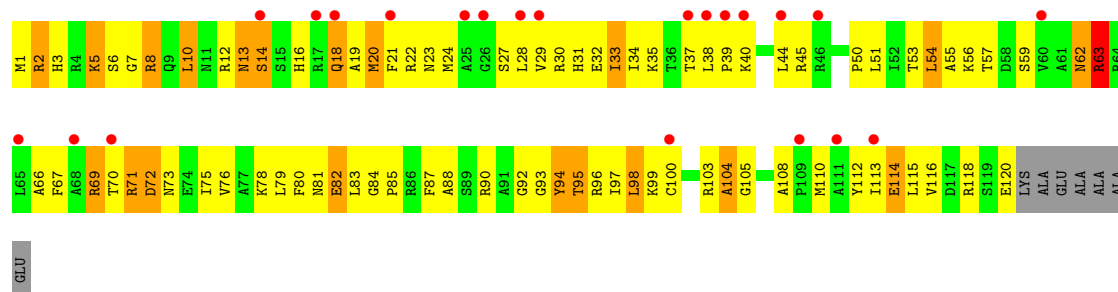
• Molecule 36: 50S ribosomal protein L16



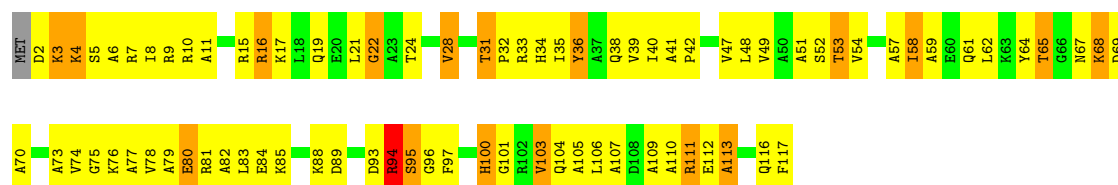
• Molecule 37: 50S ribosomal protein L17



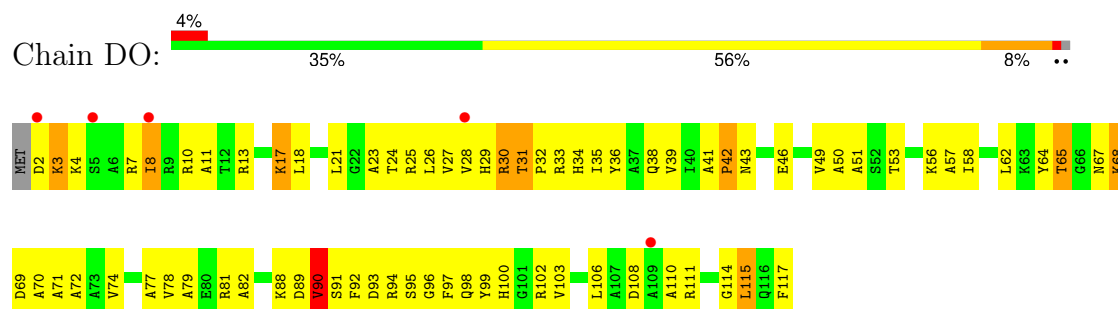
• Molecule 37: 50S ribosomal protein L17



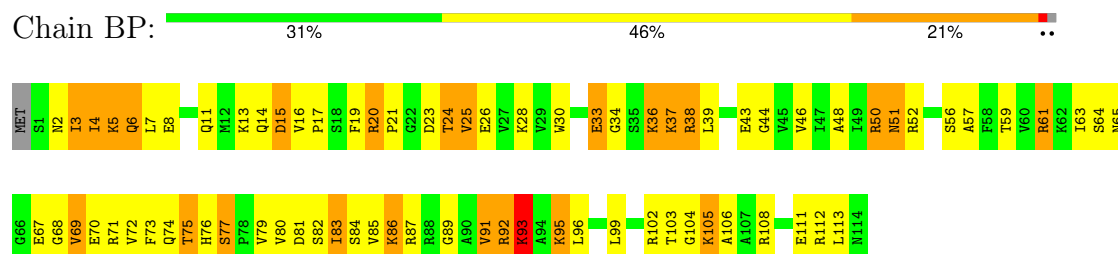
• Molecule 38: 50S ribosomal protein L18



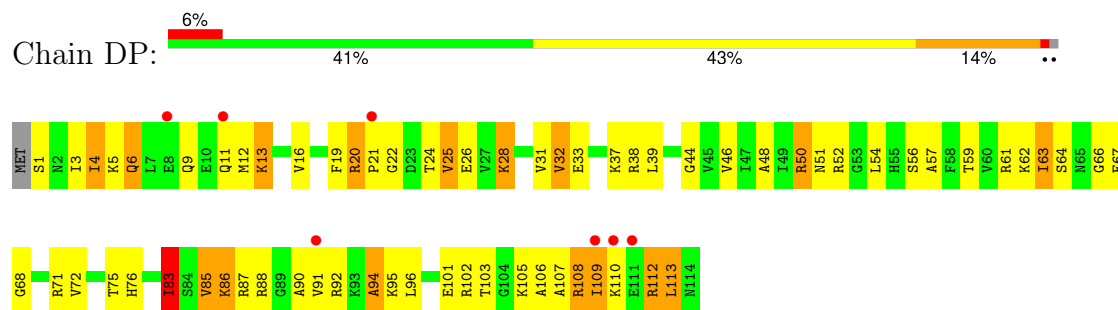
- Molecule 38: 50S ribosomal protein L18



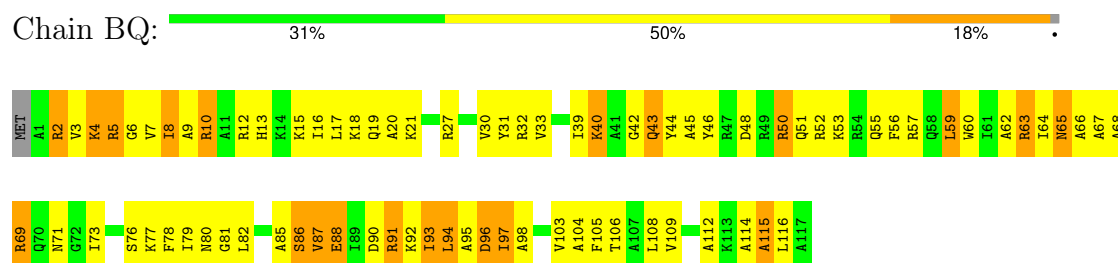
- Molecule 39: 50S ribosomal protein L19



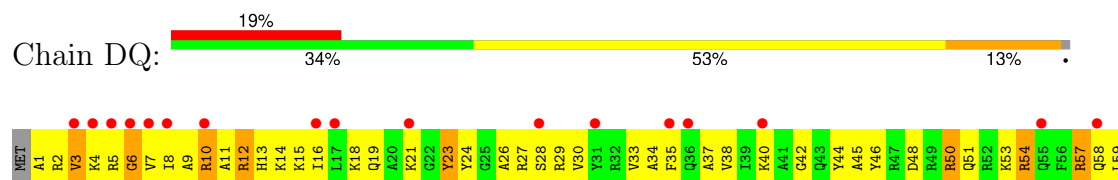
- Molecule 39: 50S ribosomal protein L19



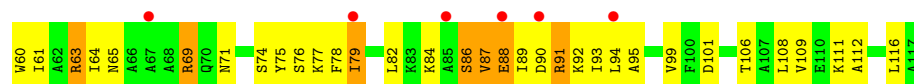
- Molecule 40: 50S ribosomal protein L20



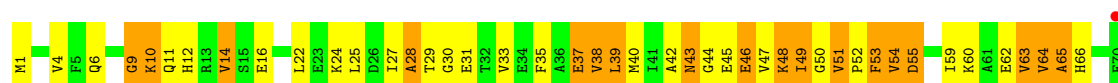
- Molecule 40: 50S ribosomal protein L20



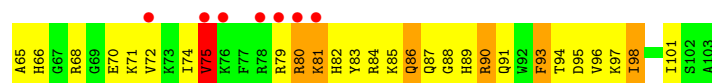
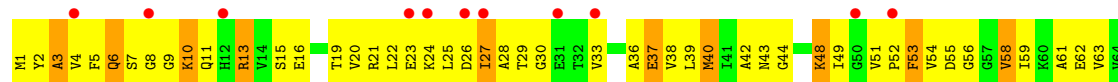




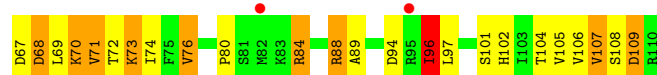
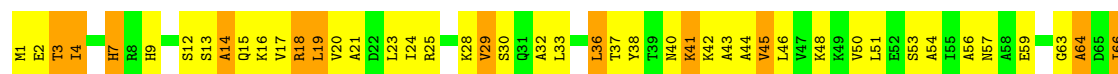
• Molecule 41: 50S ribosomal protein L21



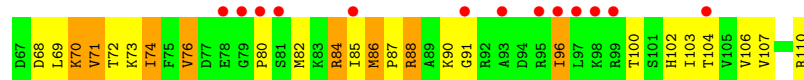
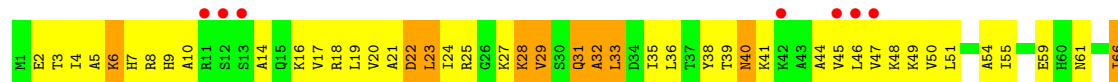
• Molecule 41: 50S ribosomal protein L21



• Molecule 42: 50S ribosomal protein L22

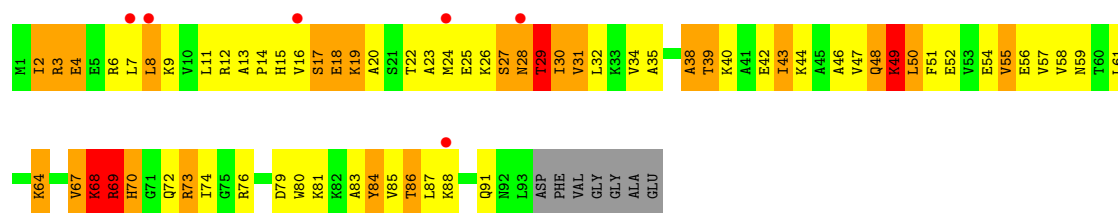


• Molecule 42: 50S ribosomal protein L22

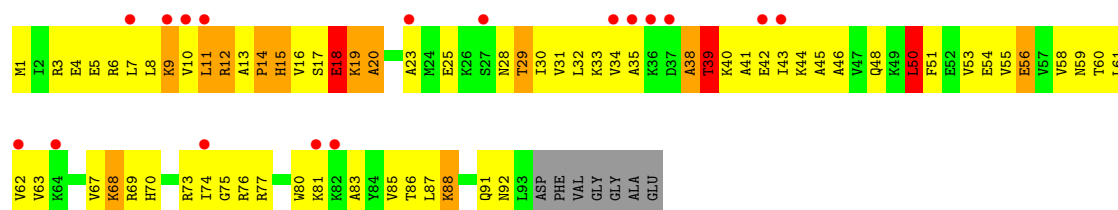


• Molecule 43: 50S ribosomal protein L23

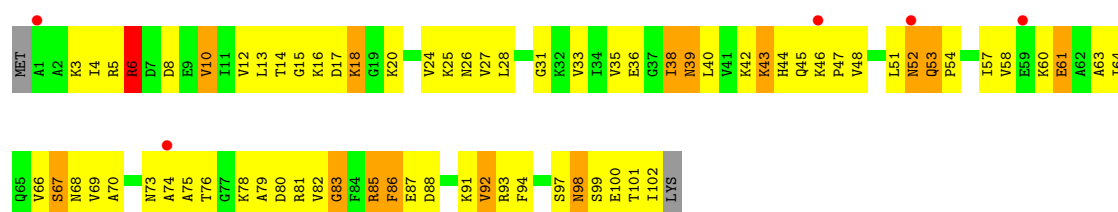




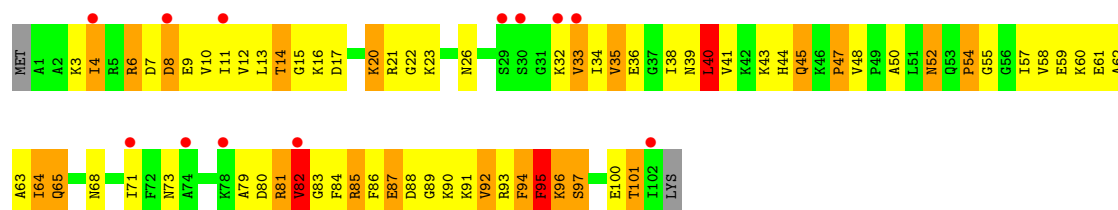
• Molecule 43: 50S ribosomal protein L23



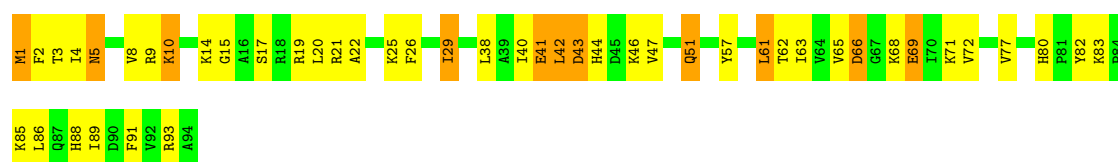
• Molecule 44: 50S ribosomal protein L24



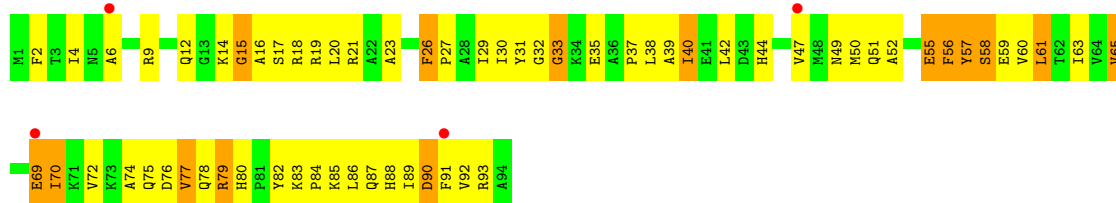
• Molecule 44: 50S ribosomal protein L24



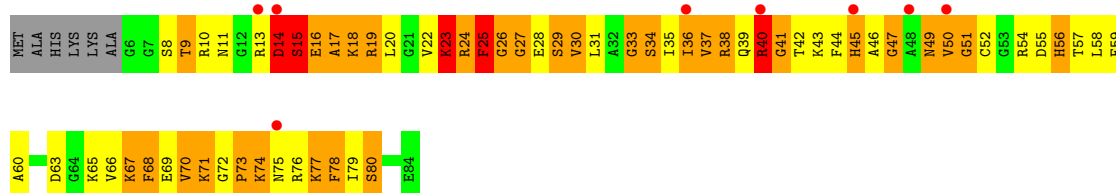
• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25



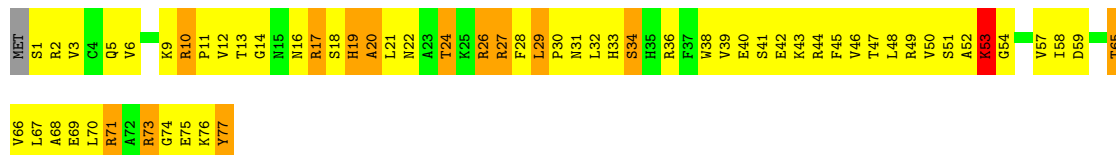
- Molecule 46: 50S ribosomal protein L27



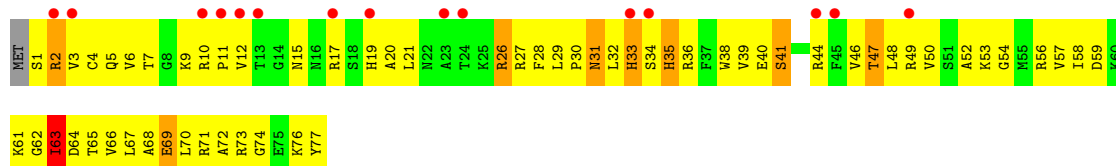
- Molecule 46: 50S ribosomal protein L27



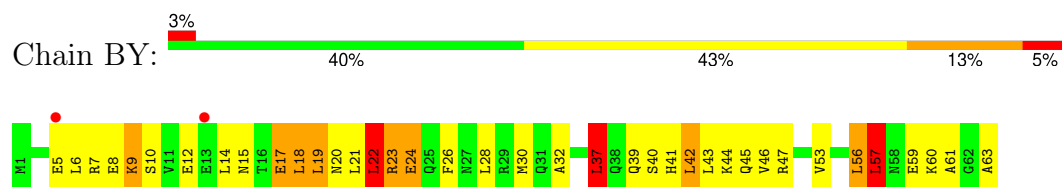
- Molecule 47: 50S ribosomal protein L28



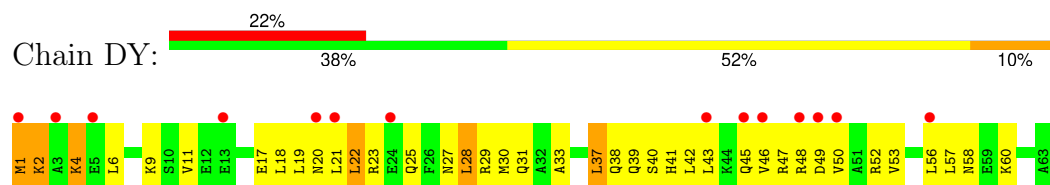
- Molecule 47: 50S ribosomal protein L28



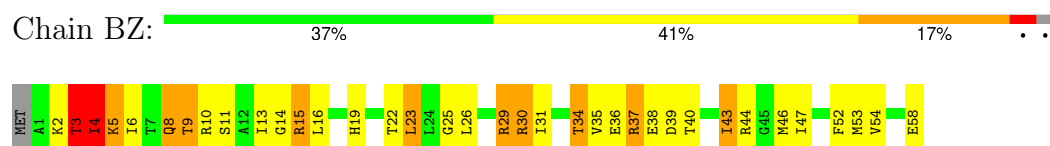
- Molecule 48: 50S ribosomal protein L29



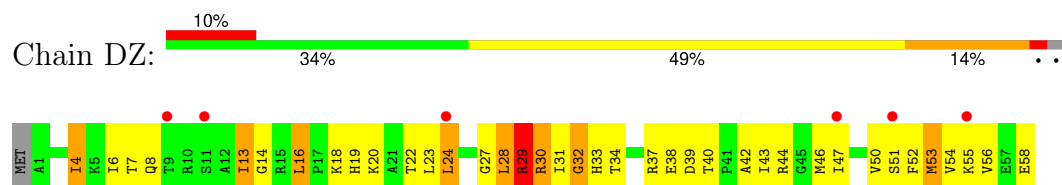
- Molecule 48: 50S ribosomal protein L29



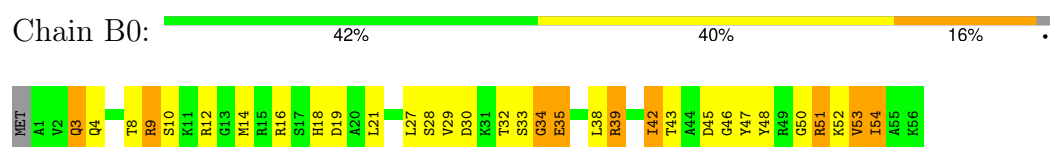
- Molecule 49: 50S ribosomal protein L30



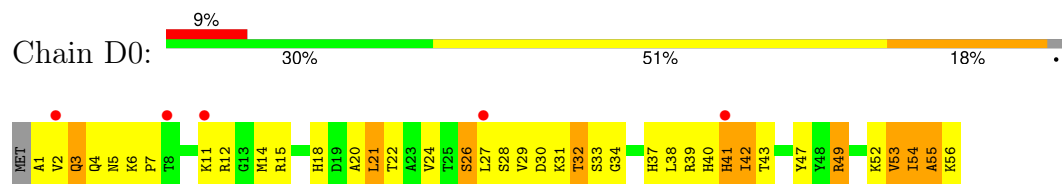
- Molecule 49: 50S ribosomal protein L30



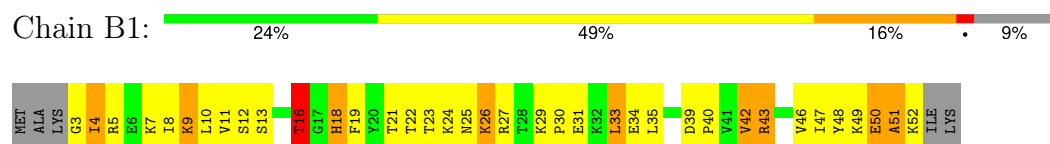
- Molecule 50: 50S ribosomal protein L32



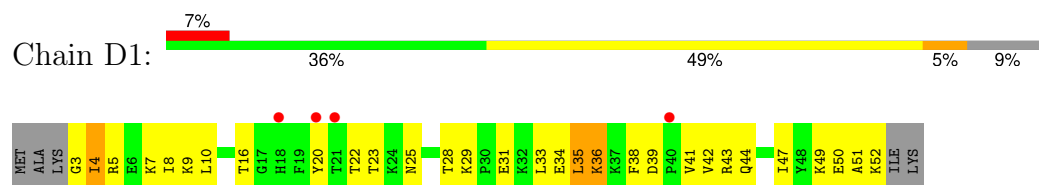
- Molecule 50: 50S ribosomal protein L32



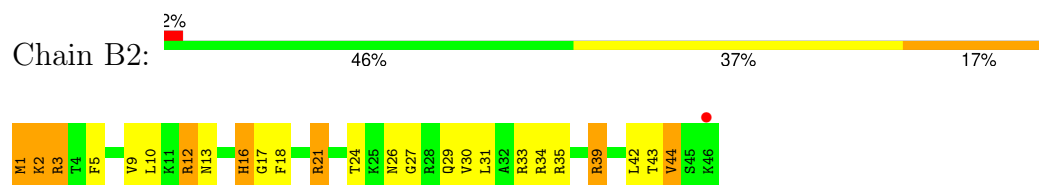
- Molecule 51: 50S ribosomal protein L33



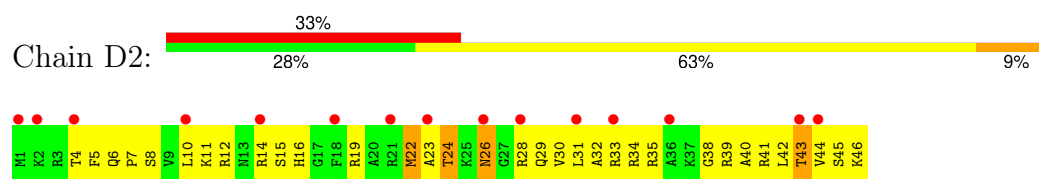
- Molecule 51: 50S ribosomal protein L33



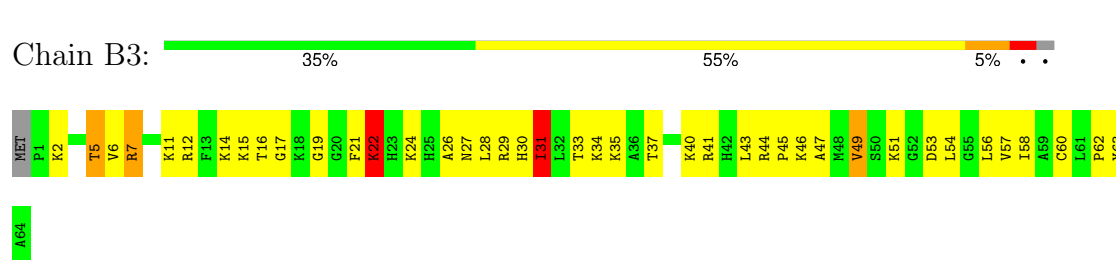
- Molecule 52: 50S ribosomal protein L34



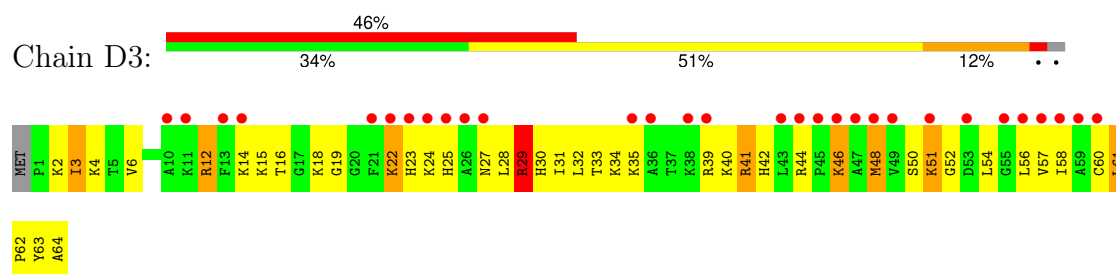
- Molecule 52: 50S ribosomal protein L34



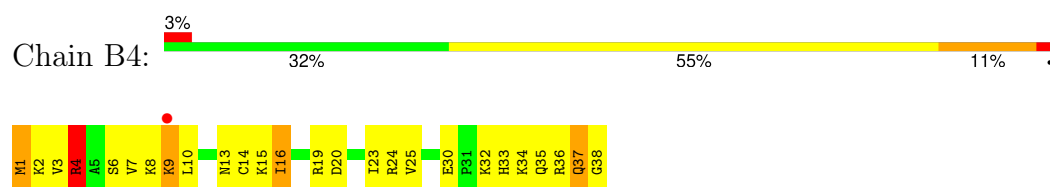
- Molecule 53: 50S ribosomal protein L35



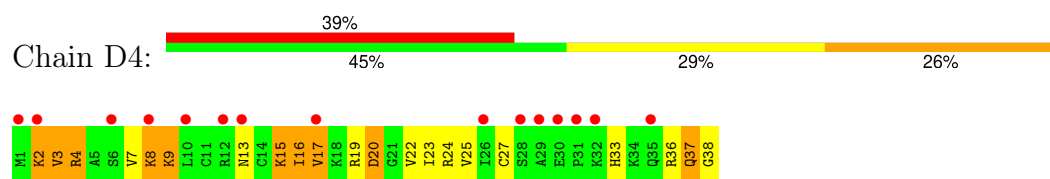
- Molecule 53: 50S ribosomal protein L35



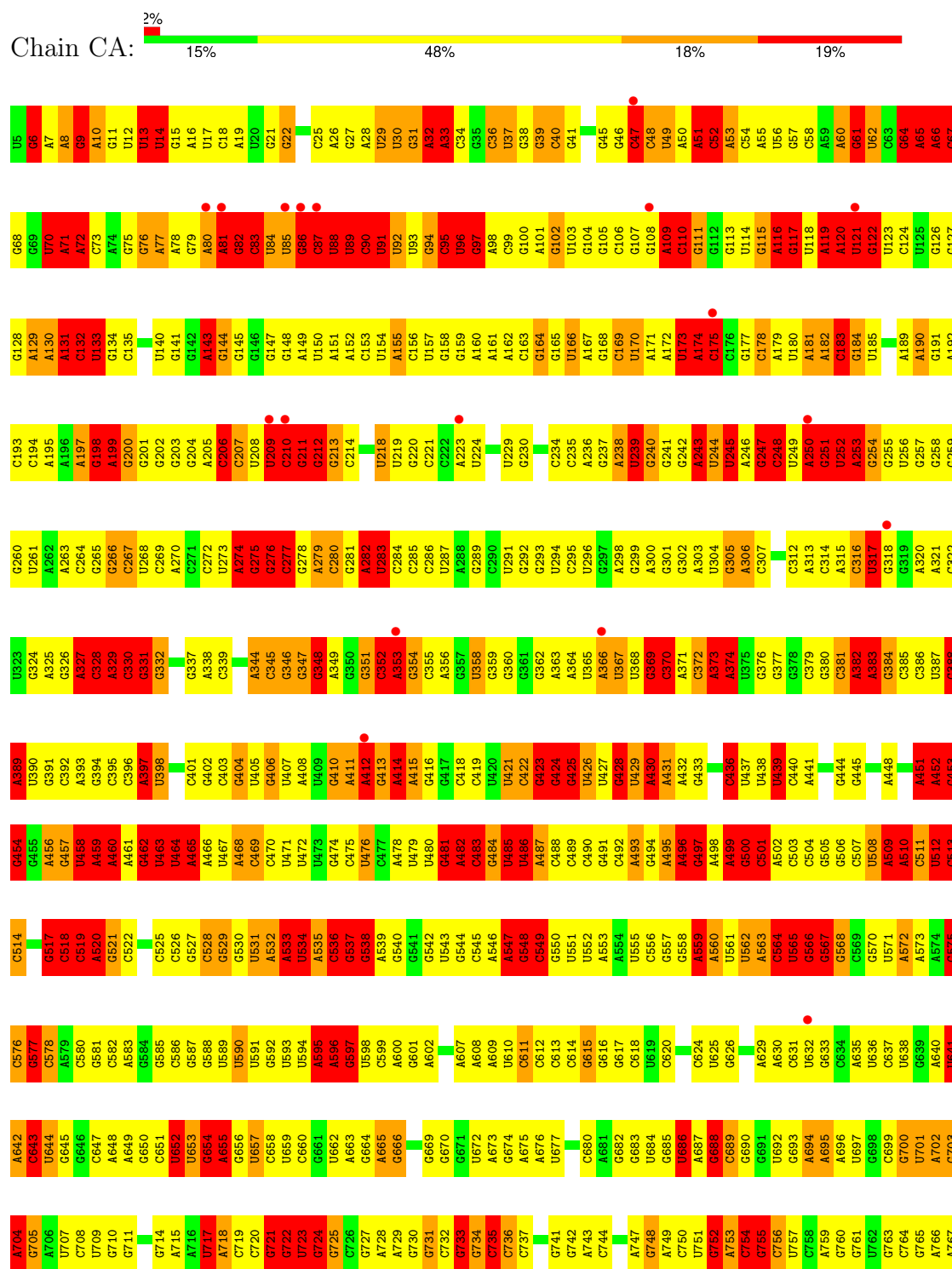
- Molecule 54: 50S ribosomal protein L36

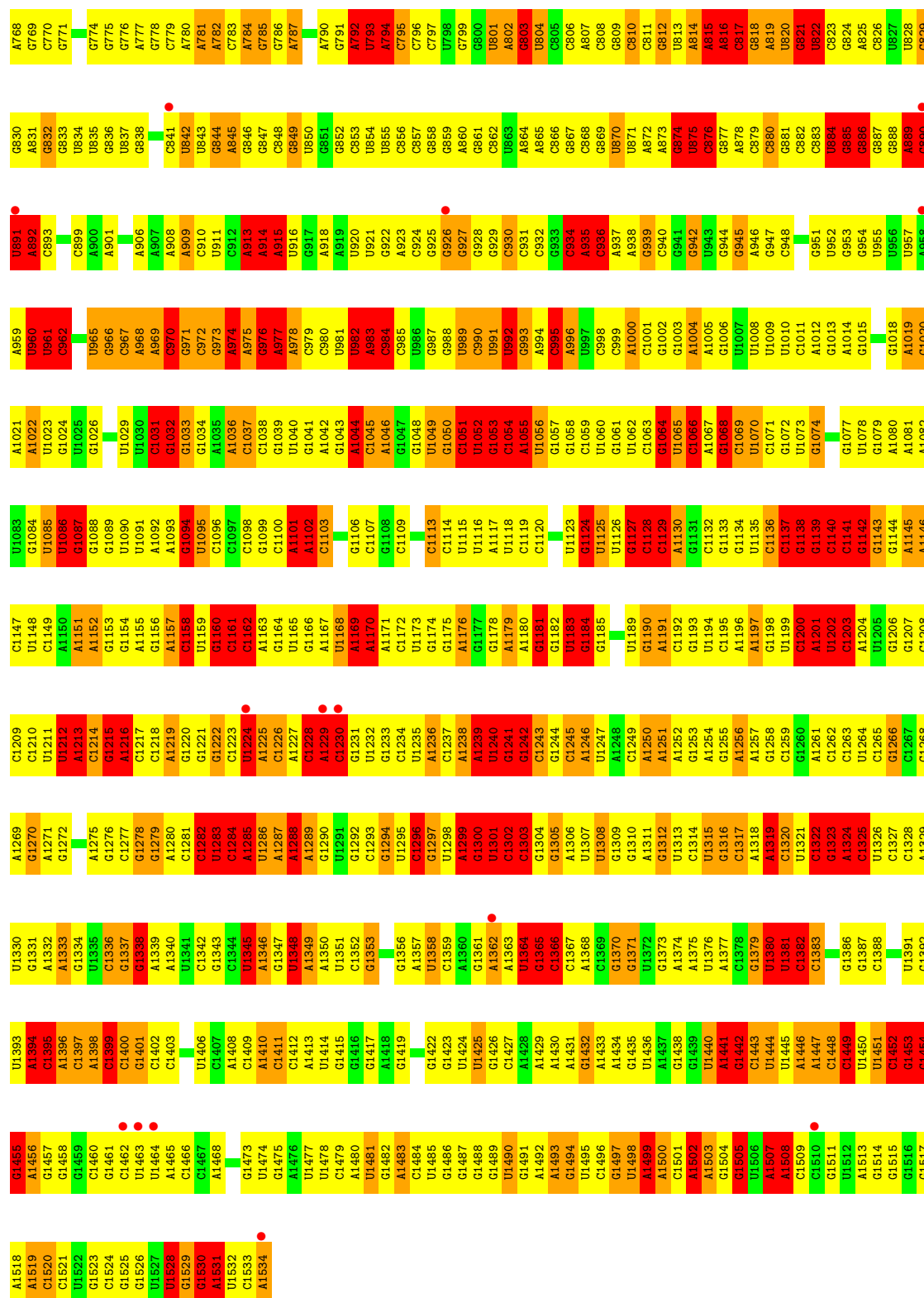


- Molecule 54: 50S ribosomal protein L36

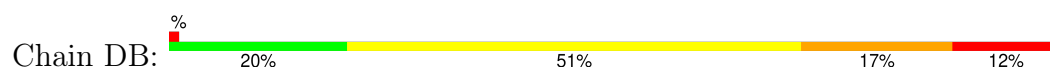


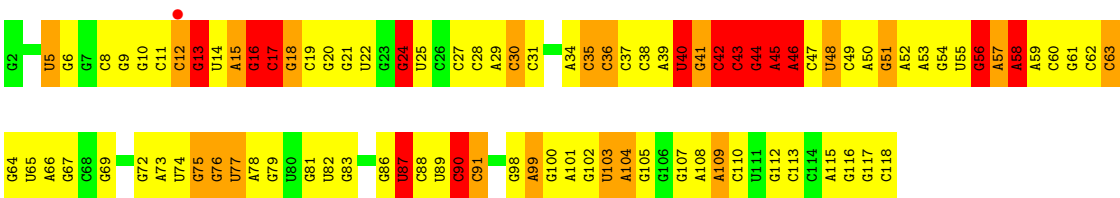
• Molecule 55: 16S rRNA





• Molecule 56: 5S rRNA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.227 , 0.268 0.235 , 0.275	Depositor DCC
$R_{free}$ test set	9161 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 87.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	286150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AB	0.25	0/1735	0.47	0/2338
1	CB	0.25	0/1735	0.46	0/2338
2	AC	0.27	0/1651	0.48	0/2225
2	CC	0.26	0/1651	0.47	0/2225
3	AD	0.27	0/1665	0.48	0/2227
3	CD	0.30	0/1665	0.50	0/2227
4	AE	0.30	0/1118	0.54	0/1504
4	CE	0.29	0/1118	0.53	0/1504
5	AF	0.26	0/835	0.46	0/1128
5	CF	0.26	0/835	0.46	0/1128
6	AG	0.25	0/1195	0.43	0/1602
6	CG	0.27	0/1187	0.50	0/1591
7	AH	0.27	0/989	0.50	0/1326
7	CH	0.25	0/989	0.47	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.25	0/1034	0.47	0/1375
9	AJ	0.25	0/796	0.48	0/1077
9	CJ	0.24	0/796	0.47	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.26	0/893	0.50	0/1205
11	AL	0.33	0/969	0.62	0/1300
11	CL	0.31	0/969	0.53	0/1300
12	AM	0.36	0/892	0.64	3/1193 (0.3%)
12	CM	0.38	0/884	0.53	0/1181
13	AN	0.26	0/785	0.48	0/1043
13	CN	0.25	0/780	0.43	0/1036
14	AO	0.26	0/722	0.48	0/964
14	CO	0.24	0/722	0.46	0/964
15	AP	0.27	0/659	0.46	0/884
15	CP	0.27	0/648	0.47	0/870
16	AQ	0.33	0/657	0.55	0/881
16	CQ	0.26	0/657	0.46	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.25	0/462	0.48	0/621
17	CR	0.27	0/462	0.49	0/621
18	AS	0.24	0/652	0.43	0/877
18	CS	0.23	0/652	0.46	0/877
19	AT	0.29	0/671	0.51	0/888
19	CT	0.24	0/671	0.44	0/888
20	AU	0.27	0/430	0.46	0/570
20	CU	0.29	0/430	0.54	0/570
21	AA	0.55	1/36834 (0.0%)	1.44	678/57462 (1.2%)
22	AV	0.59	0/408	1.14	1/634 (0.2%)
22	AX	0.52	0/408	1.04	0/634
22	CV	0.56	0/408	1.14	0/634
22	CX	0.41	0/408	0.82	0/634
23	AW	0.88	0/131	1.88	5/200 (2.5%)
23	CW	0.73	0/131	1.93	7/200 (3.5%)
24	BA	0.76	12/68626 (0.0%)	1.69	1758/107056 (1.6%)
24	DA	0.53	1/68314 (0.0%)	1.46	1365/106569 (1.3%)
25	BB	0.66	0/2828	1.67	74/4410 (1.7%)
26	BC	0.45	0/2121	0.72	1/2852 (0.0%)
26	DC	0.33	0/2121	0.54	0/2852
27	BD	0.50	0/1586	0.75	1/2134 (0.0%)
27	DD	0.31	0/1586	0.55	0/2134
28	BE	0.44	0/1571	0.67	0/2113
28	DE	0.25	0/1571	0.47	0/2113
29	BF	0.41	0/1434	0.68	3/1926 (0.2%)
29	DF	0.35	0/1444	0.73	5/1937 (0.3%)
30	BG	0.43	0/1343	0.65	0/1816
30	DG	0.23	0/1343	0.46	0/1816
31	BH	0.70	6/1122 (0.5%)	0.83	6/1515 (0.4%)
31	DH	0.53	3/1122 (0.3%)	0.67	3/1515 (0.2%)
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.23	0/1046	0.44	0/1410
33	BJ	0.55	0/1152	0.75	0/1551
33	DJ	0.28	0/1152	0.55	0/1551
34	BK	0.55	0/947	0.83	0/1268
34	DK	0.31	0/947	0.54	0/1268
35	BL	0.42	0/1054	0.77	1/1403 (0.1%)
35	DL	0.27	0/1054	0.51	0/1403
36	BM	0.51	0/1093	0.77	1/1460 (0.1%)
36	DM	0.31	0/1093	0.48	0/1460
37	BN	0.55	0/973	0.79	0/1301
37	DN	0.27	0/973	0.49	0/1301
38	BO	0.42	0/902	0.63	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DO	0.24	0/902	0.44	0/1209
39	BP	0.51	0/929	0.77	0/1242
39	DP	0.28	0/929	0.49	0/1242
40	BQ	0.60	0/960	0.71	0/1278
40	DQ	0.28	0/960	0.46	0/1278
41	BR	0.56	0/829	0.85	1/1107 (0.1%)
41	DR	0.28	0/829	0.50	0/1107
42	BS	0.50	0/864	0.75	0/1156
42	DS	0.29	0/864	0.54	0/1156
43	BT	0.48	0/744	0.70	0/994
43	DT	0.25	0/744	0.49	0/994
44	BU	0.41	0/787	0.70	0/1051
44	DU	0.25	0/787	0.47	0/1051
45	BV	0.48	0/766	0.66	0/1025
45	DV	0.38	0/766	0.54	0/1025
46	BW	0.51	0/603	0.76	0/797
46	DW	0.26	0/603	0.47	0/797
47	BX	0.42	0/635	0.67	0/848
47	DX	0.30	0/635	0.55	0/848
48	BY	0.40	0/510	0.66	0/677
48	DY	0.23	0/510	0.44	0/677
49	BZ	0.52	0/453	0.77	0/605
49	DZ	0.28	0/453	0.51	0/605
50	B0	0.45	0/450	0.79	0/599
50	D0	0.28	0/450	0.51	0/599
51	B1	0.40	0/416	0.63	0/554
51	D1	0.28	0/416	0.46	0/554
52	B2	0.47	0/380	0.73	0/498
52	D2	0.28	0/380	0.55	0/498
53	B3	0.51	0/513	0.76	0/676
53	D3	0.26	0/513	0.51	0/676
54	B4	0.47	0/303	0.76	0/397
54	D4	0.30	0/303	0.49	0/397
55	CA	0.53	0/36762	1.45	712/57350 (1.2%)
56	DB	0.52	0/2803	1.35	52/4371 (1.2%)
All	All	0.55	23/308631 (0.0%)	1.35	4677/461501 (1.0%)

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
12	AM	0	1
27	BD	0	1
31	BH	0	2
31	DH	0	3
37	BN	0	1
All	All	0	8

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-13.92	1.29	1.37
31	BH	48	GLU	C-O	9.51	1.41	1.23
24	BA	2451	A	C8-N7	9.03	1.37	1.31
31	DH	49	ALA	CA-CB	-7.88	1.35	1.52
31	BH	48	GLU	CA-CB	6.93	1.69	1.53

The worst 5 of 4677 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	2447	G	C6-N1-C2	-22.51	111.59	125.10
24	BA	2451	A	C5-N7-C8	-17.23	95.28	103.90
24	BA	2347	C	N1-C1'-C2'	-16.79	92.17	114.00
24	BA	790	U	P-O3'-C3'	-16.12	100.36	119.70
25	BB	88	C	O4'-C1'-N1	-15.24	96.01	108.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AM	70	ARG	Peptide
27	BD	10	GLY	Peptide
31	BH	48	GLU	Mainchain
31	BH	49	ALA	Mainchain
37	BN	101	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	253	0
1	CB	1704	0	1732	203	0
2	AC	1624	0	1699	133	0
2	CC	1624	0	1699	149	0
3	AD	1643	0	1710	139	0
3	CD	1643	0	1710	139	0
4	AE	1105	0	1148	196	0
4	CE	1105	0	1148	127	0
5	AF	817	0	808	91	0
5	CF	817	0	808	76	0
6	AG	1181	0	1240	100	0
6	CG	1174	0	1230	154	0
7	AH	979	0	1034	107	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	122	0
8	CI	1022	0	1070	108	0
9	AJ	786	0	828	69	0
9	CJ	786	0	828	114	0
10	AK	877	0	887	103	0
10	CK	877	0	887	82	0
11	AL	955	0	1019	97	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	69	0
12	CM	876	0	937	123	0
13	AN	774	0	827	72	0
13	CN	769	0	822	83	0
14	AO	714	0	737	50	0
14	CO	714	0	737	40	0
15	AP	649	0	666	63	0
15	CP	638	0	656	56	0
16	AQ	648	0	691	70	0
16	CQ	648	0	691	59	0
17	AR	455	0	478	36	0
17	CR	455	0	478	41	0
18	AS	637	0	665	42	0
18	CS	637	0	665	79	0
19	AT	665	0	714	56	0
19	CT	665	0	714	58	0
20	AU	425	0	449	65	0
20	CU	425	0	449	70	0
21	AA	32895	0	16553	1800	0
22	AV	365	0	185	24	0
22	AX	365	0	185	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	365	0	185	26	0
22	CX	365	0	185	11	0
23	AW	120	0	61	8	0
23	CW	120	0	61	4	0
24	BA	61274	0	30819	3133	0
24	DA	60995	0	30679	3843	0
25	BB	2529	0	1281	109	0
26	BC	2082	0	2157	226	0
26	DC	2082	0	2157	230	0
27	BD	1565	0	1616	200	0
27	DD	1565	0	1616	162	0
28	BE	1552	0	1619	158	0
28	DE	1552	0	1619	170	0
29	BF	1410	0	1447	144	0
29	DF	1420	0	1460	183	0
30	BG	1323	0	1374	149	0
30	DG	1323	0	1374	116	0
31	BH	1111	0	1148	108	0
31	DH	1111	0	1148	100	0
32	BI	1032	0	1088	116	0
32	DI	1032	0	1088	69	0
33	BJ	1129	0	1162	160	0
33	DJ	1129	0	1162	122	0
34	BK	938	0	1012	102	0
34	DK	938	0	1012	114	0
35	BL	1045	0	1117	133	0
35	DL	1045	0	1117	130	0
36	BM	1074	0	1157	129	0
36	DM	1074	0	1157	96	0
37	BN	960	0	1000	102	0
37	DN	960	0	1000	107	0
38	BO	892	0	923	82	0
38	DO	892	0	923	90	0
39	BP	917	0	965	120	0
39	DP	917	0	965	87	0
40	BQ	947	0	1022	147	0
40	DQ	947	0	1022	120	0
41	BR	816	0	839	102	0
41	DR	816	0	839	90	0
42	BS	857	0	922	89	0
42	DS	857	0	922	83	0
43	BT	738	0	807	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DT	738	0	807	96	0
44	BU	779	0	834	65	0
44	DU	779	0	834	93	0
45	BV	753	0	780	54	0
45	DV	753	0	780	98	0
46	BW	596	0	610	179	0
46	DW	596	0	610	105	0
47	BX	625	0	655	68	0
47	DX	625	0	655	76	0
48	BY	509	0	543	45	0
48	DY	509	0	543	55	0
49	BZ	449	0	491	41	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	36	0
50	D0	444	0	461	63	0
51	B1	409	0	440	43	0
51	D1	409	0	440	33	0
52	B2	377	0	418	28	0
52	D2	377	0	418	42	0
53	B3	504	0	574	41	0
53	D3	504	0	574	54	0
54	B4	302	0	340	40	0
54	D4	302	0	340	27	0
55	CA	32831	0	16521	2003	0
56	DB	2507	0	1270	160	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	D4	1	0	0	0	0
57	DA	132	0	0	0	0
57	DB	1	0	0	0	0
57	DC	2	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	196	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	0	0
59	AN	6	0	0	1	0
59	AT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AU	1	0	0	0	0
59	B2	1	0	0	0	0
59	B3	3	0	0	0	0
59	B4	2	0	0	0	0
59	BA	615	0	0	21	0
59	BB	20	0	0	1	0
59	BC	8	0	0	1	0
59	BD	3	0	0	4	0
59	BE	1	0	0	0	0
59	BL	3	0	0	0	0
59	BN	3	0	0	0	0
59	BT	1	0	0	1	0
59	CA	195	0	0	6	0
59	CE	4	0	0	0	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	600	0	0	17	0
59	DB	4	0	0	0	0
59	DC	12	0	0	0	0
59	DD	2	0	0	0	0
59	DE	3	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	6	0	0	0	0
59	DN	2	0	0	1	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	286150	0	191700	19249	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 41.

The worst 5 of 19249 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)
12:AM:67:ASP:O	12:AM:70:ARG:HD2	1.23	1.31
55:CA:1213:A:O2'	55:CA:1214:C:H5'	1.29	1.25
24:DA:604:G:O2'	24:DA:605:G:H5'	1.40	1.19
40:BQ:63:ARG:NH1	40:BQ:96:ASP:HA	1.56	1.18
24:DA:297:G:H5''	44:DU:84:PHE:HB2	1.26	1.18

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	216/241 (90%)	119 (55%)	69 (32%)	28 (13%)	0	4
1	CB	216/241 (90%)	144 (67%)	50 (23%)	22 (10%)	0	7
2	AC	204/233 (88%)	140 (69%)	48 (24%)	16 (8%)	1	11
2	CC	204/233 (88%)	136 (67%)	52 (26%)	16 (8%)	1	11
3	AD	203/206 (98%)	143 (70%)	43 (21%)	17 (8%)	0	9
3	CD	203/206 (98%)	136 (67%)	46 (23%)	21 (10%)	0	6
4	AE	148/167 (89%)	105 (71%)	27 (18%)	16 (11%)	0	5
4	CE	148/167 (89%)	100 (68%)	34 (23%)	14 (10%)	0	8
5	AF	98/135 (73%)	68 (69%)	22 (22%)	8 (8%)	1	9
5	CF	98/135 (73%)	65 (66%)	27 (28%)	6 (6%)	1	16
6	AG	149/179 (83%)	103 (69%)	36 (24%)	10 (7%)	1	14
6	CG	148/179 (83%)	84 (57%)	44 (30%)	20 (14%)	0	3
7	AH	127/130 (98%)	90 (71%)	27 (21%)	10 (8%)	1	11
7	CH	127/130 (98%)	88 (69%)	30 (24%)	9 (7%)	1	13
8	AI	125/130 (96%)	81 (65%)	32 (26%)	12 (10%)	0	7
8	CI	125/130 (96%)	88 (70%)	33 (26%)	4 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	16 (17%)	11 (12%)	0	4
9	CJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	0	4
10	AK	115/129 (89%)	84 (73%)	22 (19%)	9 (8%)	1	11
10	CK	115/129 (89%)	86 (75%)	19 (16%)	10 (9%)	0	9
11	AL	121/124 (98%)	82 (68%)	27 (22%)	12 (10%)	0	7
11	CL	121/124 (98%)	86 (71%)	26 (22%)	9 (7%)	1	12
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	1	15
12	CM	111/118 (94%)	71 (64%)	28 (25%)	12 (11%)	0	5
13	AN	92/101 (91%)	63 (68%)	18 (20%)	11 (12%)	0	4
13	CN	91/101 (90%)	62 (68%)	24 (26%)	5 (6%)	1	17
14	AO	86/89 (97%)	64 (74%)	20 (23%)	2 (2%)	5	31
14	CO	86/89 (97%)	67 (78%)	19 (22%)	0	100	100
15	AP	80/82 (98%)	52 (65%)	22 (28%)	6 (8%)	1	12
15	CP	78/82 (95%)	52 (67%)	20 (26%)	6 (8%)	1	11
16	AQ	78/84 (93%)	47 (60%)	20 (26%)	11 (14%)	0	3
16	CQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	1	15
17	AR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	16
17	CR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	1	16
18	AS	77/92 (84%)	61 (79%)	13 (17%)	3 (4%)	2	22
18	CS	77/92 (84%)	55 (71%)	20 (26%)	2 (3%)	4	29
19	AT	83/87 (95%)	63 (76%)	14 (17%)	6 (7%)	1	13
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	3	24
20	AU	49/71 (69%)	26 (53%)	16 (33%)	7 (14%)	0	3
20	CU	49/71 (69%)	23 (47%)	17 (35%)	9 (18%)	0	1
26	BC	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	0	5
26	DC	269/273 (98%)	169 (63%)	73 (27%)	27 (10%)	0	7
27	BD	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	3
27	DD	207/209 (99%)	129 (62%)	48 (23%)	30 (14%)	0	3
28	BE	199/201 (99%)	138 (69%)	41 (21%)	20 (10%)	0	7
28	DE	199/201 (99%)	129 (65%)	49 (25%)	21 (11%)	0	6
29	BF	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	94 (53%)	43 (24%)	39 (22%)	0	0
30	BG	174/177 (98%)	114 (66%)	34 (20%)	26 (15%)	0	3
30	DG	174/177 (98%)	109 (63%)	36 (21%)	29 (17%)	0	2
31	BH	147/149 (99%)	63 (43%)	53 (36%)	31 (21%)	0	1
31	DH	147/149 (99%)	78 (53%)	48 (33%)	21 (14%)	0	3
32	BI	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	0	8
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	3
33	BJ	140/142 (99%)	100 (71%)	22 (16%)	18 (13%)	0	4
33	DJ	140/142 (99%)	95 (68%)	31 (22%)	14 (10%)	0	7
34	BK	120/123 (98%)	86 (72%)	17 (14%)	17 (14%)	0	3
34	DK	120/123 (98%)	79 (66%)	22 (18%)	19 (16%)	0	2
35	BL	141/144 (98%)	106 (75%)	23 (16%)	12 (8%)	0	9
35	DL	141/144 (98%)	80 (57%)	42 (30%)	19 (14%)	0	3
36	BM	134/136 (98%)	95 (71%)	16 (12%)	23 (17%)	0	2
36	DM	134/136 (98%)	89 (66%)	32 (24%)	13 (10%)	0	7
37	BN	118/127 (93%)	85 (72%)	23 (20%)	10 (8%)	0	9
37	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	0	5
38	BO	114/117 (97%)	84 (74%)	20 (18%)	10 (9%)	0	9
38	DO	114/117 (97%)	80 (70%)	28 (25%)	6 (5%)	1	18
39	BP	112/115 (97%)	74 (66%)	23 (20%)	15 (13%)	0	3
39	DP	112/115 (97%)	67 (60%)	30 (27%)	15 (13%)	0	3
40	BQ	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	16
40	DQ	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	1	13
41	BR	101/103 (98%)	75 (74%)	14 (14%)	12 (12%)	0	4
41	DR	101/103 (98%)	71 (70%)	20 (20%)	10 (10%)	0	7
42	BS	108/110 (98%)	81 (75%)	20 (18%)	7 (6%)	1	15
42	DS	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	0	8
43	BT	91/100 (91%)	55 (60%)	20 (22%)	16 (18%)	0	2
43	DT	91/100 (91%)	47 (52%)	30 (33%)	14 (15%)	0	3
44	BU	100/104 (96%)	68 (68%)	16 (16%)	16 (16%)	0	2
44	DU	100/104 (96%)	49 (49%)	29 (29%)	22 (22%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	12	43
45	DV	92/94 (98%)	59 (64%)	25 (27%)	8 (9%)	0	9
46	BW	77/85 (91%)	32 (42%)	18 (23%)	27 (35%)	0	0
46	DW	77/85 (91%)	34 (44%)	25 (32%)	18 (23%)	0	0
47	BX	75/78 (96%)	58 (77%)	12 (16%)	5 (7%)	1	14
47	DX	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	0	8
48	BY	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	0	4
48	DY	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	1	9
49	BZ	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	1	17
49	DZ	56/59 (95%)	35 (62%)	14 (25%)	7 (12%)	0	4
50	B0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	4
50	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	4
51	B1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	3
51	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	0	9
52	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	2	20
52	D2	44/46 (96%)	30 (68%)	9 (20%)	5 (11%)	0	5
53	B3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	3	26
53	D3	62/65 (95%)	42 (68%)	15 (24%)	5 (8%)	1	10
54	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	0	9
54	D4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	2
All	All	11238/11970 (94%)	7515 (67%)	2516 (22%)	1207 (11%)	0	5

5 of 1207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	37	VAL
1	AB	71	THR
1	AB	125	PHE

### 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	
1	AB	180/199 (90%)	147 (82%)	33 (18%)	1	9
1	CB	180/199 (90%)	158 (88%)	22 (12%)	4	20
2	AC	170/190 (90%)	148 (87%)	22 (13%)	3	19
2	CC	170/190 (90%)	146 (86%)	24 (14%)	3	17
3	AD	172/173 (99%)	147 (86%)	25 (14%)	2	16
3	CD	172/173 (99%)	152 (88%)	20 (12%)	4	22
4	AE	113/126 (90%)	93 (82%)	20 (18%)	1	10
4	CE	113/126 (90%)	100 (88%)	13 (12%)	4	22
5	AF	87/116 (75%)	75 (86%)	12 (14%)	3	17
5	CF	87/116 (75%)	74 (85%)	13 (15%)	2	15
6	AG	124/147 (84%)	117 (94%)	7 (6%)	17	45
6	CG	123/147 (84%)	95 (77%)	28 (23%)	0	5
7	AH	104/105 (99%)	92 (88%)	12 (12%)	4	22
7	CH	104/105 (99%)	91 (88%)	13 (12%)	3	19
8	AI	105/107 (98%)	90 (86%)	15 (14%)	2	16
8	CI	105/107 (98%)	91 (87%)	14 (13%)	3	18
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	17
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	5	25
10	AK	90/99 (91%)	80 (89%)	10 (11%)	5	24
10	CK	90/99 (91%)	80 (89%)	10 (11%)	5	24
11	AL	103/104 (99%)	85 (82%)	18 (18%)	1	10
11	CL	103/104 (99%)	88 (85%)	15 (15%)	2	15
12	AM	92/96 (96%)	87 (95%)	5 (5%)	18	46
12	CM	91/96 (95%)	74 (81%)	17 (19%)	1	8
13	AN	79/84 (94%)	73 (92%)	6 (8%)	11	36
13	CN	79/84 (94%)	68 (86%)	11 (14%)	3	17
14	AO	76/77 (99%)	72 (95%)	4 (5%)	19	46
14	CO	76/77 (99%)	72 (95%)	4 (5%)	19	46
15	AP	65/65 (100%)	60 (92%)	5 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	59 (91%)	6 (9%)	7	30
16	AQ	74/78 (95%)	60 (81%)	14 (19%)	1	8
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	3	18
17	AR	48/65 (74%)	46 (96%)	2 (4%)	25	51
17	CR	48/65 (74%)	46 (96%)	2 (4%)	25	51
18	AS	70/79 (89%)	63 (90%)	7 (10%)	6	26
18	CS	70/79 (89%)	59 (84%)	11 (16%)	2	14
19	AT	65/66 (98%)	55 (85%)	10 (15%)	2	14
19	CT	65/66 (98%)	56 (86%)	9 (14%)	3	17
20	AU	44/61 (72%)	37 (84%)	7 (16%)	2	13
20	CU	44/61 (72%)	35 (80%)	9 (20%)	1	7
26	BC	216/218 (99%)	173 (80%)	43 (20%)	1	7
26	DC	216/218 (99%)	191 (88%)	25 (12%)	4	22
27	BD	164/164 (100%)	136 (83%)	28 (17%)	1	11
27	DD	164/164 (100%)	144 (88%)	20 (12%)	4	20
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	6
28	DE	165/165 (100%)	152 (92%)	13 (8%)	10	35
29	BF	148/150 (99%)	130 (88%)	18 (12%)	4	20
29	DF	149/150 (99%)	124 (83%)	25 (17%)	1	11
30	BG	137/138 (99%)	107 (78%)	30 (22%)	1	6
30	DG	137/138 (99%)	120 (88%)	17 (12%)	4	20
31	BH	114/114 (100%)	97 (85%)	17 (15%)	2	15
31	DH	114/114 (100%)	95 (83%)	19 (17%)	2	12
32	BI	109/110 (99%)	94 (86%)	15 (14%)	3	17
32	DI	109/110 (99%)	102 (94%)	7 (6%)	14	41
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	5
33	DJ	116/116 (100%)	106 (91%)	10 (9%)	8	33
34	BK	103/104 (99%)	84 (82%)	19 (18%)	1	8
34	DK	103/104 (99%)	85 (82%)	18 (18%)	1	10
35	BL	102/103 (99%)	81 (79%)	21 (21%)	1	6
35	DL	102/103 (99%)	90 (88%)	12 (12%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	90 (83%)	19 (17%)	1	10
36	DM	109/109 (100%)	100 (92%)	9 (8%)	9	34
37	BN	100/103 (97%)	81 (81%)	19 (19%)	1	8
37	DN	100/103 (97%)	85 (85%)	15 (15%)	2	15
38	BO	86/87 (99%)	69 (80%)	17 (20%)	1	7
38	DO	86/87 (99%)	78 (91%)	8 (9%)	7	29
39	BP	99/100 (99%)	79 (80%)	20 (20%)	1	7
39	DP	99/100 (99%)	91 (92%)	8 (8%)	9	34
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	1	9
40	DQ	89/90 (99%)	79 (89%)	10 (11%)	5	23
41	BR	84/84 (100%)	69 (82%)	15 (18%)	1	9
41	DR	84/84 (100%)	70 (83%)	14 (17%)	2	12
42	BS	93/93 (100%)	73 (78%)	20 (22%)	1	6
42	DS	93/93 (100%)	79 (85%)	14 (15%)	2	15
43	BT	80/84 (95%)	61 (76%)	19 (24%)	0	4
43	DT	80/84 (95%)	74 (92%)	6 (8%)	11	37
44	BU	83/85 (98%)	69 (83%)	14 (17%)	1	11
44	DU	83/85 (98%)	72 (87%)	11 (13%)	3	18
45	BV	78/78 (100%)	64 (82%)	14 (18%)	1	9
45	DV	78/78 (100%)	68 (87%)	10 (13%)	3	19
46	BW	59/63 (94%)	43 (73%)	16 (27%)	0	2
46	DW	59/63 (94%)	44 (75%)	15 (25%)	0	4
47	BX	67/68 (98%)	53 (79%)	14 (21%)	1	6
47	DX	67/68 (98%)	58 (87%)	9 (13%)	3	18
48	BY	55/55 (100%)	44 (80%)	11 (20%)	1	7
48	DY	55/55 (100%)	52 (94%)	3 (6%)	18	46
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	2
49	DZ	48/49 (98%)	41 (85%)	7 (15%)	2	15
50	B0	47/48 (98%)	42 (89%)	5 (11%)	5	25
50	D0	47/48 (98%)	42 (89%)	5 (11%)	5	25
51	B1	45/49 (92%)	37 (82%)	8 (18%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	D1	45/49 (92%)	41 (91%)	4 (9%)	8	31
52	B2	38/38 (100%)	32 (84%)	6 (16%)	2	14
52	D2	38/38 (100%)	34 (90%)	4 (10%)	5	25
53	B3	51/52 (98%)	44 (86%)	7 (14%)	3	18
53	D3	51/52 (98%)	42 (82%)	9 (18%)	1	10
54	B4	34/34 (100%)	30 (88%)	4 (12%)	4	21
54	D4	34/34 (100%)	29 (85%)	5 (15%)	2	15
All	All	9331/9756 (96%)	7983 (86%)	1348 (14%)	2	16

5 of 1348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	CL	28	GLN
33	DJ	54	ILE
12	CM	113	LYS
11	CL	19	ASN
26	DC	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
26	DC	57	HIS
41	DR	86	GLN
27	DD	49	GLN
34	DK	3	GLN
45	DV	80	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	465 (30%)	230 (15%)
22	AV	17/17 (100%)	2 (11%)	1 (5%)
22	AX	17/17 (100%)	2 (11%)	1 (5%)
22	CV	17/17 (100%)	3 (17%)	1 (5%)
22	CX	16/17 (94%)	2 (12%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	1 (20%)	1 (20%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	BA	2850/2903 (98%)	925 (32%)	497 (17%)
24	DA	2838/2903 (97%)	1020 (35%)	505 (17%)
25	BB	117/118 (99%)	32 (27%)	22 (18%)
55	CA	1529/1530 (99%)	516 (33%)	245 (16%)
56	DB	116/117 (99%)	29 (25%)	13 (11%)
All	All	9059/9184 (98%)	3000 (33%)	1517 (16%)

5 of 3000 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U

5 of 1517 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	CA	1053	G
24	DA	778	G
55	CA	1213	A
55	CA	1051	C
24	DA	223	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 365 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AB	218/241 (90%)	0.81	31 (14%) 7 10	170, 274, 284, 290	0
1	CB	218/241 (90%)	0.25	9 (4%) 42 31	159, 222, 233, 241	0
2	AC	206/233 (88%)	-0.35	0 100 100	133, 162, 187, 202	0
2	CC	206/233 (88%)	0.03	1 (0%) 87 72	140, 172, 212, 228	0
3	AD	205/206 (99%)	-0.04	4 (1%) 64 47	122, 157, 195, 218	0
3	CD	205/206 (99%)	0.06	6 (2%) 54 38	112, 131, 152, 165	0
4	AE	150/167 (89%)	1.60	43 (28%) 1 3	108, 211, 223, 227	0
4	CE	150/167 (89%)	0.49	10 (6%) 25 21	100, 156, 171, 176	0
5	AF	100/135 (74%)	-0.01	2 (2%) 64 47	197, 229, 250, 260	0
5	CF	100/135 (74%)	-0.02	3 (3%) 52 38	164, 186, 203, 209	0
6	AG	151/179 (84%)	-0.05	3 (1%) 64 47	158, 192, 220, 237	0
6	CG	150/179 (83%)	0.59	11 (7%) 22 19	142, 194, 228, 244	0
7	AH	129/130 (99%)	-0.18	0 100 100	127, 155, 181, 193	0
7	CH	129/130 (99%)	0.01	1 (0%) 82 66	152, 177, 195, 203	0
8	AI	127/130 (97%)	0.36	7 (5%) 32 24	142, 193, 220, 233	0
8	CI	127/130 (97%)	0.53	12 (9%) 15 14	155, 195, 223, 232	0
9	AJ	98/103 (95%)	0.32	5 (5%) 34 26	135, 181, 216, 239	0
9	CJ	98/103 (95%)	0.34	5 (5%) 34 26	155, 196, 230, 240	0
10	AK	117/129 (90%)	-0.26	1 (0%) 81 64	132, 195, 243, 254	0
10	CK	117/129 (90%)	-0.05	1 (0%) 81 64	125, 155, 181, 196	0
11	AL	123/124 (99%)	0.07	5 (4%) 42 31	89, 106, 131, 150	0
11	CL	123/124 (99%)	0.32	5 (4%) 42 31	117, 139, 155, 161	0
12	AM	114/118 (96%)	0.05	2 (1%) 67 49	157, 219, 252, 264	0
12	CM	113/118 (95%)	0.44	7 (6%) 28 22	195, 269, 309, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/101 (95%)	0.42	6 (6%) 27 22	142, 165, 217, 227	0
13	CN	95/101 (94%)	0.66	6 (6%) 27 22	155, 207, 265, 284	0
14	AO	88/89 (98%)	-0.17	1 (1%) 77 59	138, 168, 199, 219	0
14	CO	88/89 (98%)	0.05	3 (3%) 48 35	142, 174, 193, 201	0
15	AP	82/82 (100%)	0.01	1 (1%) 76 57	117, 144, 178, 192	0
15	CP	80/82 (97%)	0.47	4 (5%) 35 27	151, 180, 203, 207	0
16	AQ	80/84 (95%)	0.16	1 (1%) 74 55	90, 113, 135, 144	0
16	CQ	80/84 (95%)	0.02	0 100 100	99, 123, 145, 163	0
17	AR	55/75 (73%)	-0.06	0 100 100	175, 198, 219, 234	0
17	CR	55/75 (73%)	-0.16	0 100 100	148, 165, 180, 187	0
18	AS	79/92 (85%)	0.07	2 (2%) 58 42	171, 203, 244, 257	0
18	CS	79/92 (85%)	0.40	7 (8%) 17 15	223, 265, 319, 334	0
19	AT	85/87 (97%)	0.06	3 (3%) 47 34	114, 141, 164, 180	0
19	CT	85/87 (97%)	0.76	11 (12%) 9 11	194, 242, 275, 283	0
20	AU	51/71 (71%)	0.48	5 (9%) 14 14	133, 168, 248, 252	0
20	CU	51/71 (71%)	0.25	4 (7%) 20 17	126, 150, 183, 193	0
21	AA	1533/1533 (100%)	-0.33	18 (1%) 76 57	76, 150, 233, 282	0
22	AV	17/17 (100%)	0.08	0 100 100	142, 154, 182, 203	0
22	AX	17/17 (100%)	-0.53	0 100 100	139, 144, 186, 195	0
22	CV	17/17 (100%)	0.05	1 (5%) 29 23	158, 162, 193, 208	0
22	CX	17/17 (100%)	0.15	0 100 100	187, 193, 221, 222	0
23	AW	6/6 (100%)	0.41	0 100 100	136, 138, 143, 152	0
23	CW	6/6 (100%)	0.41	0 100 100	160, 160, 168, 179	0
24	BA	2854/2903 (98%)	-0.53	33 (1%) 76 57	52, 81, 194, 355	0
24	DA	2841/2903 (97%)	0.52	126 (4%) 39 29	132, 200, 303, 402	0
25	BB	118/118 (100%)	-0.53	0 100 100	66, 101, 133, 171	0
26	BC	271/273 (99%)	0.02	8 (2%) 52 38	60, 99, 129, 161	0
26	DC	271/273 (99%)	0.76	35 (12%) 9 11	133, 157, 179, 190	0
27	BD	209/209 (100%)	-0.25	0 100 100	55, 75, 114, 129	0
27	DD	209/209 (100%)	0.85	29 (13%) 7 10	147, 200, 232, 242	0
28	BE	201/201 (100%)	-0.31	0 100 100	56, 96, 129, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	201/201 (100%)	0.93	38 (18%) 4 6	154, 282, 335, 351	0
29	BF	177/179 (98%)	0.12	3 (1%) 69 50	120, 166, 201, 215	0
29	DF	178/179 (99%)	0.16	5 (2%) 55 40	307, 314, 321, 323	0
30	BG	176/177 (99%)	-0.25	1 (0%) 85 70	83, 108, 134, 152	0
30	DG	176/177 (99%)	0.23	6 (3%) 48 35	186, 221, 245, 259	0
31	BH	149/149 (100%)	0.26	3 (2%) 64 47	110, 239, 259, 264	0
31	DH	149/149 (100%)	0.66	16 (10%) 12 13	186, 240, 256, 260	0
32	BI	141/142 (99%)	0.48	6 (4%) 40 30	243, 307, 359, 366	0
32	DI	141/142 (99%)	0.28	4 (2%) 55 40	367, 394, 412, 419	0
33	BJ	142/142 (100%)	-0.23	0 100 100	59, 76, 102, 132	0
33	DJ	142/142 (100%)	0.65	13 (9%) 16 15	161, 201, 223, 233	0
34	BK	122/123 (99%)	-0.26	4 (3%) 49 35	55, 73, 113, 169	0
34	DK	122/123 (99%)	0.18	4 (3%) 49 35	151, 171, 189, 198	0
35	BL	143/144 (99%)	-0.02	4 (2%) 55 40	55, 93, 124, 136	0
35	DL	143/144 (99%)	1.23	35 (24%) 2 3	166, 240, 288, 297	0
36	BM	136/136 (100%)	-0.26	0 100 100	58, 81, 111, 138	0
36	DM	136/136 (100%)	0.43	8 (5%) 29 23	144, 181, 210, 232	0
37	BN	120/127 (94%)	-0.21	1 (0%) 82 66	61, 76, 96, 141	0
37	DN	120/127 (94%)	0.98	22 (18%) 4 6	183, 222, 252, 266	0
38	BO	116/117 (99%)	-0.15	0 100 100	96, 105, 123, 147	0
38	DO	116/117 (99%)	0.48	5 (4%) 40 30	286, 293, 297, 303	0
39	BP	114/115 (99%)	-0.42	0 100 100	64, 81, 119, 134	0
39	DP	114/115 (99%)	0.56	7 (6%) 28 22	179, 203, 220, 230	0
40	BQ	117/118 (99%)	-0.24	0 100 100	56, 77, 99, 120	0
40	DQ	117/118 (99%)	1.14	23 (19%) 3 6	184, 211, 240, 247	0
41	BR	103/103 (100%)	-0.16	1 (0%) 79 62	55, 87, 114, 131	0
41	DR	103/103 (100%)	0.88	18 (17%) 5 7	173, 249, 271, 277	0
42	BS	110/110 (100%)	-0.34	2 (1%) 67 49	55, 70, 105, 159	0
42	DS	110/110 (100%)	1.07	20 (18%) 4 7	159, 223, 269, 278	0
43	BT	93/100 (93%)	0.43	6 (6%) 26 21	65, 105, 142, 151	0
43	DT	93/100 (93%)	0.95	17 (18%) 4 6	206, 253, 285, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BU	102/104 (98%)	0.20	5 (4%) 36 27	89, 114, 136, 158	0
44	DU	102/104 (98%)	0.98	12 (11%) 10 12	272, 312, 355, 358	0
45	BV	94/94 (100%)	-0.33	0 100 100	71, 90, 116, 126	0
45	DV	94/94 (100%)	0.36	4 (4%) 40 30	228, 241, 252, 254	0
46	BW	79/85 (92%)	0.40	8 (10%) 14 14	68, 86, 136, 156	0
46	DW	79/85 (92%)	0.77	10 (12%) 9 11	156, 216, 233, 252	0
47	BX	77/78 (98%)	-0.03	0 100 100	65, 101, 124, 137	0
47	DX	77/78 (98%)	1.19	15 (19%) 4 6	157, 185, 209, 224	0
48	BY	63/63 (100%)	-0.04	2 (3%) 50 36	101, 123, 149, 159	0
48	DY	63/63 (100%)	1.27	14 (22%) 3 4	264, 288, 316, 329	0
49	BZ	58/59 (98%)	-0.10	0 100 100	64, 74, 111, 141	0
49	DZ	58/59 (98%)	0.91	6 (10%) 13 13	188, 215, 238, 248	0
50	B0	56/57 (98%)	-0.47	0 100 100	54, 77, 113, 132	0
50	D0	56/57 (98%)	0.66	5 (8%) 17 15	157, 230, 260, 265	0
51	B1	50/55 (90%)	-0.29	0 100 100	76, 100, 118, 132	0
51	D1	50/55 (90%)	0.42	4 (8%) 20 16	174, 207, 228, 238	0
52	B2	46/46 (100%)	-0.09	1 (2%) 62 44	62, 75, 103, 137	0
52	D2	46/46 (100%)	1.56	15 (32%) 1 2	155, 182, 198, 202	0
53	B3	64/65 (98%)	-0.04	0 100 100	58, 73, 96, 120	0
53	D3	64/65 (98%)	1.99	30 (46%) 0 1	180, 194, 211, 215	0
54	B4	38/38 (100%)	0.06	1 (2%) 57 41	69, 84, 110, 120	0
54	D4	38/38 (100%)	1.95	15 (39%) 1 1	171, 187, 198, 203	0
55	CA	1530/1530 (100%)	0.11	32 (2%) 63 45	109, 171, 272, 362	0
56	DB	117/117 (100%)	0.34	1 (0%) 81 64	219, 294, 300, 302	0
All	All	20511/21154 (96%)	0.14	930 (4%) 39 29	52, 166, 293, 419	0

The worst 5 of 930 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AE	114	LEU	10.8
8	CI	129	ARG	7.7
11	CL	123	ALA	7.7
4	AE	130	THR	7.4
39	DP	109	ILE	7.4

## 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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	CA	1636	1/1	-0.09	0.74	120,120,120,120	0
57	MG	DA	3020	1/1	-0.01	0.32	229,229,229,229	0
57	MG	DA	3128	1/1	0.01	0.42	132,132,132,132	0
57	MG	DA	3058	1/1	0.18	0.42	162,162,162,162	0
57	MG	DA	3060	1/1	0.19	0.68	132,132,132,132	0
57	MG	DA	3072	1/1	0.26	0.18	182,182,182,182	0
57	MG	BA	3131	1/1	0.27	0.54	68,68,68,68	0
57	MG	DA	3129	1/1	0.28	0.63	132,132,132,132	0
57	MG	DA	3074	1/1	0.29	0.37	187,187,187,187	0
57	MG	CA	1640	1/1	0.30	0.39	118,118,118,118	0
57	MG	DA	3063	1/1	0.30	0.78	157,157,157,157	0
57	MG	DA	3003	1/1	0.31	0.21	229,229,229,229	0
57	MG	CA	1619	1/1	0.37	0.30	135,135,135,135	0
57	MG	CA	1617	1/1	0.40	0.10	183,183,183,183	0
57	MG	DA	3002	1/1	0.42	0.34	212,212,212,212	0
57	MG	DA	3015	1/1	0.42	0.28	164,164,164,164	0
57	MG	CA	1627	1/1	0.44	0.20	136,136,136,136	0
57	MG	DA	3094	1/1	0.44	0.17	173,173,173,173	0
57	MG	DA	3092	1/1	0.45	0.15	198,198,198,198	0
57	MG	D4	101	1/1	0.45	0.35	183,183,183,183	0
57	MG	BA	3124	1/1	0.46	0.59	59,59,59,59	0
57	MG	AA	1627	1/1	0.47	0.48	142,142,142,142	0
57	MG	CA	1610	1/1	0.48	0.15	181,181,181,181	0
57	MG	BA	3062	1/1	0.49	0.51	55,55,55,55	0
57	MG	DA	3013	1/1	0.50	0.17	165,165,165,165	0
57	MG	DA	3005	1/1	0.51	0.23	197,197,197,197	0
57	MG	DA	3132	1/1	0.52	0.15	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3070	1/1	0.52	0.15	158,158,158,158	0
57	MG	DA	3030	1/1	0.53	0.21	164,164,164,164	0
57	MG	DA	3059	1/1	0.53	0.20	136,136,136,136	0
57	MG	DA	3082	1/1	0.53	0.14	220,220,220,220	0
57	MG	DA	3045	1/1	0.54	0.16	188,188,188,188	0
57	MG	DA	3078	1/1	0.54	0.33	144,144,144,144	0
57	MG	CA	1614	1/1	0.54	0.29	146,146,146,146	0
57	MG	DA	3069	1/1	0.55	0.24	139,139,139,139	0
57	MG	CA	1628	1/1	0.56	0.38	99,99,99,99	0
57	MG	DA	3007	1/1	0.58	0.14	250,250,250,250	0
57	MG	AA	1630	1/1	0.59	0.26	99,99,99,99	0
57	MG	DA	3016	1/1	0.60	0.23	175,175,175,175	0
57	MG	DA	3042	1/1	0.61	0.12	179,179,179,179	0
57	MG	DA	3108	1/1	0.61	0.19	172,172,172,172	0
57	MG	BA	3058	1/1	0.61	0.47	63,63,63,63	0
57	MG	DA	3022	1/1	0.62	0.21	152,152,152,152	0
57	MG	CA	1625	1/1	0.62	0.21	127,127,127,127	0
57	MG	CA	1629	1/1	0.63	0.13	157,157,157,157	0
57	MG	AA	1641	1/1	0.64	0.30	108,108,108,108	0
57	MG	AA	1607	1/1	0.64	0.19	113,113,113,113	0
57	MG	DA	3076	1/1	0.65	0.30	145,145,145,145	0
57	MG	CA	1603	1/1	0.65	0.19	141,141,141,141	0
57	MG	DA	3039	1/1	0.66	0.11	186,186,186,186	0
57	MG	DA	3109	1/1	0.66	0.21	145,145,145,145	0
57	MG	DA	3091	1/1	0.66	0.20	174,174,174,174	0
57	MG	AA	1637	1/1	0.67	0.21	118,118,118,118	0
57	MG	CA	1602	1/1	0.67	0.14	177,177,177,177	0
57	MG	DA	3064	1/1	0.67	0.10	157,157,157,157	0
57	MG	DA	3111	1/1	0.68	0.11	160,160,160,160	0
57	MG	DA	3123	1/1	0.68	0.17	225,225,225,225	0
57	MG	DA	3075	1/1	0.68	0.25	155,155,155,155	0
57	MG	DA	3097	1/1	0.68	0.18	156,156,156,156	0
57	MG	AA	1619	1/1	0.68	0.22	162,162,162,162	0
57	MG	DC	301	1/1	0.68	0.09	135,135,135,135	0
57	MG	DJ	201	1/1	0.68	0.11	183,183,183,183	0
57	MG	DA	3006	1/1	0.68	0.09	296,296,296,296	0
57	MG	DA	3018	1/1	0.69	0.18	248,248,248,248	0
57	MG	DA	3036	1/1	0.70	0.22	212,212,212,212	0
57	MG	DA	3026	1/1	0.70	0.23	160,160,160,160	0
57	MG	DA	3096	1/1	0.71	0.14	190,190,190,190	0
57	MG	BA	3075	1/1	0.72	0.28	58,58,58,58	0
57	MG	DA	3011	1/1	0.72	0.25	184,184,184,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3049	1/1	0.72	0.07	249,249,249,249	0
57	MG	DA	3019	1/1	0.72	0.16	245,245,245,245	0
57	MG	DA	3106	1/1	0.72	0.17	228,228,228,228	0
57	MG	DA	3014	1/1	0.73	0.14	162,162,162,162	0
57	MG	DA	3071	1/1	0.73	0.15	184,184,184,184	0
57	MG	DA	3083	1/1	0.74	0.07	303,303,303,303	0
57	MG	DA	3110	1/1	0.74	0.10	219,219,219,219	0
57	MG	AA	1636	1/1	0.74	0.13	154,154,154,154	0
57	MG	CA	1620	1/1	0.74	0.18	150,150,150,150	0
57	MG	AA	1621	1/1	0.74	0.16	80,80,80,80	0
57	MG	DA	3073	1/1	0.75	0.11	312,312,312,312	0
57	MG	DA	3098	1/1	0.75	0.13	170,170,170,170	0
57	MG	DA	3010	1/1	0.76	0.16	210,210,210,210	0
57	MG	DA	3057	1/1	0.76	0.24	133,133,133,133	0
57	MG	CA	1622	1/1	0.76	0.11	216,216,216,216	0
57	MG	CA	1601	1/1	0.76	0.12	224,224,224,224	0
57	MG	AA	1617	1/1	0.76	0.20	150,150,150,150	0
57	MG	DA	3062	1/1	0.76	0.24	160,160,160,160	0
57	MG	DA	3095	1/1	0.77	0.10	152,152,152,152	0
57	MG	DA	3125	1/1	0.77	0.13	187,187,187,187	0
57	MG	AA	1624	1/1	0.77	0.10	131,131,131,131	0
57	MG	DA	3028	1/1	0.77	0.14	165,165,165,165	0
57	MG	BA	3004	1/1	0.78	0.18	86,86,86,86	0
57	MG	CA	1607	1/1	0.78	0.10	134,134,134,134	0
57	MG	BA	3035	1/1	0.78	0.29	72,72,72,72	0
57	MG	DA	3027	1/1	0.78	0.10	171,171,171,171	0
57	MG	DA	3038	1/1	0.79	0.12	197,197,197,197	0
57	MG	DA	3107	1/1	0.79	0.12	137,137,137,137	0
57	MG	BB	201	1/1	0.80	0.30	118,118,118,118	0
57	MG	DA	3084	1/1	0.80	0.17	214,214,214,214	0
57	MG	DA	3043	1/1	0.80	0.08	208,208,208,208	0
57	MG	BA	3061	1/1	0.80	0.32	56,56,56,56	0
57	MG	DA	3100	1/1	0.80	0.12	150,150,150,150	0
57	MG	DA	3113	1/1	0.80	0.10	182,182,182,182	0
57	MG	BA	3098	1/1	0.80	0.30	72,72,72,72	0
57	MG	DA	3121	1/1	0.81	0.19	206,206,206,206	0
57	MG	DA	3088	1/1	0.81	0.10	180,180,180,180	0
57	MG	AA	1628	1/1	0.81	0.10	134,134,134,134	0
57	MG	DA	3029	1/1	0.81	0.15	179,179,179,179	0
57	MG	BA	3112	1/1	0.81	0.12	64,64,64,64	0
57	MG	CA	1616	1/1	0.81	0.17	199,199,199,199	0
57	MG	BA	3115	1/1	0.81	0.30	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1625	1/1	0.81	0.18	114,114,114,114	0
57	MG	BA	3028	1/1	0.81	0.26	57,57,57,57	0
57	MG	DA	3131	1/1	0.82	0.22	181,181,181,181	0
57	MG	CA	1606	1/1	0.82	0.09	124,124,124,124	0
57	MG	DB	201	1/1	0.82	0.14	224,224,224,224	0
57	MG	BA	3093	1/1	0.82	0.17	104,104,104,104	0
57	MG	BA	3015	1/1	0.82	0.40	55,55,55,55	0
57	MG	DA	3130	1/1	0.82	0.13	170,170,170,170	0
57	MG	DA	3048	1/1	0.83	0.10	203,203,203,203	0
57	MG	BA	3133	1/1	0.83	0.38	73,73,73,73	0
57	MG	DA	3079	1/1	0.83	0.10	148,148,148,148	0
57	MG	DA	3114	1/1	0.83	0.16	135,135,135,135	0
57	MG	DA	3093	1/1	0.83	0.16	208,208,208,208	0
57	MG	BA	3136	1/1	0.83	0.38	64,64,64,64	0
57	MG	DA	3044	1/1	0.83	0.15	210,210,210,210	0
57	MG	CA	1637	1/1	0.83	0.17	112,112,112,112	0
57	MG	DA	3017	1/1	0.84	0.13	187,187,187,187	0
57	MG	DA	3052	1/1	0.84	0.09	144,144,144,144	0
57	MG	BA	3030	1/1	0.84	0.33	58,58,58,58	0
57	MG	DA	3103	1/1	0.84	0.12	150,150,150,150	0
57	MG	CA	1615	1/1	0.84	0.11	156,156,156,156	0
57	MG	AA	1604	1/1	0.84	0.07	157,157,157,157	0
57	MG	CA	1611	1/1	0.84	0.11	132,132,132,132	0
57	MG	CA	1613	1/1	0.84	0.10	121,121,121,121	0
57	MG	DA	3047	1/1	0.85	0.18	208,208,208,208	0
57	MG	AA	1610	1/1	0.85	0.10	155,155,155,155	0
57	MG	DA	3080	1/1	0.85	0.09	134,134,134,134	0
57	MG	DA	3001	1/1	0.85	0.16	206,206,206,206	0
57	MG	DA	3117	1/1	0.85	0.15	170,170,170,170	0
57	MG	DA	3118	1/1	0.85	0.16	181,181,181,181	0
57	MG	AA	1616	1/1	0.85	0.20	161,161,161,161	0
57	MG	AA	1620	1/1	0.85	0.09	186,186,186,186	0
57	MG	CA	1608	1/1	0.85	0.11	121,121,121,121	0
57	MG	CA	1632	1/1	0.86	0.12	210,210,210,210	0
57	MG	CA	1612	1/1	0.86	0.09	124,124,124,124	0
57	MG	DA	3086	1/1	0.86	0.11	196,196,196,196	0
57	MG	BA	3060	1/1	0.86	0.31	56,56,56,56	0
57	MG	AA	1629	1/1	0.86	0.16	161,161,161,161	0
57	MG	CA	1623	1/1	0.86	0.16	123,123,123,123	0
57	MG	AA	1611	1/1	0.87	0.14	126,126,126,126	0
57	MG	AA	1602	1/1	0.87	0.24	97,97,97,97	0
57	MG	DA	3033	1/1	0.87	0.12	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	1630	1/1	0.87	0.20	99,99,99,99	0
57	MG	DA	3037	1/1	0.87	0.12	204,204,204,204	0
57	MG	CA	1642	1/1	0.87	0.07	170,170,170,170	0
57	MG	DA	3068	1/1	0.87	0.19	143,143,143,143	0
57	MG	DA	3085	1/1	0.87	0.12	167,167,167,167	0
57	MG	DA	3051	1/1	0.87	0.08	160,160,160,160	0
57	MG	BA	3007	1/1	0.87	0.14	111,111,111,111	0
57	MG	DA	3054	1/1	0.87	0.12	155,155,155,155	0
57	MG	DA	3055	1/1	0.87	0.07	136,136,136,136	0
57	MG	DA	3056	1/1	0.87	0.12	141,141,141,141	0
57	MG	CA	1634	1/1	0.87	0.07	153,153,153,153	0
57	MG	DA	3101	1/1	0.88	0.10	155,155,155,155	0
57	MG	BA	3056	1/1	0.88	0.25	64,64,64,64	0
57	MG	BA	3088	1/1	0.88	0.15	77,77,77,77	0
57	MG	DA	3032	1/1	0.89	0.11	161,161,161,161	0
57	MG	BA	3046	1/1	0.89	0.11	77,77,77,77	0
57	MG	AA	1614	1/1	0.89	0.08	150,150,150,150	0
57	MG	BA	3014	1/1	0.89	0.28	55,55,55,55	0
57	MG	DA	3127	1/1	0.89	0.23	138,138,138,138	0
57	MG	DC	302	1/1	0.89	0.12	140,140,140,140	0
57	MG	BA	3092	1/1	0.89	0.08	127,127,127,127	0
57	MG	DA	3099	1/1	0.89	0.07	211,211,211,211	0
57	MG	DA	3004	1/1	0.90	0.16	206,206,206,206	0
57	MG	DA	3023	1/1	0.90	0.11	148,148,148,148	0
57	MG	DA	3025	1/1	0.90	0.08	135,135,135,135	0
57	MG	DA	3065	1/1	0.90	0.08	152,152,152,152	0
57	MG	DA	3067	1/1	0.90	0.08	147,147,147,147	0
57	MG	DA	3034	1/1	0.90	0.14	158,158,158,158	0
57	MG	BA	3113	1/1	0.90	0.09	54,54,54,54	0
57	MG	AA	1609	1/1	0.90	0.09	118,118,118,118	0
57	MG	BA	3003	1/1	0.90	0.10	90,90,90,90	0
57	MG	DA	3009	1/1	0.90	0.18	199,199,199,199	0
57	MG	DA	3087	1/1	0.90	0.06	208,208,208,208	0
57	MG	DA	3061	1/1	0.90	0.09	134,134,134,134	0
57	MG	BA	3095	1/1	0.91	0.10	92,92,92,92	0
57	MG	DA	3115	1/1	0.91	0.07	154,154,154,154	0
57	MG	BA	3077	1/1	0.91	0.15	63,63,63,63	0
57	MG	BA	3101	1/1	0.91	0.15	54,54,54,54	0
57	MG	BA	3019	1/1	0.91	0.09	86,86,86,86	0
57	MG	CA	1631	1/1	0.91	0.09	130,130,130,130	0
57	MG	AA	1615	1/1	0.91	0.06	153,153,153,153	0
57	MG	BA	3011	1/1	0.91	0.28	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	1635	1/1	0.91	0.07	142,142,142,142	0
57	MG	DA	3050	1/1	0.92	0.07	180,180,180,180	0
57	MG	BA	3081	1/1	0.92	0.14	56,56,56,56	0
57	MG	BA	3085	1/1	0.92	0.36	59,59,59,59	0
57	MG	DA	3053	1/1	0.92	0.12	144,144,144,144	0
57	MG	BA	3086	1/1	0.92	0.10	60,60,60,60	0
57	MG	DA	3081	1/1	0.92	0.08	182,182,182,182	0
57	MG	DA	3012	1/1	0.92	0.15	168,168,168,168	0
57	MG	AA	1608	1/1	0.92	0.13	105,105,105,105	0
57	MG	CA	1638	1/1	0.92	0.08	226,226,226,226	0
57	MG	DA	3035	1/1	0.92	0.13	155,155,155,155	0
57	MG	CA	1639	1/1	0.92	0.05	266,266,266,266	0
57	MG	BA	3048	1/1	0.92	0.14	91,91,91,91	0
57	MG	DA	3119	1/1	0.92	0.08	147,147,147,147	0
57	MG	AA	1631	1/1	0.92	0.17	114,114,114,114	0
57	MG	DA	3089	1/1	0.92	0.12	179,179,179,179	0
57	MG	CA	1609	1/1	0.92	0.08	131,131,131,131	0
57	MG	DA	3040	1/1	0.92	0.09	171,171,171,171	0
57	MG	DA	3041	1/1	0.92	0.11	176,176,176,176	0
57	MG	BA	3032	1/1	0.92	0.10	57,57,57,57	0
57	MG	BA	3135	1/1	0.92	0.31	60,60,60,60	0
57	MG	AA	1601	1/1	0.92	0.07	133,133,133,133	0
57	MG	BA	3099	1/1	0.92	0.11	58,58,58,58	0
57	MG	DA	3046	1/1	0.92	0.12	172,172,172,172	0
57	MG	BB	202	1/1	0.92	0.11	127,127,127,127	0
57	MG	BD	301	1/1	0.92	0.15	55,55,55,55	0
57	MG	DA	3008	1/1	0.92	0.06	198,198,198,198	0
57	MG	DA	3102	1/1	0.92	0.07	141,141,141,141	0
57	MG	BA	3051	1/1	0.93	0.15	57,57,57,57	0
57	MG	DA	3124	1/1	0.93	0.18	168,168,168,168	0
57	MG	BA	3005	1/1	0.93	0.09	91,91,91,91	0
57	MG	BA	3071	1/1	0.93	0.30	55,55,55,55	0
57	MG	BA	3089	1/1	0.93	0.18	66,66,66,66	0
57	MG	DA	3066	1/1	0.93	0.09	150,150,150,150	0
57	MG	BA	3119	1/1	0.93	0.28	68,68,68,68	0
57	MG	BA	3123	1/1	0.93	0.07	79,79,79,79	0
57	MG	CA	1604	1/1	0.93	0.06	117,117,117,117	0
57	MG	AA	1632	1/1	0.93	0.09	117,117,117,117	0
57	MG	BA	3047	1/1	0.93	0.09	78,78,78,78	0
57	MG	BA	3079	1/1	0.93	0.07	110,110,110,110	0
57	MG	BA	3080	1/1	0.93	0.10	93,93,93,93	0
57	MG	BA	3002	1/1	0.93	0.35	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3076	1/1	0.94	0.07	62,62,62,62	0
57	MG	BA	3021	1/1	0.94	0.24	59,59,59,59	0
57	MG	BA	3026	1/1	0.94	0.34	59,59,59,59	0
57	MG	DA	3077	1/1	0.94	0.07	162,162,162,162	0
57	MG	DA	3024	1/1	0.94	0.07	162,162,162,162	0
57	MG	BB	204	1/1	0.94	0.07	74,74,74,74	0
57	MG	CA	1633	1/1	0.94	0.09	123,123,123,123	0
57	MG	BA	3009	1/1	0.94	0.07	61,61,61,61	0
57	MG	AA	1613	1/1	0.94	0.10	95,95,95,95	0
57	MG	BA	3114	1/1	0.94	0.07	88,88,88,88	0
57	MG	AA	1603	1/1	0.94	0.07	93,93,93,93	0
57	MG	DA	3105	1/1	0.94	0.06	159,159,159,159	0
57	MG	AA	1633	1/1	0.94	0.08	128,128,128,128	0
57	MG	CA	1621	1/1	0.94	0.08	115,115,115,115	0
57	MG	BA	3037	1/1	0.94	0.26	58,58,58,58	0
57	MG	BA	3066	1/1	0.94	0.10	61,61,61,61	0
57	MG	BA	3044	1/1	0.94	0.08	88,88,88,88	0
57	MG	BA	3016	1/1	0.94	0.27	56,56,56,56	0
57	MG	DA	3112	1/1	0.94	0.07	143,143,143,143	0
57	MG	AA	1635	1/1	0.94	0.07	148,148,148,148	0
57	MG	BA	3022	1/1	0.95	0.16	55,55,55,55	0
57	MG	BA	3064	1/1	0.95	0.09	55,55,55,55	0
57	MG	BA	3103	1/1	0.95	0.10	81,81,81,81	0
57	MG	DA	3126	1/1	0.95	0.12	199,199,199,199	0
57	MG	CA	1626	1/1	0.95	0.16	139,139,139,139	0
57	MG	DA	3070	1/1	0.95	0.05	147,147,147,147	0
57	MG	BA	3132	1/1	0.95	0.25	61,61,61,61	0
57	MG	BA	3107	1/1	0.95	0.09	67,67,67,67	0
57	MG	AA	1612	1/1	0.95	0.06	106,106,106,106	0
57	MG	CA	1641	1/1	0.95	0.07	151,151,151,151	0
57	MG	DA	3116	1/1	0.95	0.09	133,133,133,133	0
57	MG	BA	3059	1/1	0.95	0.13	69,69,69,69	0
57	MG	AA	1639	1/1	0.95	0.07	143,143,143,143	0
57	MG	BA	3083	1/1	0.95	0.11	59,59,59,59	0
57	MG	AA	1634	1/1	0.95	0.05	121,121,121,121	0
57	MG	DA	3090	1/1	0.96	0.05	200,200,200,200	0
57	MG	DA	3122	1/1	0.96	0.13	146,146,146,146	0
57	MG	BA	3053	1/1	0.96	0.10	57,57,57,57	0
57	MG	BA	3072	1/1	0.96	0.30	55,55,55,55	0
57	MG	AA	1606	1/1	0.96	0.06	119,119,119,119	0
57	MG	AA	1638	1/1	0.96	0.10	107,107,107,107	0
57	MG	AA	1623	1/1	0.96	0.07	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3068	1/1	0.96	0.08	65,65,65,65	0
57	MG	DA	3031	1/1	0.96	0.06	159,159,159,159	0
57	MG	CA	1624	1/1	0.96	0.15	99,99,99,99	0
57	MG	BA	3105	1/1	0.96	0.07	55,55,55,55	0
57	MG	BA	3127	1/1	0.96	0.09	57,57,57,57	0
57	MG	BA	3128	1/1	0.96	0.06	64,64,64,64	0
57	MG	BA	3045	1/1	0.96	0.21	80,80,80,80	0
57	MG	BA	3111	1/1	0.96	0.12	55,55,55,55	0
57	MG	DA	3104	1/1	0.96	0.12	142,142,142,142	0
57	MG	DA	3120	1/1	0.96	0.11	159,159,159,159	0
57	MG	BA	3074	1/1	0.97	0.13	54,54,54,54	0
57	MG	BA	3042	1/1	0.97	0.05	68,68,68,68	0
57	MG	BA	3125	1/1	0.97	0.11	58,58,58,58	0
57	MG	BA	3126	1/1	0.97	0.07	70,70,70,70	0
57	MG	AA	1618	1/1	0.97	0.06	131,131,131,131	0
57	MG	AA	1605	1/1	0.97	0.10	124,124,124,124	0
57	MG	AA	1643	1/1	0.97	0.05	101,101,101,101	0
57	MG	AA	1622	1/1	0.97	0.05	113,113,113,113	0
57	MG	BA	3010	1/1	0.97	0.05	64,64,64,64	0
57	MG	BA	3049	1/1	0.97	0.07	61,61,61,61	0
57	MG	BA	3109	1/1	0.97	0.07	60,60,60,60	0
57	MG	BA	3110	1/1	0.97	0.06	61,61,61,61	0
57	MG	CA	1618	1/1	0.97	0.09	148,148,148,148	0
57	MG	AA	1626	1/1	0.97	0.14	136,136,136,136	0
57	MG	BA	3069	1/1	0.97	0.05	65,65,65,65	0
57	MG	DA	3021	1/1	0.97	0.21	151,151,151,151	0
57	MG	BA	3039	1/1	0.97	0.06	57,57,57,57	0
57	MG	BA	3040	1/1	0.97	0.07	58,58,58,58	0
57	MG	BA	3090	1/1	0.97	0.07	63,63,63,63	0
57	MG	BA	3057	1/1	0.97	0.26	61,61,61,61	0
57	MG	BA	3122	1/1	0.97	0.06	57,57,57,57	0
57	MG	CA	1605	1/1	0.97	0.05	115,115,115,115	0
58	ZN	D4	102	1/1	0.97	0.14	99,99,99,99	0
57	MG	BA	3006	1/1	0.98	0.04	101,101,101,101	0
57	MG	BA	3106	1/1	0.98	0.05	58,58,58,58	0
57	MG	BA	3087	1/1	0.98	0.05	61,61,61,61	0
57	MG	BA	3020	1/1	0.98	0.22	63,63,63,63	0
57	MG	AA	1640	1/1	0.98	0.04	160,160,160,160	0
57	MG	BA	3063	1/1	0.98	0.09	54,54,54,54	0
57	MG	BA	3091	1/1	0.98	0.05	88,88,88,88	0
57	MG	BA	3052	1/1	0.98	0.04	54,54,54,54	0
57	MG	BA	3078	1/1	0.98	0.04	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3094	1/1	0.98	0.05	92,92,92,92	0
57	MG	BA	3118	1/1	0.98	0.06	60,60,60,60	0
57	MG	BA	3043	1/1	0.98	0.07	68,68,68,68	0
57	MG	BA	3120	1/1	0.98	0.04	59,59,59,59	0
57	MG	BA	3121	1/1	0.98	0.10	64,64,64,64	0
57	MG	BA	3034	1/1	0.98	0.04	57,57,57,57	0
57	MG	BA	3001	1/1	0.98	0.11	61,61,61,61	0
57	MG	BA	3100	1/1	0.98	0.05	74,74,74,74	0
57	MG	BA	3036	1/1	0.98	0.05	65,65,65,65	0
57	MG	BA	3102	1/1	0.98	0.17	57,57,57,57	0
57	MG	AA	1642	1/1	0.98	0.09	90,90,90,90	0
57	MG	BA	3104	1/1	0.98	0.06	55,55,55,55	0
57	MG	BA	3067	1/1	0.99	0.06	57,57,57,57	0
57	MG	BA	3134	1/1	0.99	0.04	55,55,55,55	0
57	MG	BA	3029	1/1	0.99	0.07	54,54,54,54	0
57	MG	BA	3041	1/1	0.99	0.06	60,60,60,60	0
57	MG	BA	3054	1/1	0.99	0.03	62,62,62,62	0
57	MG	BA	3055	1/1	0.99	0.07	62,62,62,62	0
57	MG	BB	203	1/1	0.99	0.04	69,69,69,69	0
57	MG	BA	3017	1/1	0.99	0.04	56,56,56,56	0
57	MG	BA	3073	1/1	0.99	0.03	61,61,61,61	0
57	MG	BA	3018	1/1	0.99	0.03	80,80,80,80	0
57	MG	BA	3116	1/1	0.99	0.09	55,55,55,55	0
57	MG	BA	3117	1/1	0.99	0.04	67,67,67,67	0
57	MG	BA	3033	1/1	0.99	0.06	56,56,56,56	0
57	MG	BA	3024	1/1	0.99	0.06	60,60,60,60	0
57	MG	BA	3096	1/1	0.99	0.17	61,61,61,61	0
57	MG	BA	3097	1/1	0.99	0.06	65,65,65,65	0
57	MG	BA	3025	1/1	0.99	0.03	59,59,59,59	0
57	MG	BA	3012	1/1	0.99	0.04	54,54,54,54	0
57	MG	BA	3027	1/1	0.99	0.09	59,59,59,59	0
57	MG	BA	3038	1/1	0.99	0.03	59,59,59,59	0
57	MG	BA	3050	1/1	0.99	0.05	56,56,56,56	0
57	MG	BA	3082	1/1	0.99	0.04	55,55,55,55	0
57	MG	BA	3065	1/1	0.99	0.08	55,55,55,55	0
57	MG	BA	3129	1/1	0.99	0.04	55,55,55,55	0
57	MG	BA	3130	1/1	0.99	0.09	68,68,68,68	0
57	MG	BA	3084	1/1	0.99	0.18	61,61,61,61	0
58	ZN	B4	101	1/1	0.99	0.02	99,99,99,99	0
57	MG	BA	3008	1/1	0.99	0.04	59,59,59,59	0
57	MG	BA	3023	1/1	1.00	0.05	59,59,59,59	0
57	MG	BA	3108	1/1	1.00	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3013	1/1	1.00	0.05	55,55,55,55	0
57	MG	BA	3031	1/1	1.00	0.08	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.