



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 12:17 AM EDT

PDB ID : 4V6D
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 : 2009-06-27
Resolution : 3.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-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

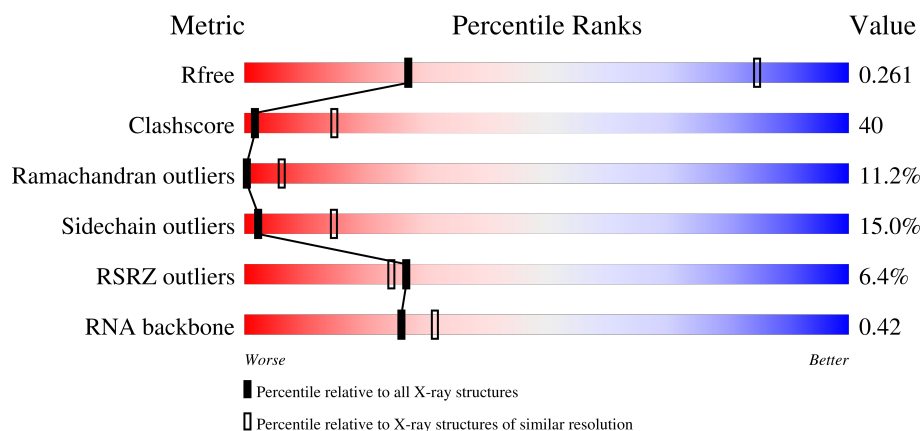
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1155 (4.00-3.64)
Clashscore	180529	1222 (4.00-3.64)
Ramachandran outliers	177936	1182 (4.00-3.64)
Sidechain outliers	177891	1174 (4.00-3.64)
RSRZ outliers	164620	1156 (4.00-3.64)
RNA backbone	3690	1132 (4.62-3.00)

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 ≥ 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	<div> <div>24%</div> <div>17% 55% 15% • 10%</div> </div>
1	CB	241	<div> <div>7%</div> <div>20% 56% 13% • 10%</div> </div>
2	AC	233	<div> <div>33% 44% 10% • 12%</div> </div>
2	CC	233	<div> <div>% 32% 45% 11% • 12%</div> </div>

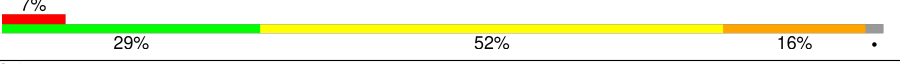
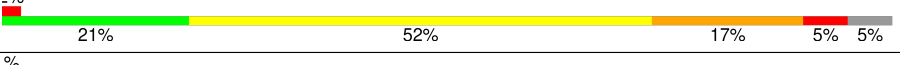
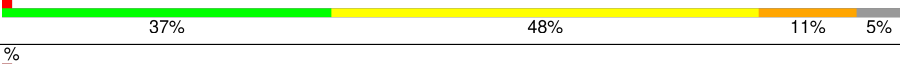
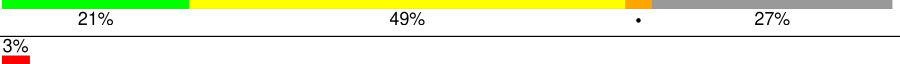
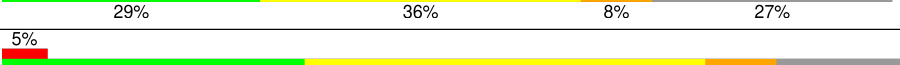
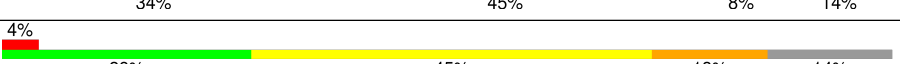
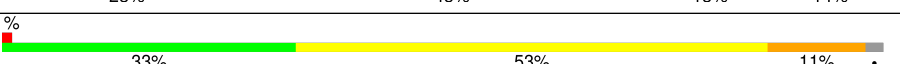
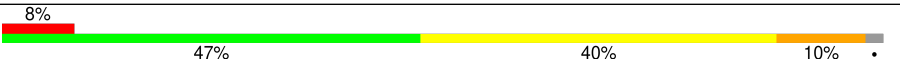


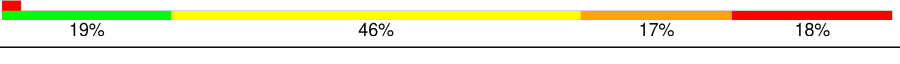
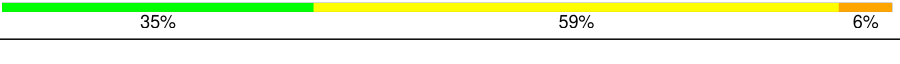

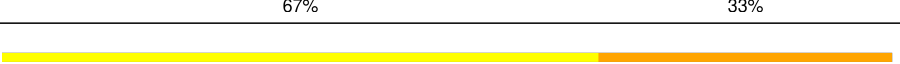
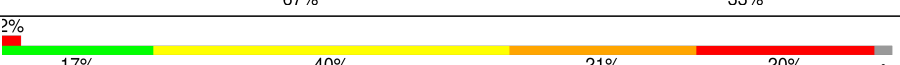
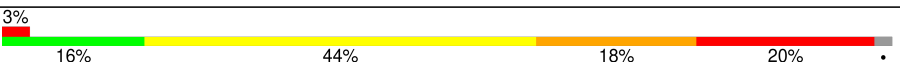
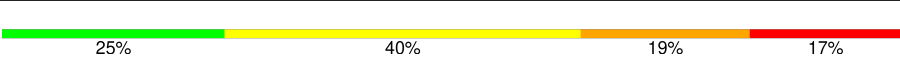
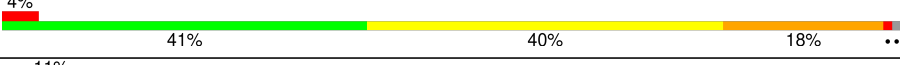
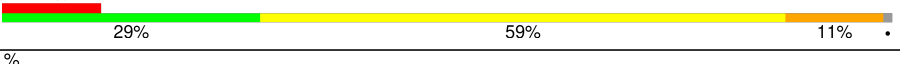
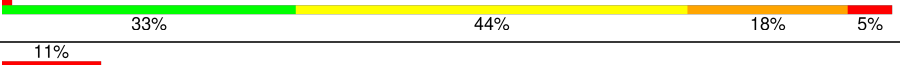

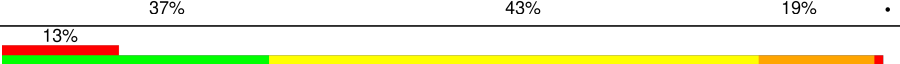



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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
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	CV	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	
28	BE	201	
28	DE	201	

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Mol	Chain	Length	Quality of chain
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	
40	DQ	118	
41	BR	103	

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Mol	Chain	Length	Quality of chain
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	
53	B3	65	
53	D3	65	

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Mol	Chain	Length	Quality of chain
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	BA	3015	-	-	-	X
57	MG	BA	3131	-	-	-	X
57	MG	BA	3132	-	-	-	X
57	MG	BA	3133	-	-	-	X
57	MG	CA	1624	-	-	-	X
57	MG	DA	3004	-	-	-	X
57	MG	DA	3016	-	-	-	X
57	MG	DA	3062	-	-	-	X
57	MG	DA	3065	-	-	-	X
57	MG	DA	3076	-	-	-	X
57	MG	DA	3110	-	-	-	X
57	MG	DA	3131	-	-	-	X
57	MG	DA	3134	-	-	-	X

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 285420 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
			360	161	64	118	17			
22	CV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	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
			125	56	18	45	6			
23	CW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	DC	1	Total	Mg	0	0
			1	1		
57	DJ	1	Total	Mg	0	0
			1	1		
57	DA	134	Total	Mg	0	0
			134	134		
57	DB	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 1 1	0	0
58	D4	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AE	1	Total O 1 1	0	0
59	AL	3	Total O 3 3	0	0
59	AN	5	Total O 5 5	0	0
59	AT	3	Total O 3 3	0	0
59	AU	1	Total O 1 1	0	0
59	AA	195	Total O 195 195	0	0
59	BA	615	Total O 615 615	0	0
59	BB	19	Total O 19 19	0	0
59	BC	7	Total O 7 7	0	0
59	BD	2	Total O 2 2	0	0
59	BE	1	Total O 1 1	0	0
59	BL	4	Total O 4 4	0	0
59	BN	2	Total O 2 2	0	0
59	BQ	1	Total O 1 1	0	0
59	BT	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	B2	2	Total O 2 2	0	0
59	B3	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	2	Total 2	O 2	0	0
59	CE	3	Total 3	O 3	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	196	Total 196	O 196	0	0
59	DC	14	Total 14	O 14	0	0
59	DD	4	Total 4	O 4	0	0
59	DE	2	Total 2	O 2	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	5	Total 5	O 5	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0
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
59	DA	598	Total 598	O 598	0	0

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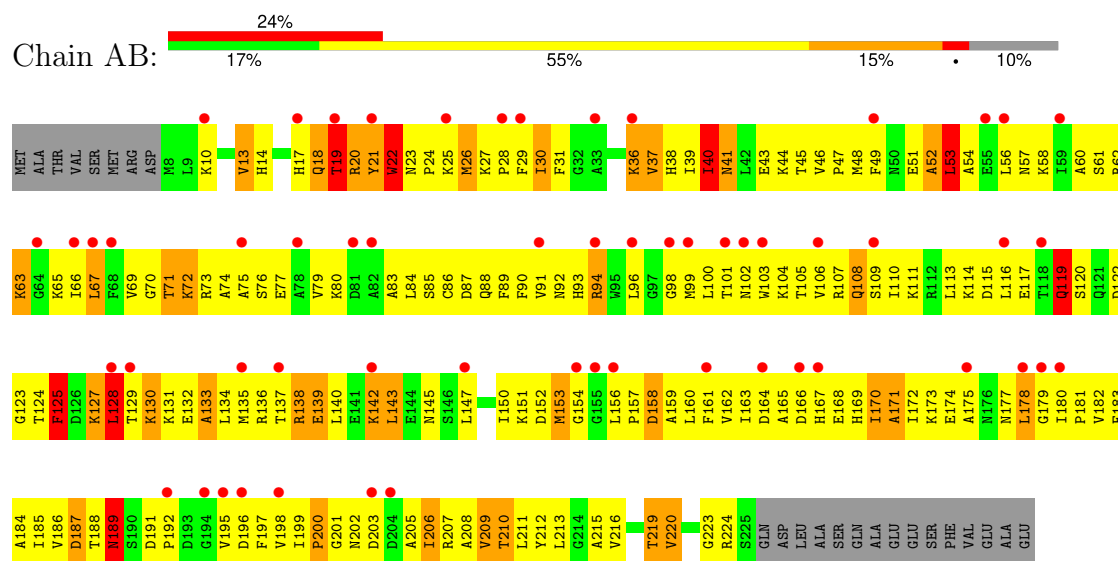
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	4	Total	O	0	0
			4	4		

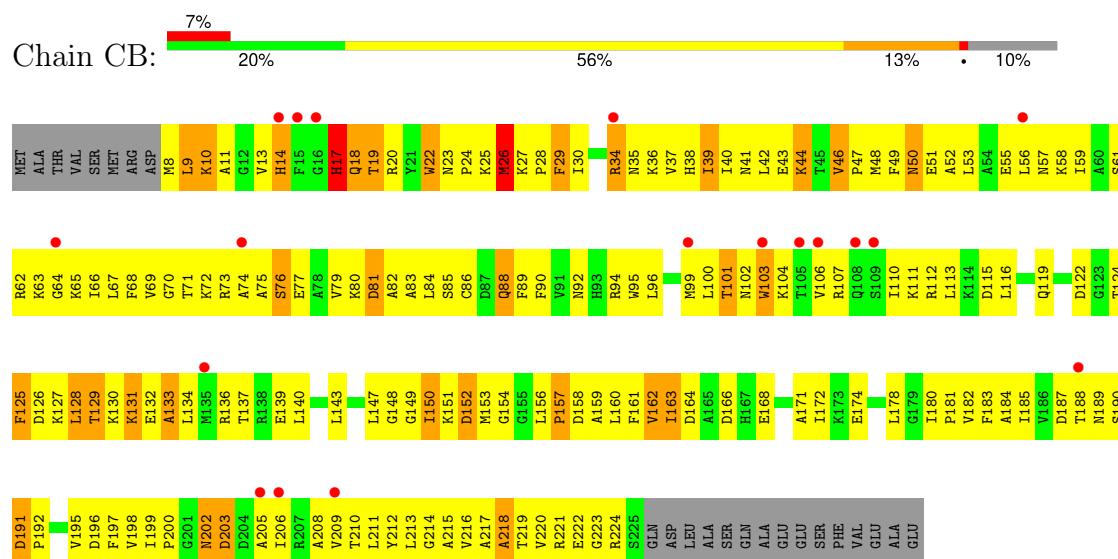
3 Residue-property plots [i](#)

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

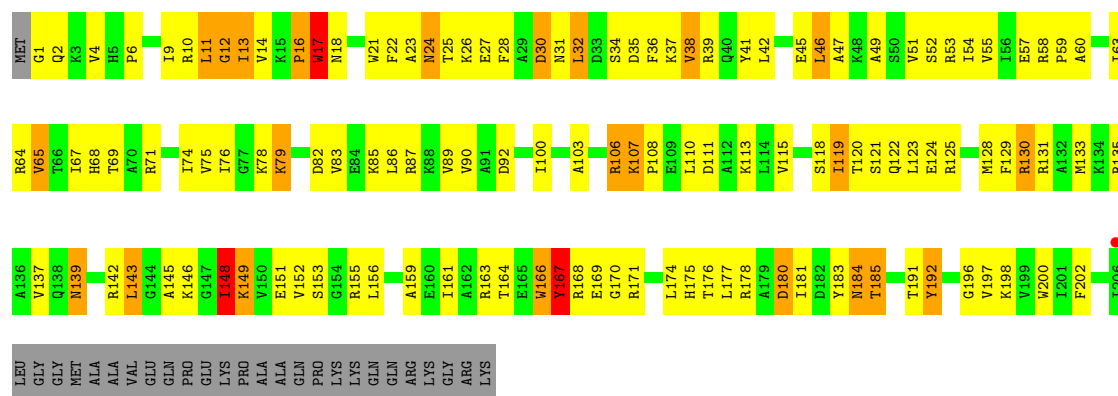


• Molecule 1: 30S ribosomal protein S2



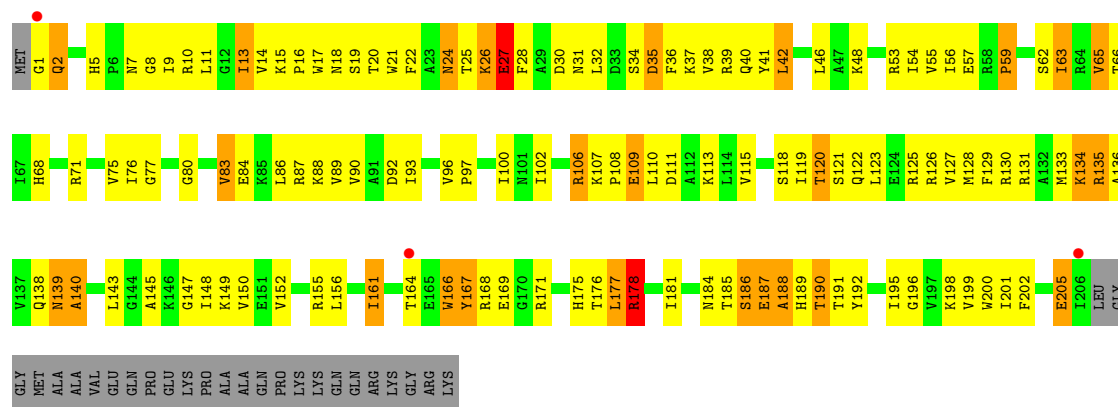
• Molecule 2: 30S ribosomal protein S3

Chain AC: 



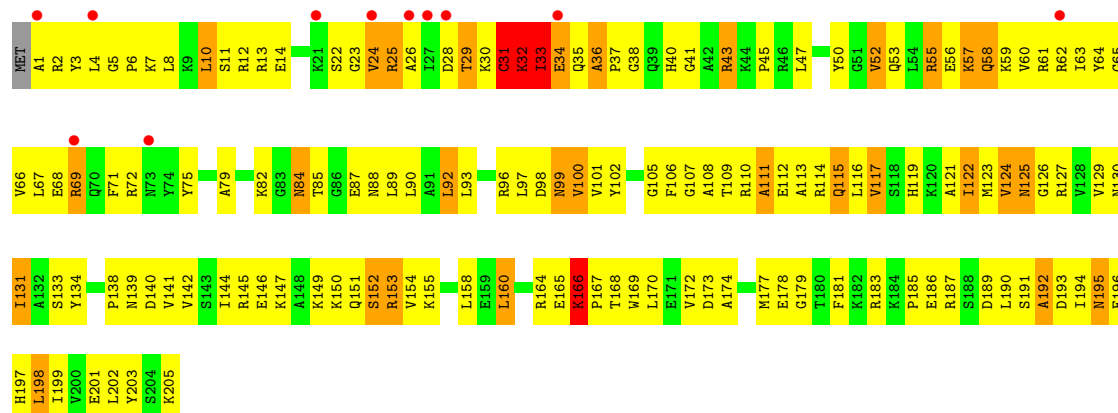
• Molecule 2: 30S ribosomal protein S3

Chain CC: 

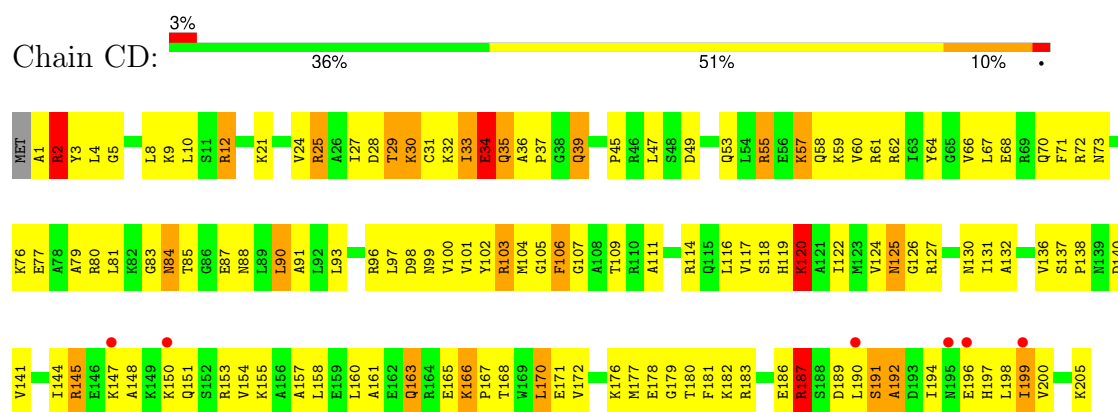


• Molecule 3: 30S ribosomal protein S4

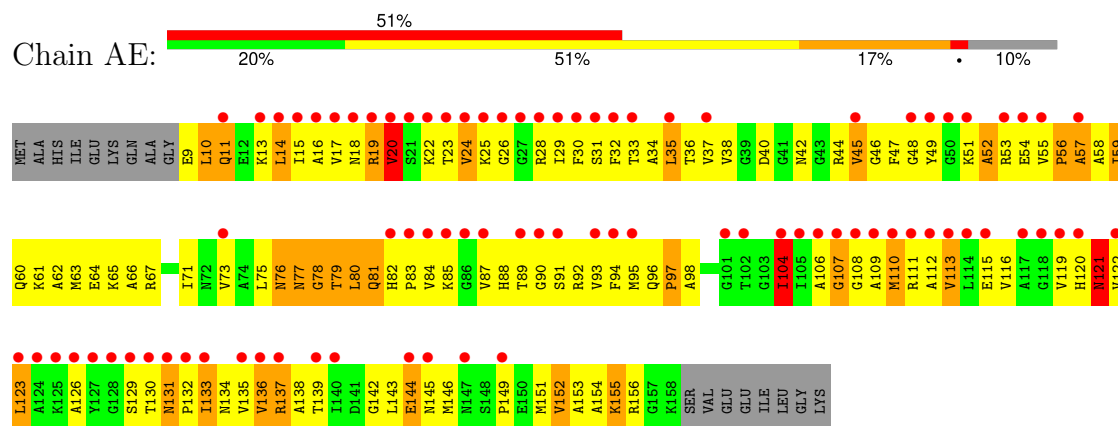
Chain AD: 



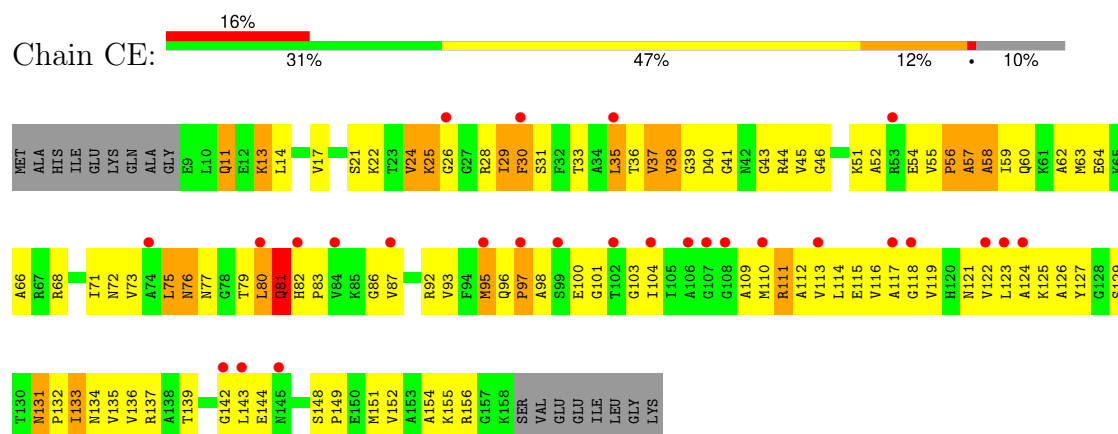
• Molecule 3: 30S ribosomal protein S4



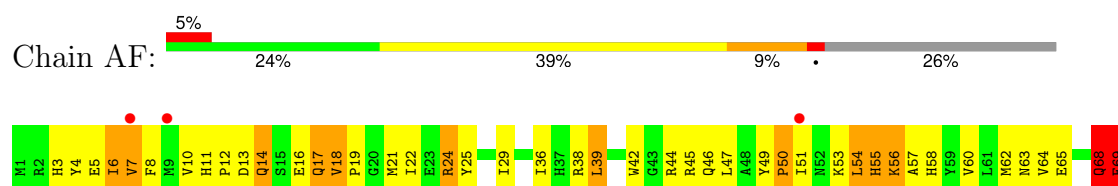
• Molecule 4: 30S ribosomal protein S5

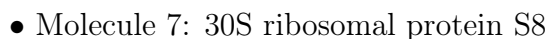
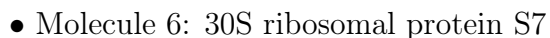
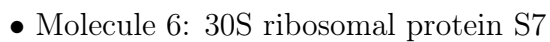
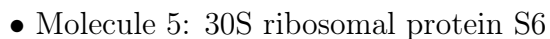


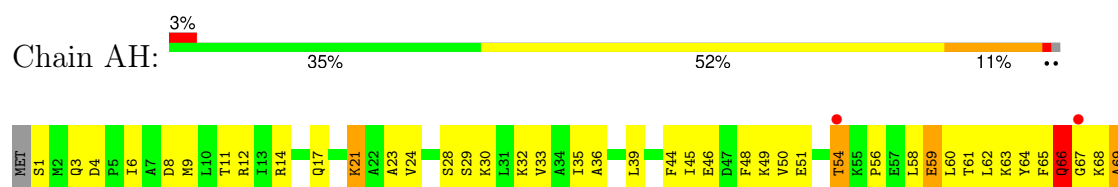
• Molecule 4: 30S ribosomal protein S5



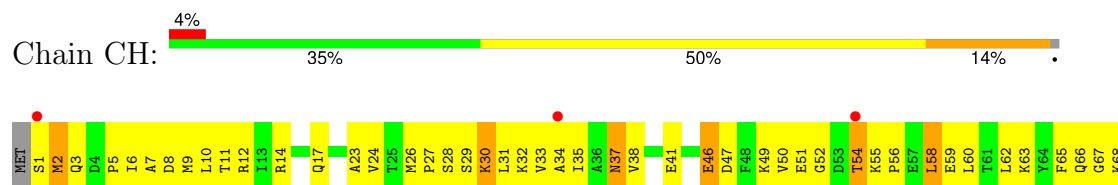
• Molecule 5: 30S ribosomal protein S6



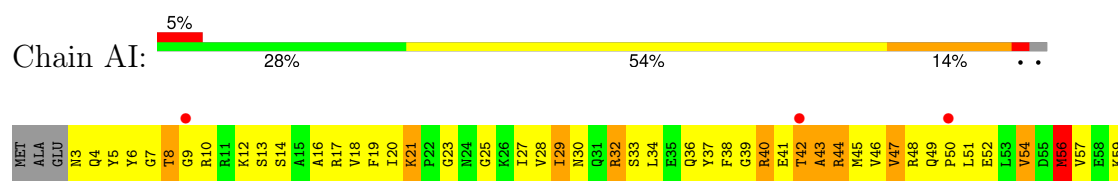




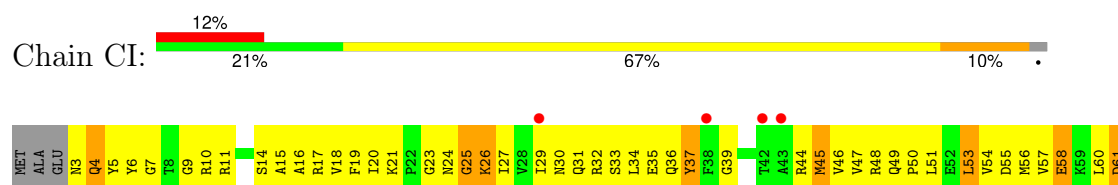
- Molecule 7: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S9

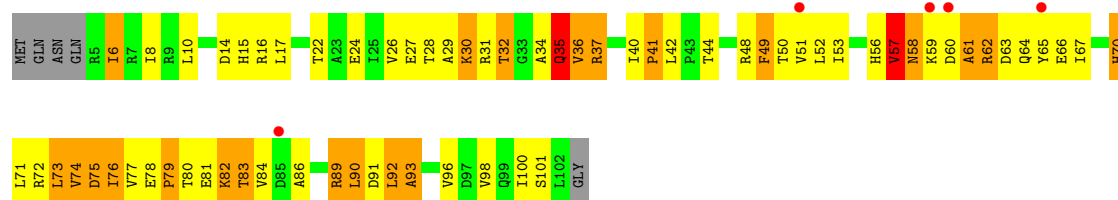


- Molecule 8: 30S ribosomal protein S9

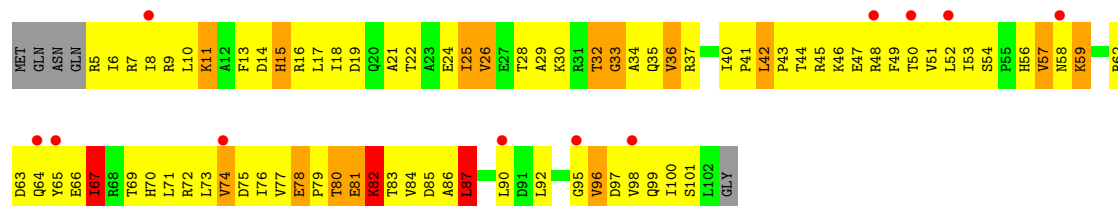


- Molecule 9: 30S ribosomal protein S10

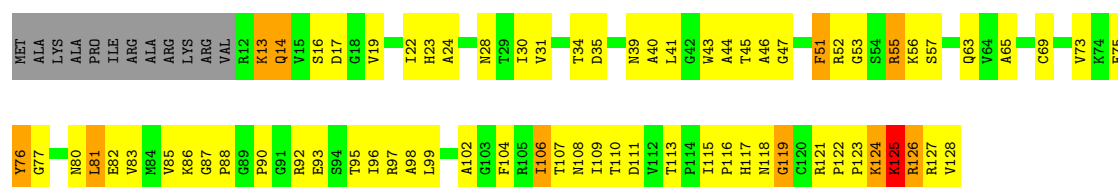




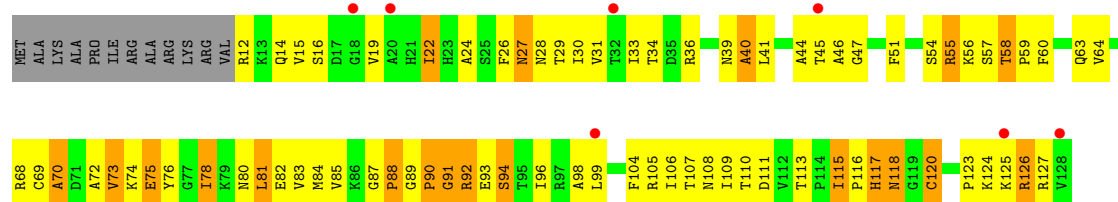
• Molecule 9: 30S ribosomal protein S10



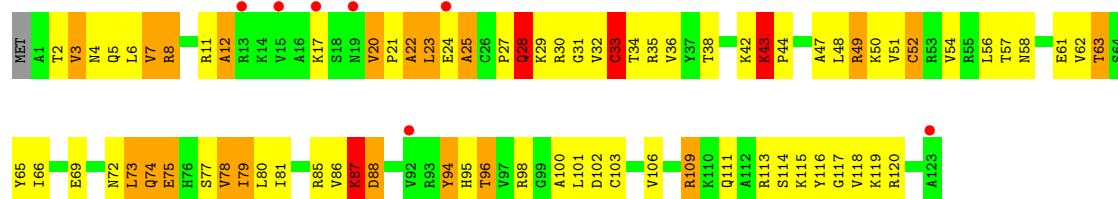
• Molecule 10: 30S ribosomal protein S11



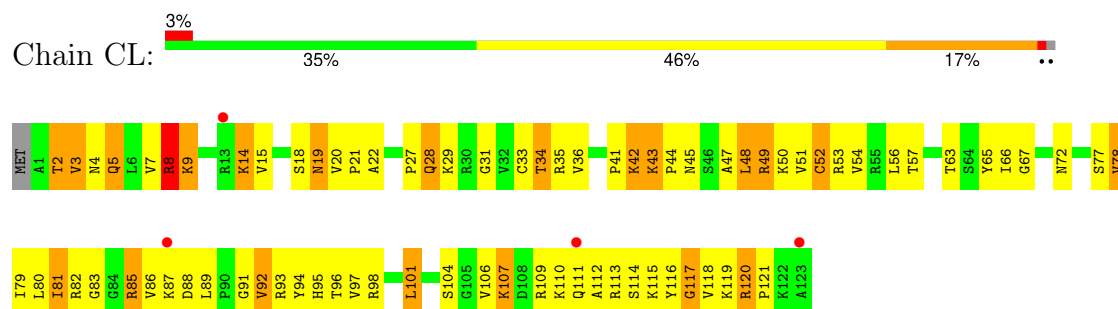
• Molecule 10: 30S ribosomal protein S11



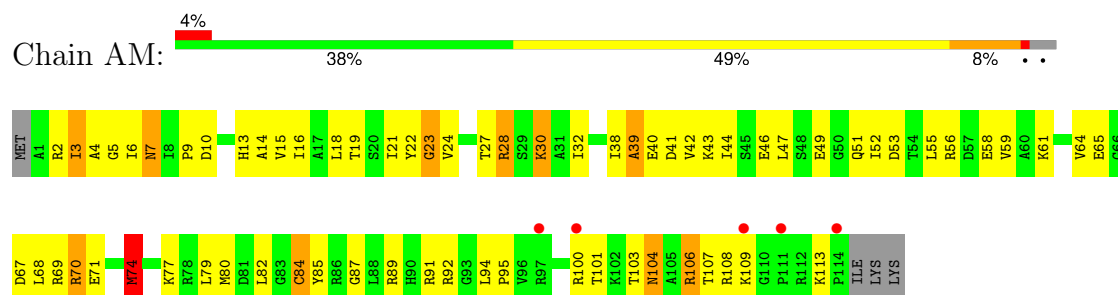
• Molecule 11: 30S ribosomal protein S12



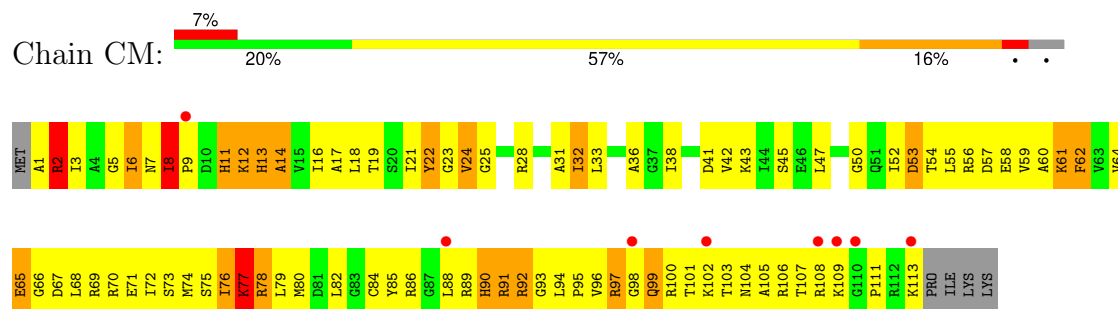
- Molecule 11: 30S ribosomal protein S12



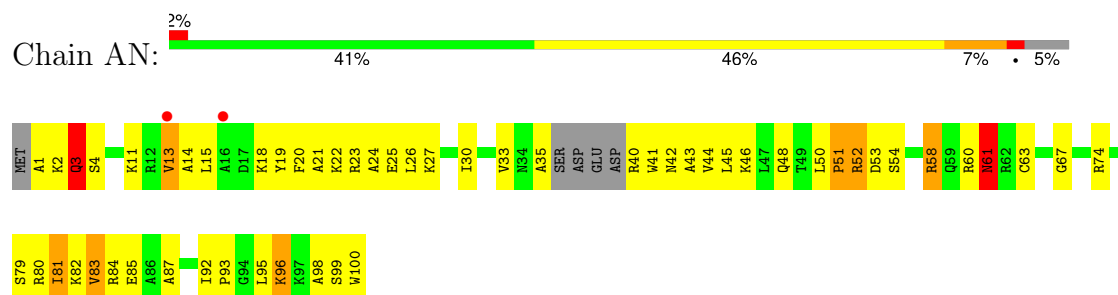
- Molecule 12: 30S ribosomal protein S13



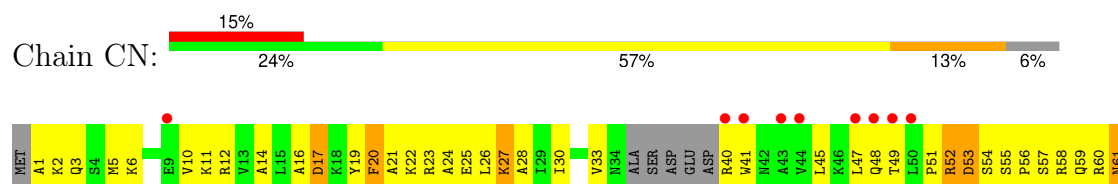
- Molecule 12: 30S ribosomal protein S13

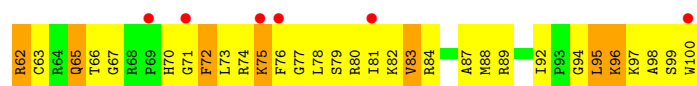


- Molecule 13: 30S ribosomal protein S14

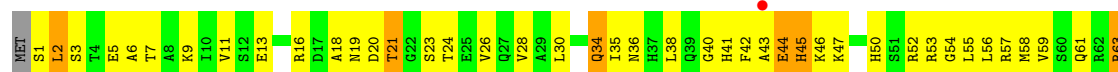


- Molecule 13: 30S ribosomal protein S14

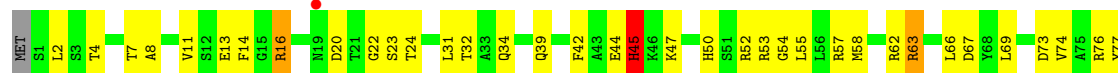




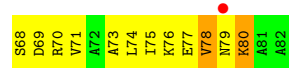
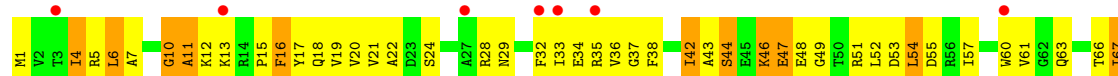
- Molecule 14: 30S ribosomal protein S15



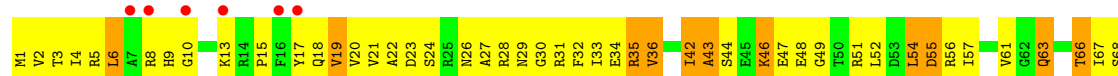
- Molecule 14: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S16

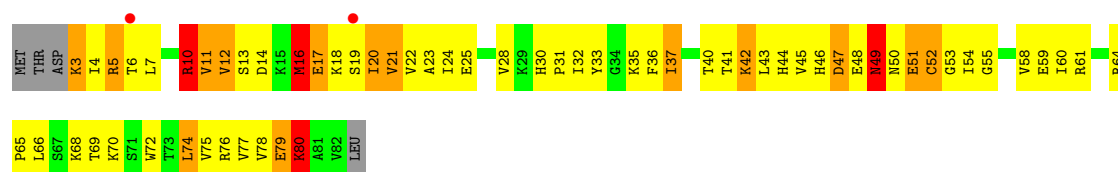


- Molecule 15: 30S ribosomal protein S16

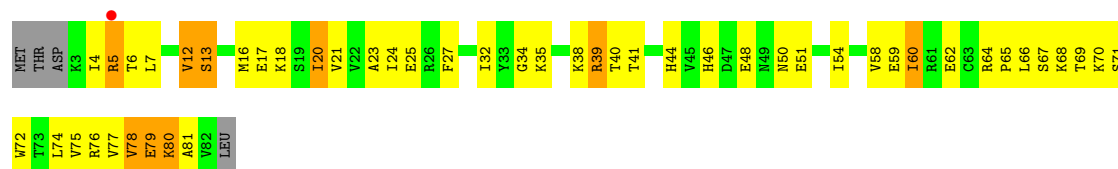


- Molecule 16: 30S ribosomal protein S17

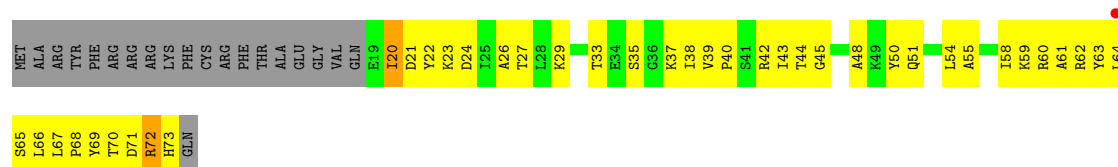




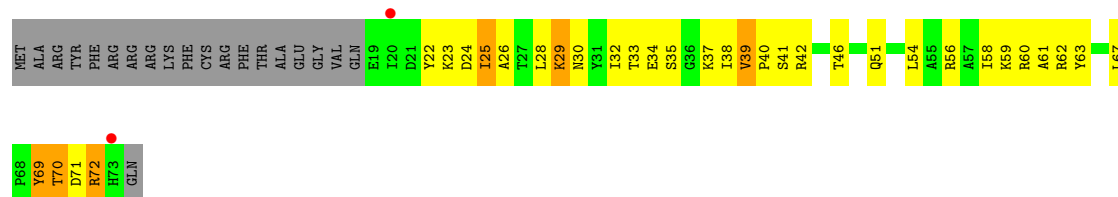
- Molecule 16: 30S ribosomal protein S17



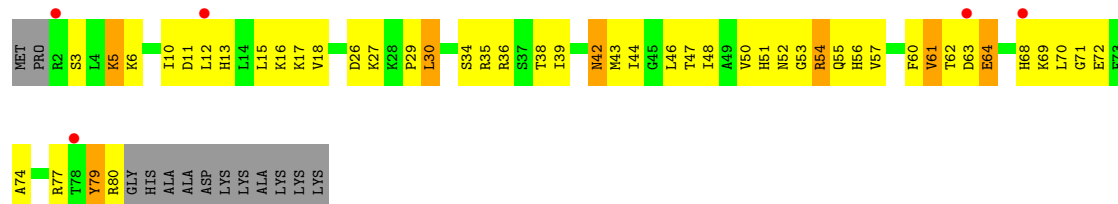
- Molecule 17: 30S ribosomal protein S18



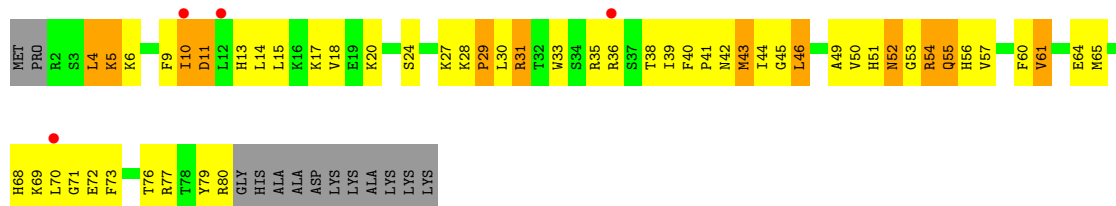
- Molecule 17: 30S ribosomal protein S18



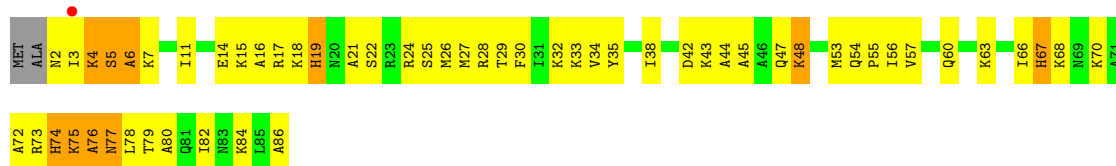
- Molecule 18: 30S ribosomal protein S19



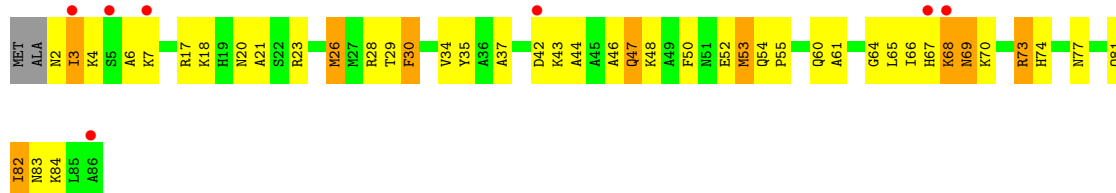
- Molecule 18: 30S ribosomal protein S19



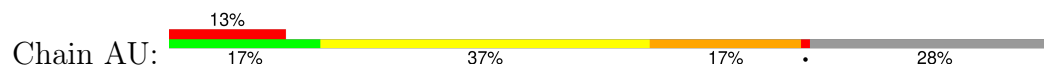
- Molecule 19: 30S ribosomal protein S20



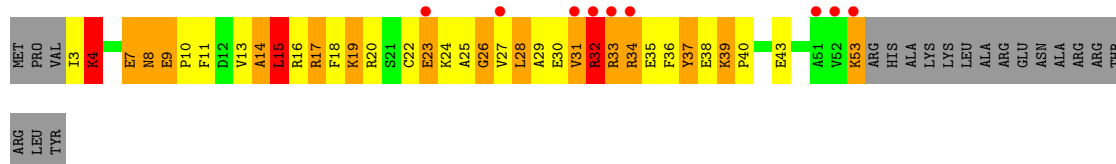
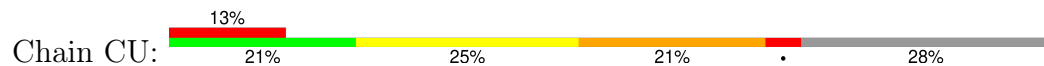
- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S21

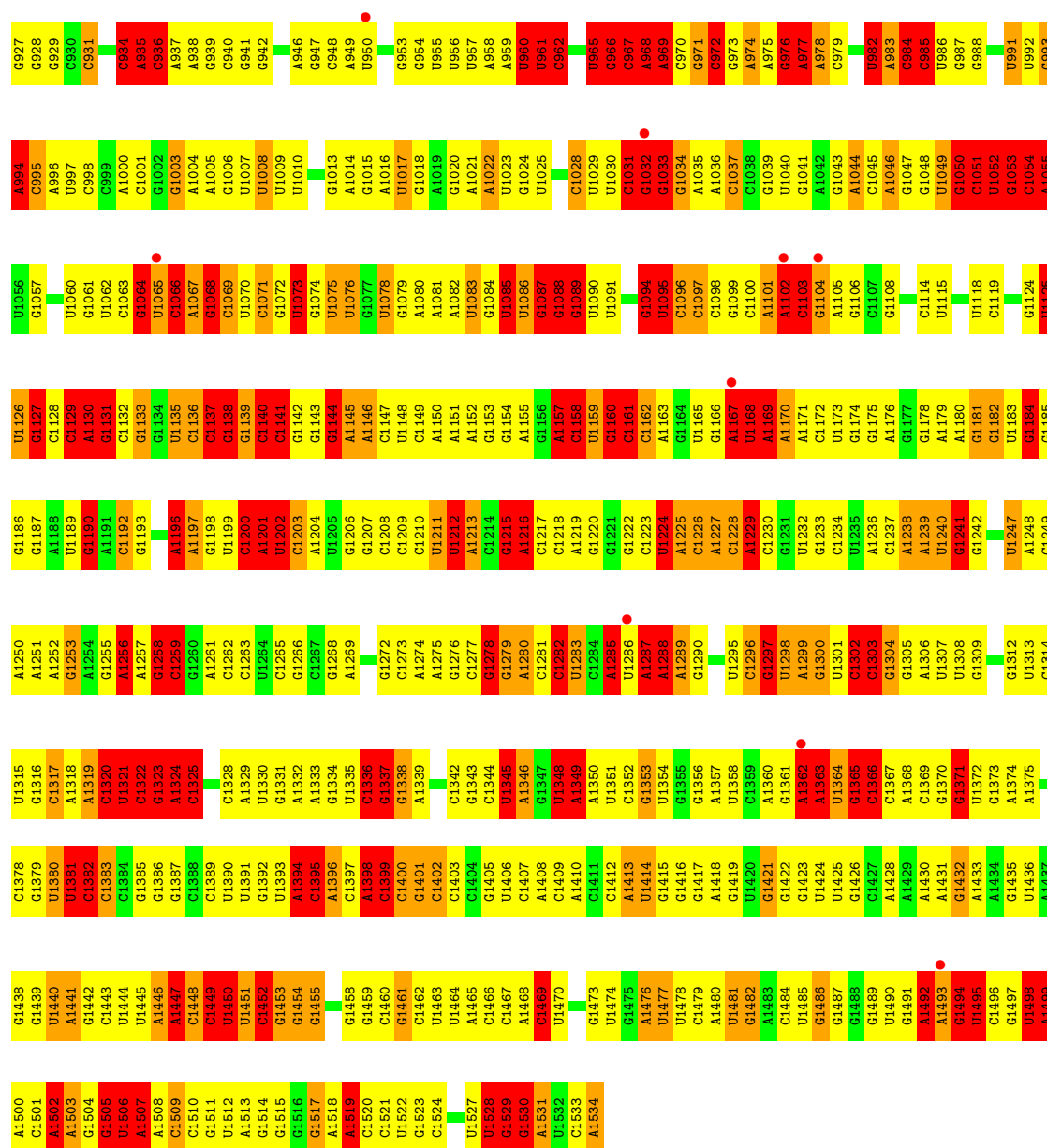


- Molecule 20: 30S ribosomal protein S21



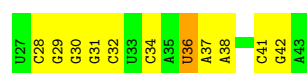
- Molecule 21: 16S rRNA





• Molecule 22: P-site tRNA ASL fragment

Chain AV: 35% 59% 6%

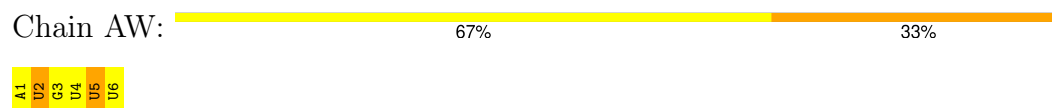


• Molecule 22: P-site tRNA ASL fragment

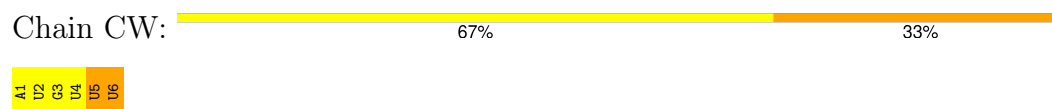
Chain CV: 41% 53% 6%



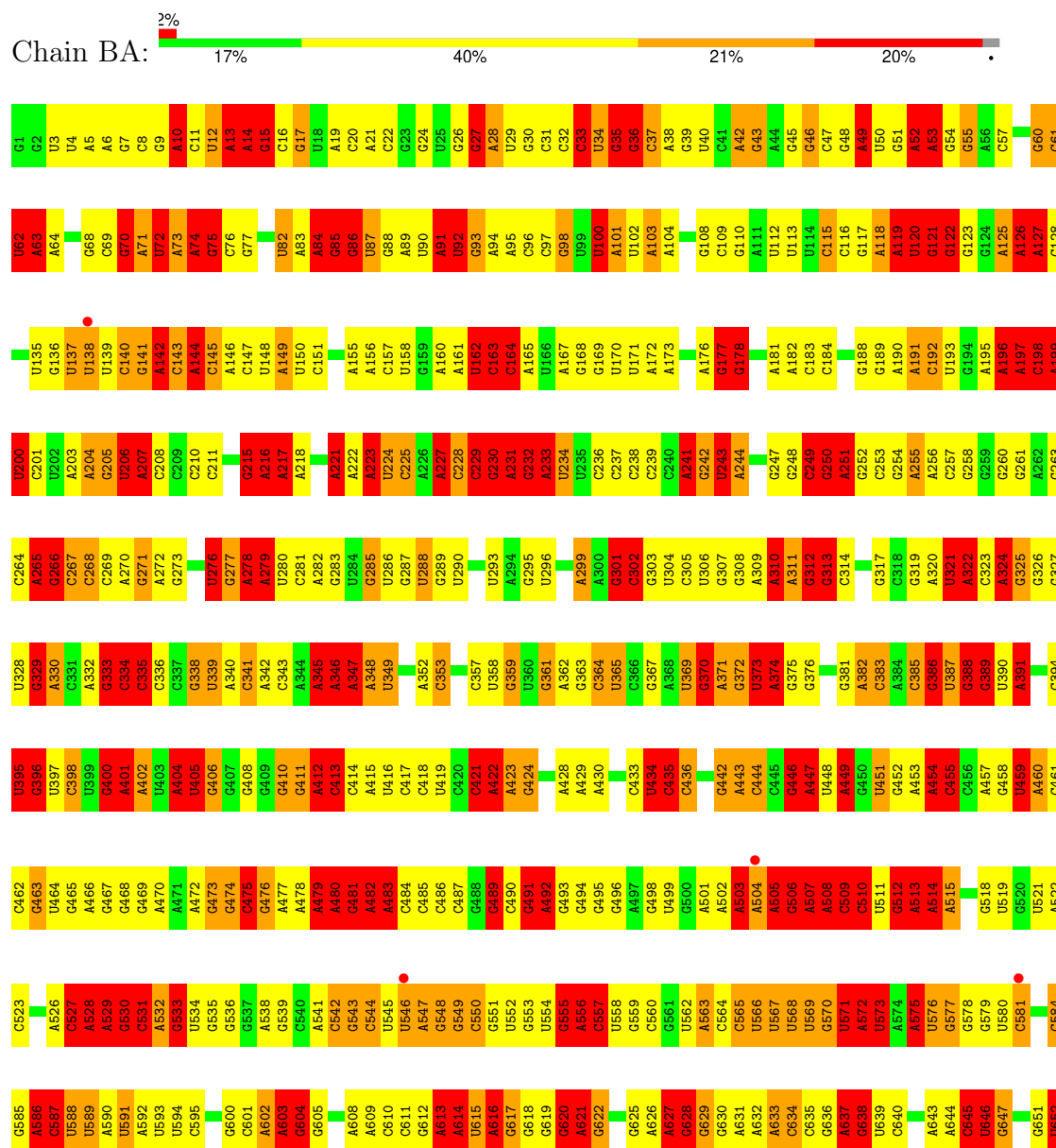
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA

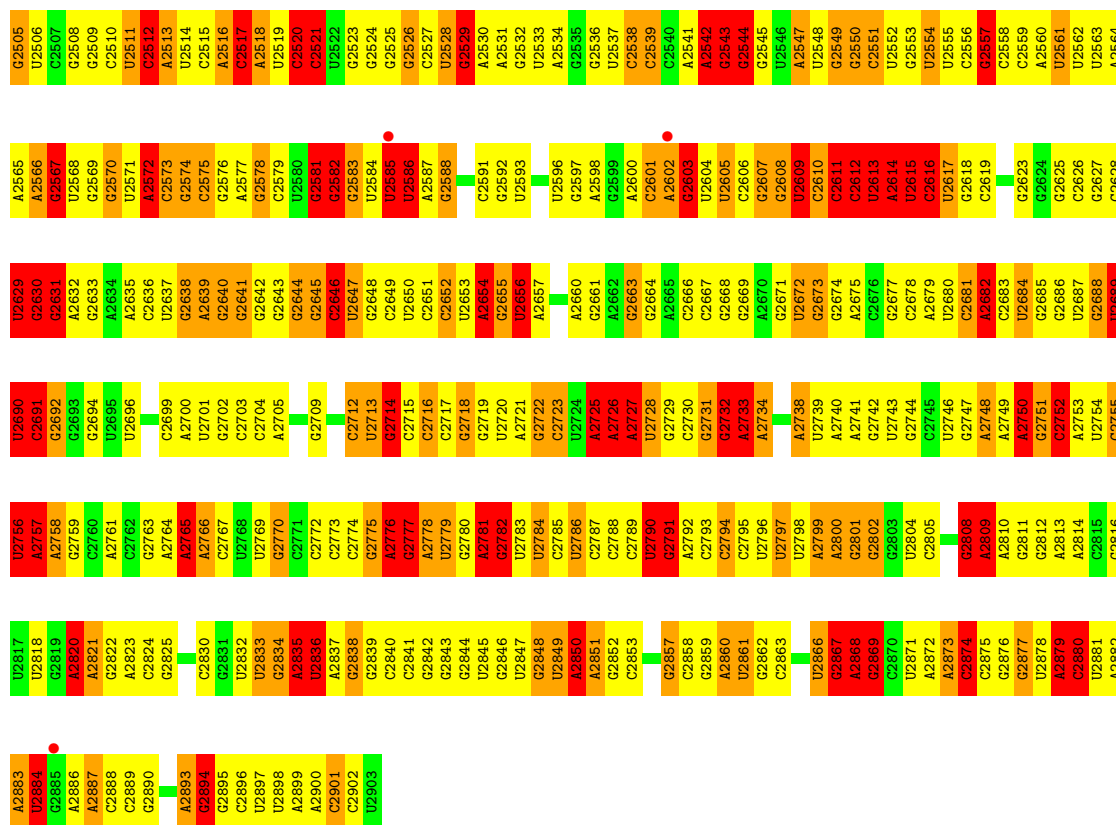


- Molecule 24: 23S rRNA

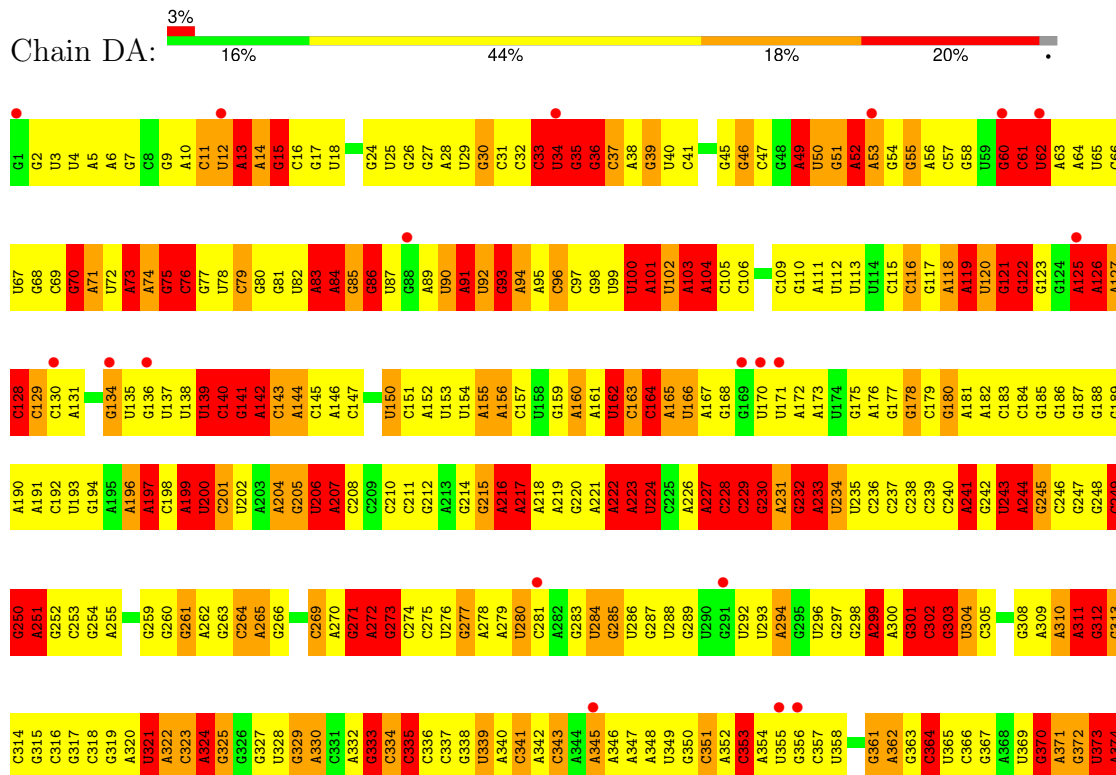






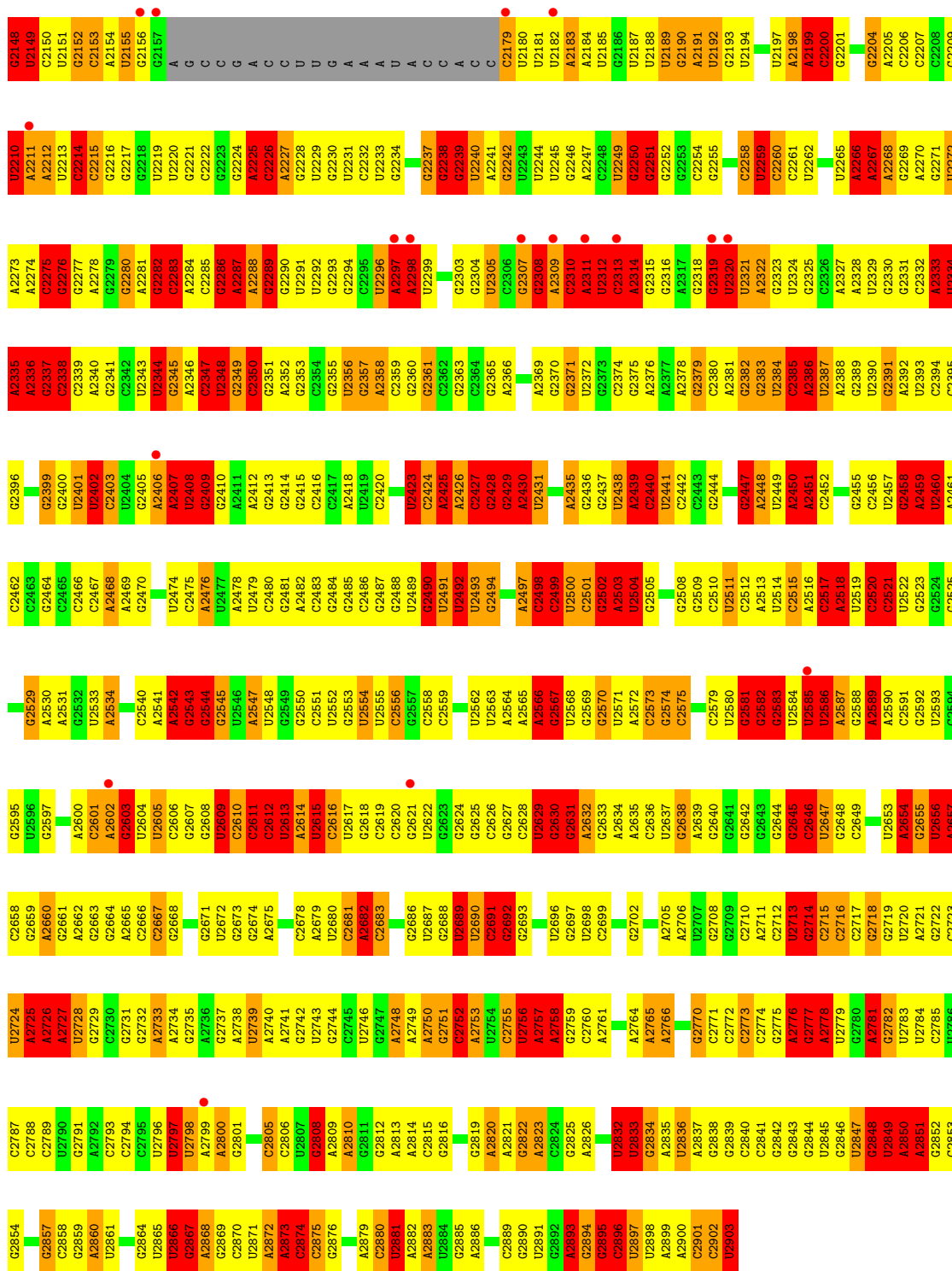


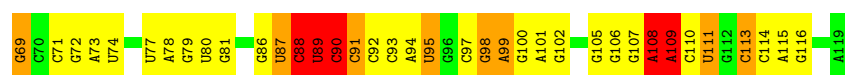
• Molecule 24: 23S rRNA



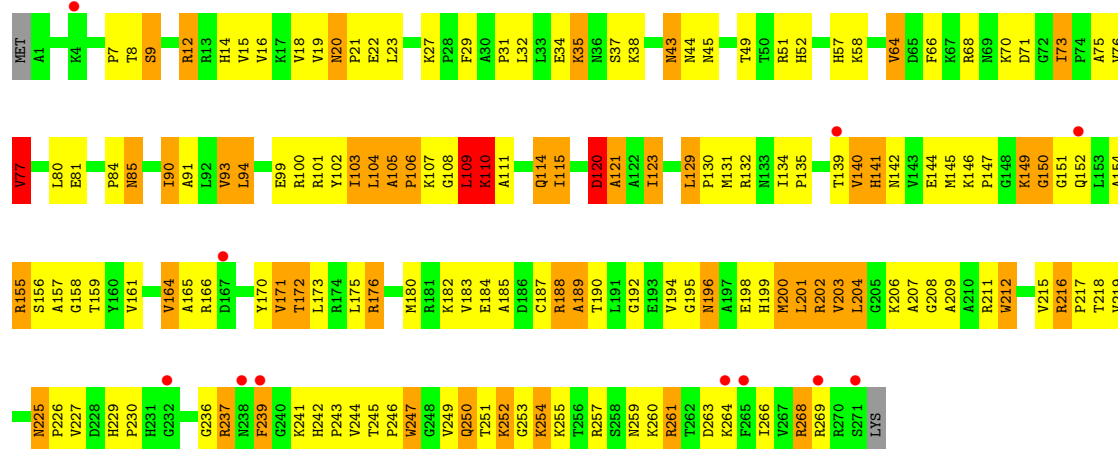
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G1201	G1139	U1077	G1016	U955	C	G823	A761	G696	G630	U567	A502	G438	G377
G1202	G1140	U1078	G1017	G956	A	U824	U762	G697	A631	U568	A503	U439	G378
U1203	U1141	C1079	U1018	C957	U	G825	G763	C698	A632	U569	A504	C440	G379
A1204	A1142	A1080	U1019	U958	C	U826	A764	A699	A633	G570	A505	U441	G380
A1205	A1143	U1081	A1020	A959	C	U827	G765	G700	G634	U571	A506	G442	G381
G1206	A1144	U1082	A1021	A960	C	U828	U766	G701	C635	A572	A507	G443	A382
C1207	C1145	U1083	G1022	G961	G	A829	U767		G636	U573	A508	C444	A383
C1208	C1146	A1084	U1023	G962	A	G830	G768	G704	A637	A574	C509	C445	
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G1210	G1087	G1087	G1025	G964	U	U832	U773	G705	G640	G577	C512	A448	U387
C1211	A1088	A1088	A1026	C965	U	A833	G774	A706		G578	G512	A449	G388
G1212	C1152	A1089	A1027	G966	A	G834	G775	G707		G579	A513	A450	U390
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A1214	G1154	U1091	A1029	G968			G777	G711	U646	U581		C445	U392
G1215	G1031	G1031	G1030	G969	G	U839	G778		G647	A582	G518	C446	U393
U1219	G1032	G1032	G904	U970	C903	C840	G779	A715	G648	A583	U519	A447	C394
G1220	A1032	U1033	G904	G971	G904	G841	U779	A716	G649	G583	G520	A454	C395
C1221	U1033	A972	G907	A972	G907	U842	G780	C717	C650	C584	U521	C455	U396
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G1224	A975	A975	A909	A975	A909	A845	A783	G726	U653	G587	G524	C458	U399
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A1226	G977	G977	A911	G977	A911	U847	G785	A722	A655	U589	A526	A460	A401
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C1239	C991	C991	A925	C991	A925	G859	C797	A734	G669	G604	A538	C473	A412
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A1241	C993	C993	A927	C993	A927	A861	G799	C736	G671	U607	C540	C475	C414
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G1245	C996	C996	U930	C996	U930	G864	A802	A739	C673	A609	C545	A477	U417
A1246	U997	U997	U931	U997	U931	C865	A804	C740	G674	C610	U545	A478	C418
C1247	C998	C998	U932	C998	U932	A866	A804	U741	A675	G611	U546	A480	U419
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A1253	U1003	U1003	G942	U1003	G942	U871	G809	U746	G683	A616	G553	C485	G424
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G1255	A1006	A1006	A943	A1006	A943	C873	U811	G748	G685	G618	U554	C489	C426
C1256	C1007	C1007	G944	C1007	G944	G874	C812	A749	A686	G619	G555	C490	U427
A1257	U1009	U1009	A945	U1009	A945	U875	U813	A750	U687	G620		G491	A428
U1258	A1010	A1010	C946	A1010	C946	C876	C814	A751	C687	A821	U558	A492	A429
G1259	C1013	C1013	A947	C1013	A947	A877	C815	A752	U688	G622	G559	C493	A430
A1260	U1012	U1012	G948	U1012	G948	A878	C816	A753	A689	C623	C560	C494	U431
C1261	G1071	G1071	C948	G1071	C948	G	C817	U754	G690	C624	G561	A497	A432
U1262	A1070	A1070	G949	U1070	G949	G	G818	U755	C691	G625	U562	C496	C433
A1263	A1073	A1073	G952	U1073	G952	G	A819	A756	C692	A626	A563	U499	U434
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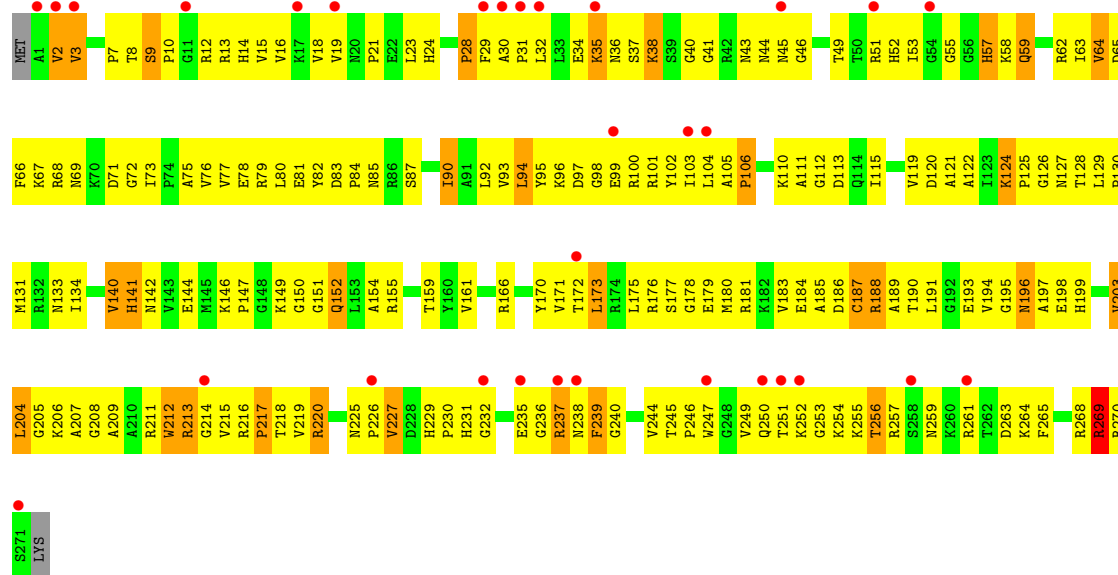




• Molecule 26: 50S ribosomal protein L2

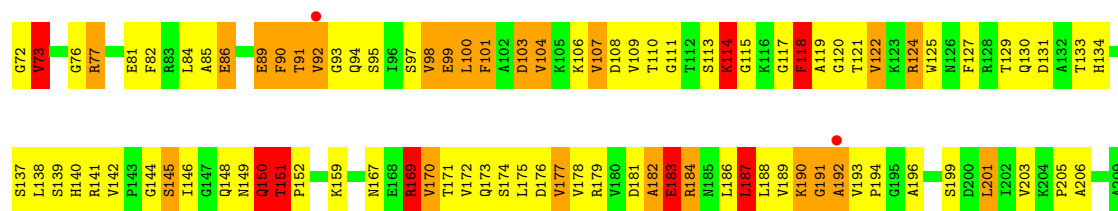


• Molecule 26: 50S ribosomal protein L2

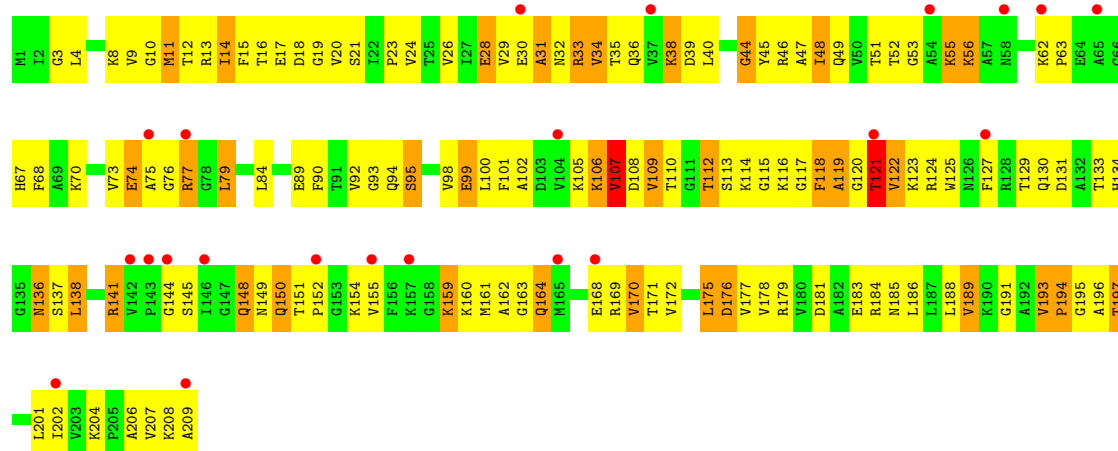


• Molecule 27: 50S ribosomal protein L3

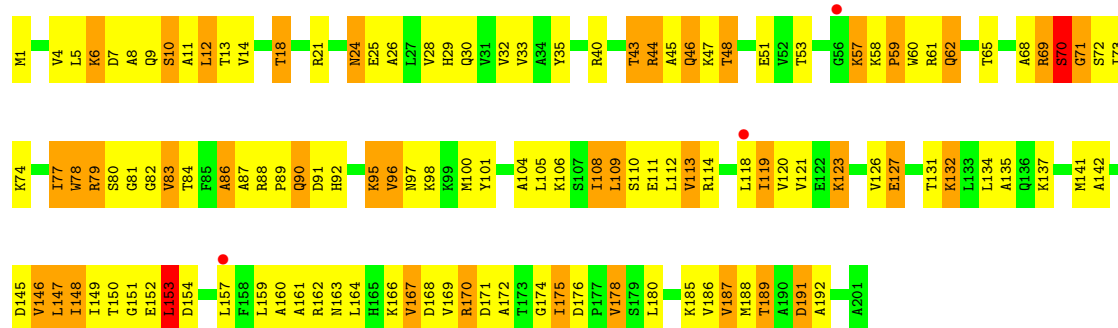




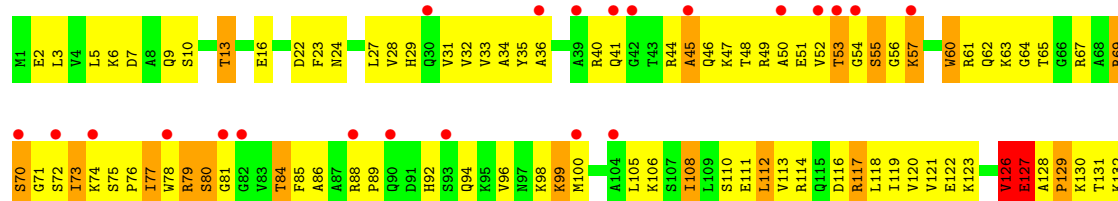
• Molecule 27: 50S ribosomal protein L3

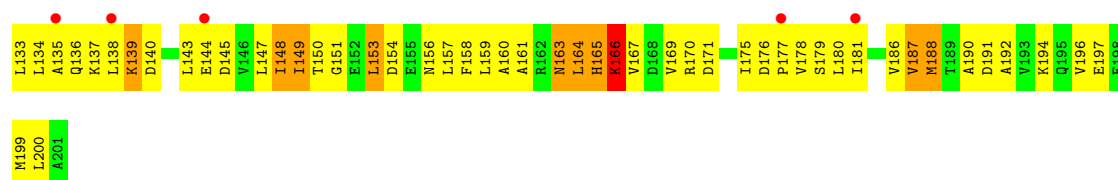


• Molecule 28: 50S ribosomal protein L4

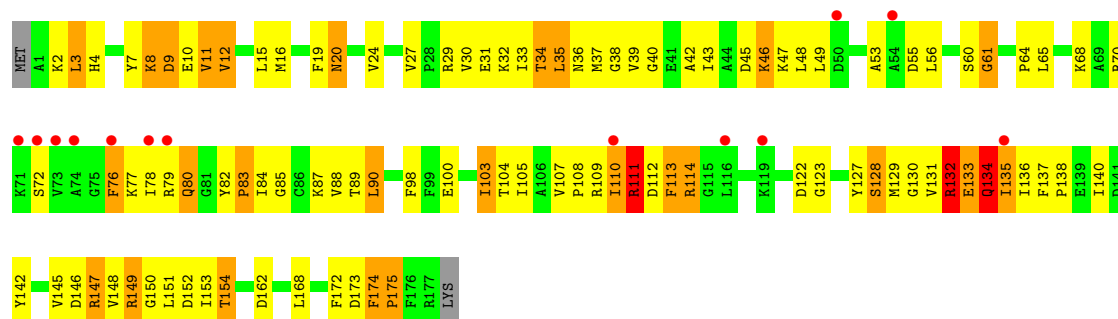
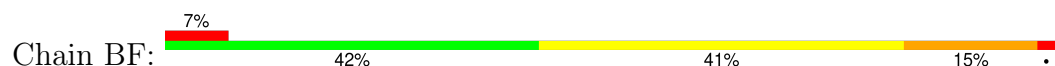


• Molecule 28: 50S ribosomal protein L4

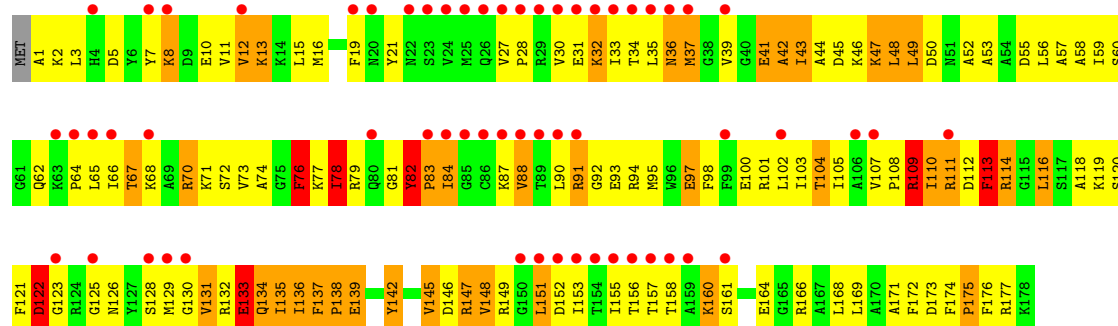




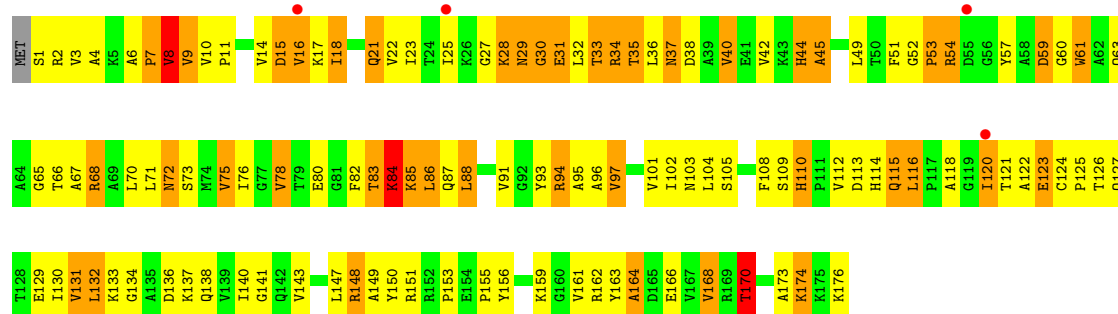
• Molecule 29: 50S ribosomal protein L5



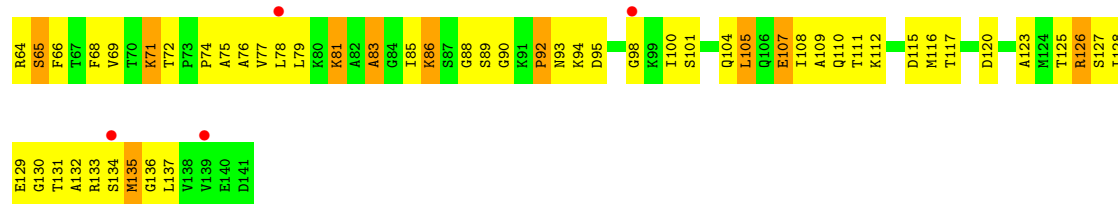
• Molecule 29: 50S ribosomal protein L5



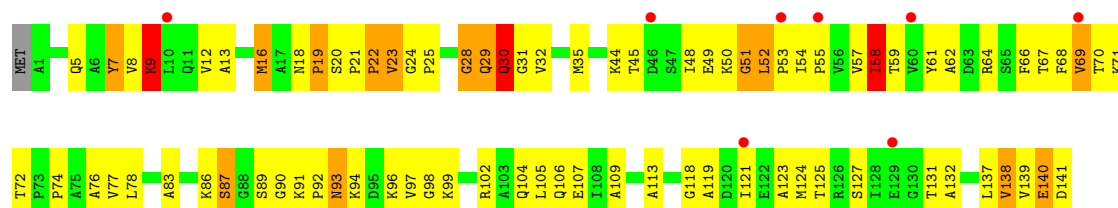
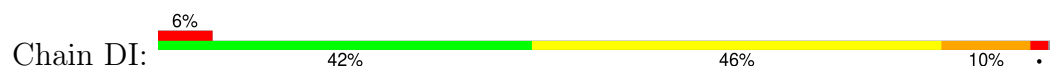
• Molecule 30: 50S ribosomal protein L6



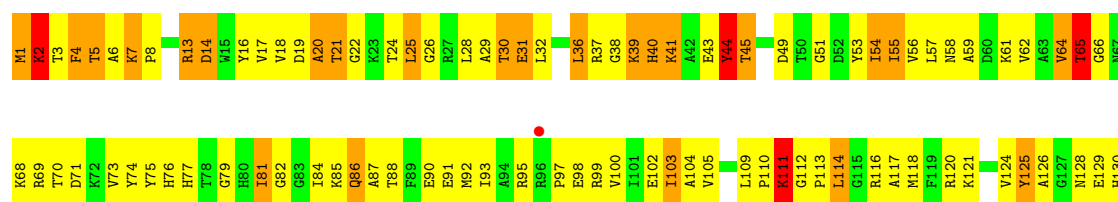
• Molecule 30: 50S ribosomal protein L6



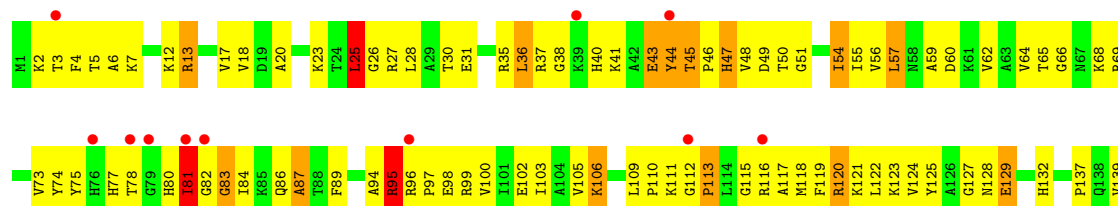
• Molecule 32: 50S ribosomal protein L11



• Molecule 33: 50S ribosomal protein L13

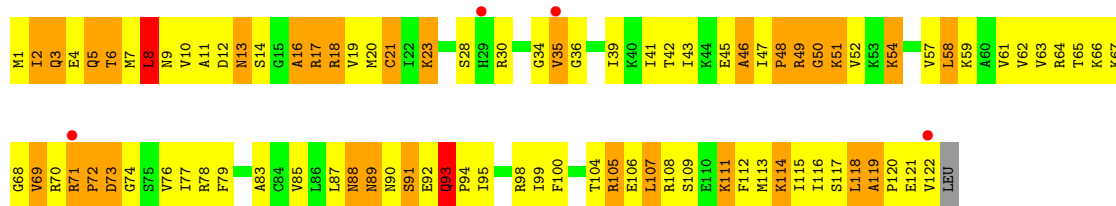


• Molecule 33: 50S ribosomal protein L13

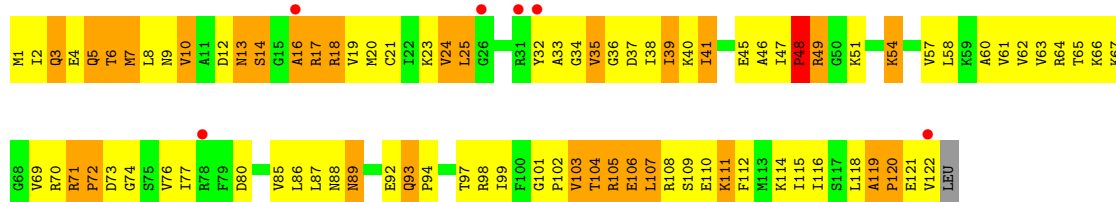


• Molecule 34: 50S ribosomal protein L14

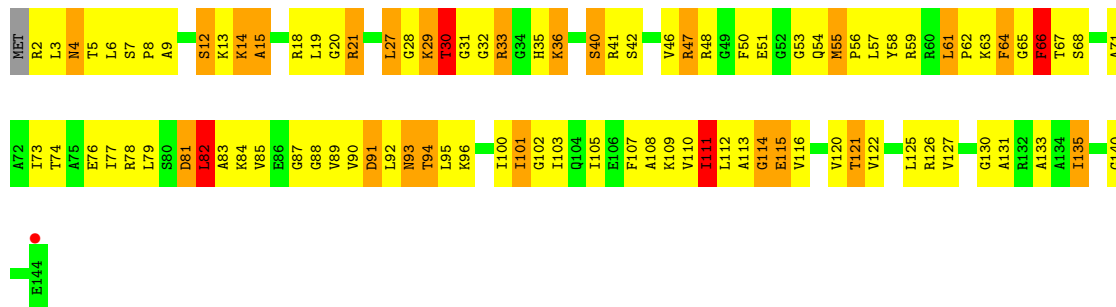




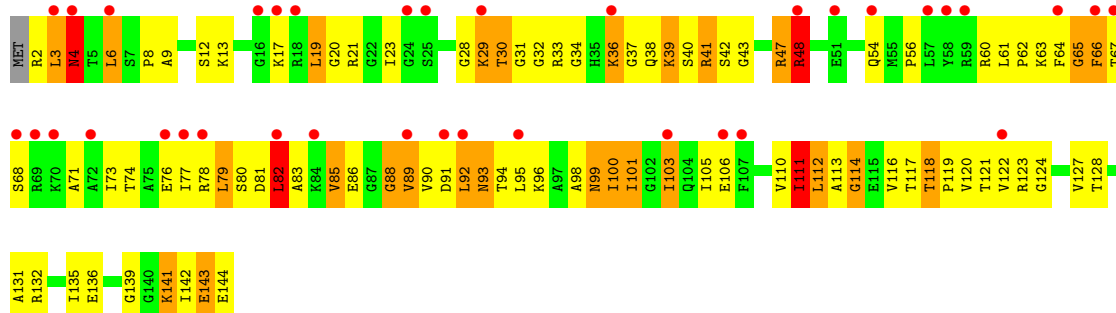
• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15

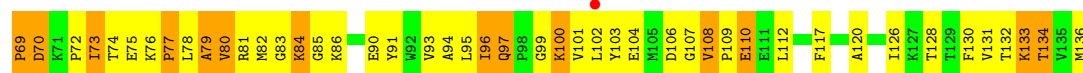


• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

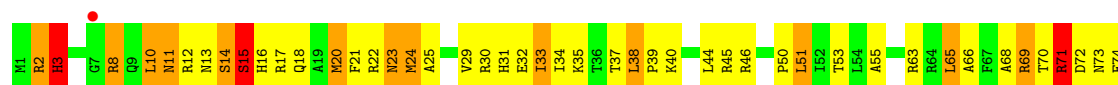




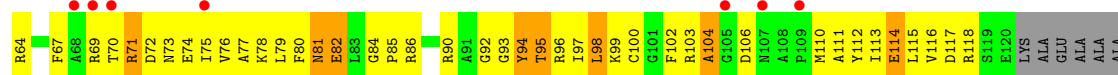
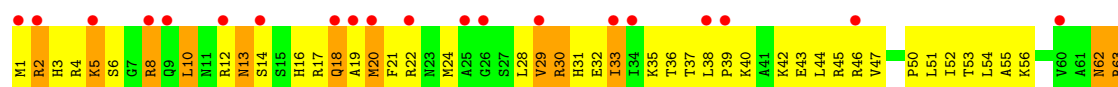
• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17

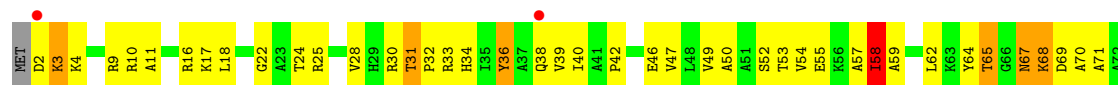


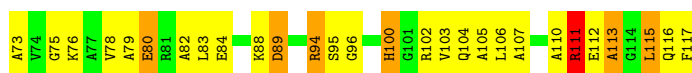
• Molecule 37: 50S ribosomal protein L17



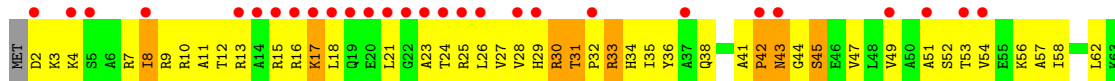
GLU

• Molecule 38: 50S ribosomal protein L18

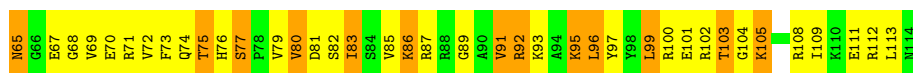
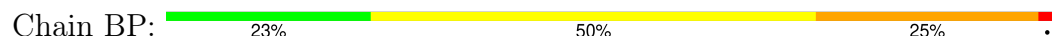




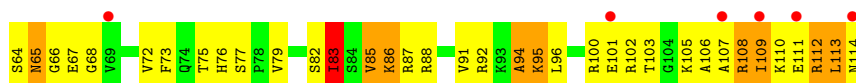
• Molecule 38: 50S ribosomal protein L18



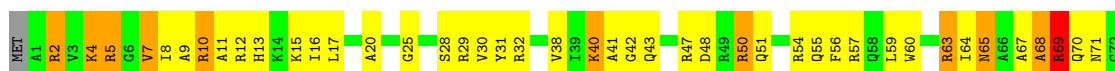
• Molecule 39: 50S ribosomal protein L19



• Molecule 39: 50S ribosomal protein L19



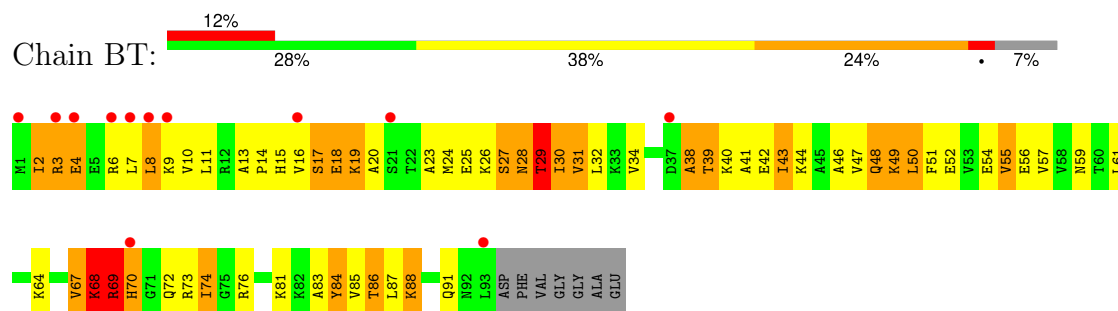
• Molecule 40: 50S ribosomal protein L20



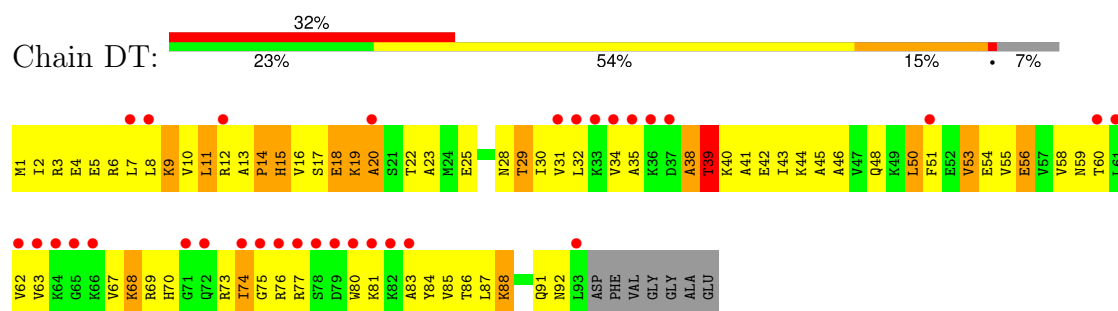
• Molecule 40: 50S ribosomal protein L20



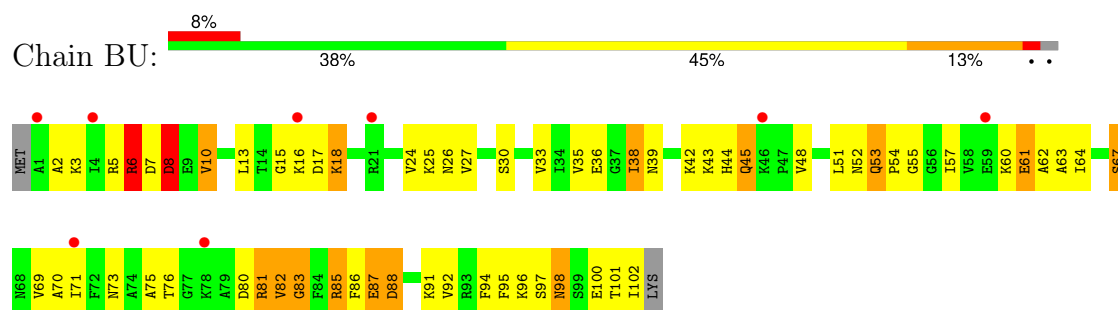
- Molecule 43: 50S ribosomal protein L23

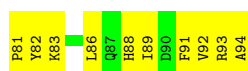


- Molecule 43: 50S ribosomal protein L23

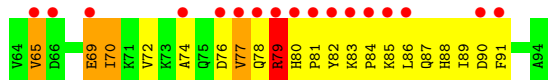


- Molecule 44: 50S ribosomal protein L24

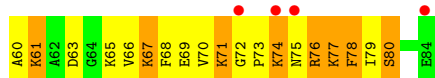
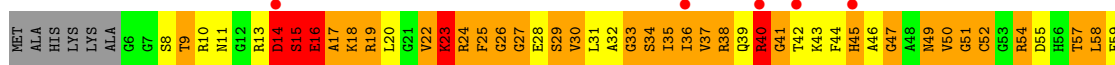




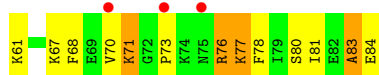
- Molecule 45: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27

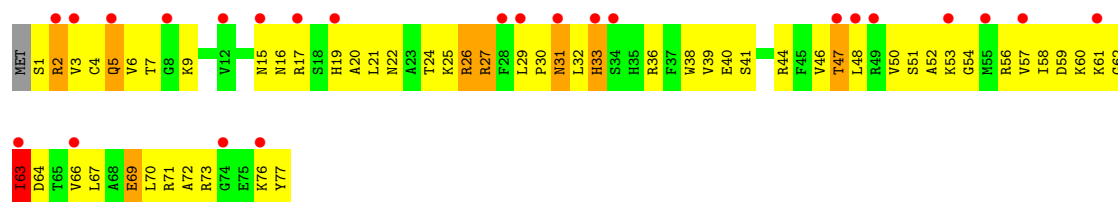


- Molecule 47: 50S ribosomal protein L28

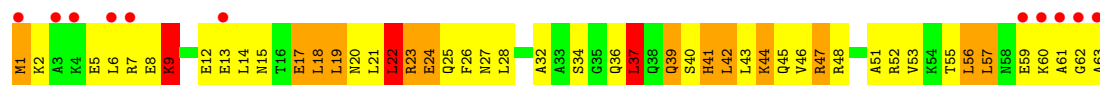


- Molecule 47: 50S ribosomal protein L28





- Molecule 48: 50S ribosomal protein L29



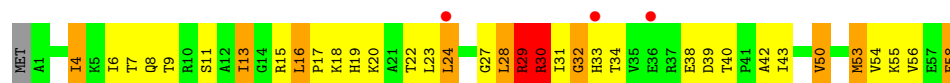
- Molecule 48: 50S ribosomal protein L29



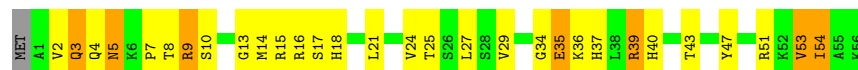
- Molecule 49: 50S ribosomal protein L30



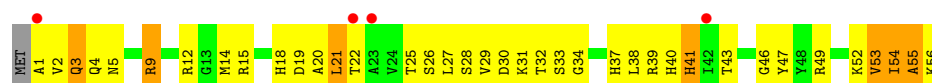
- Molecule 49: 50S ribosomal protein L30



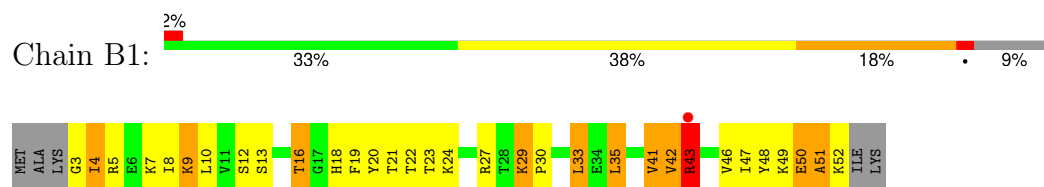
- Molecule 50: 50S ribosomal protein L32



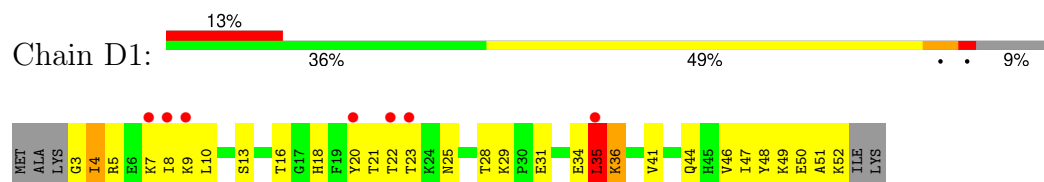
- Molecule 50: 50S ribosomal protein L32



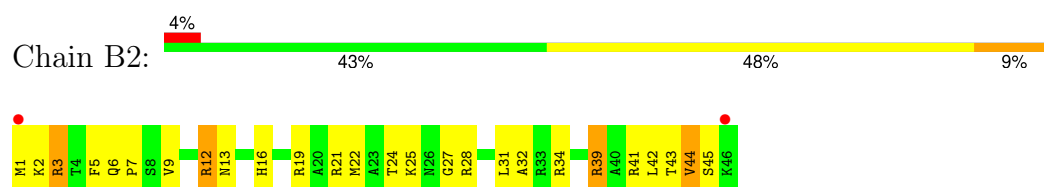
- Molecule 51: 50S ribosomal protein L33



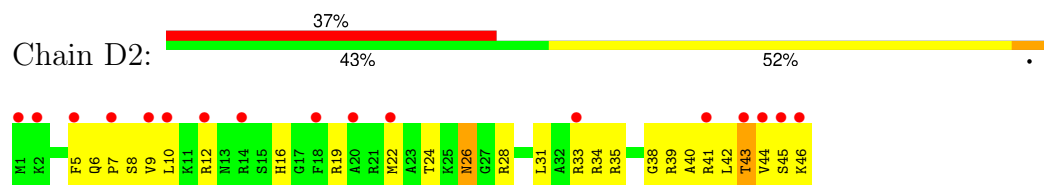
- Molecule 51: 50S ribosomal protein L33



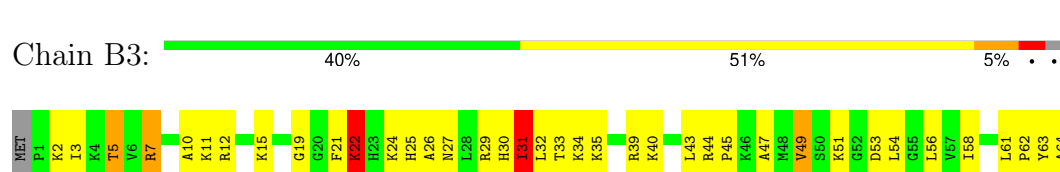
- Molecule 52: 50S ribosomal protein L34



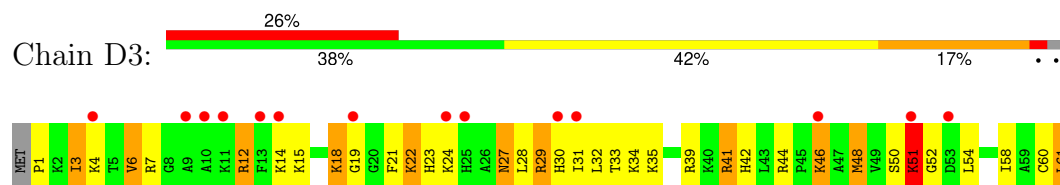
- Molecule 52: 50S ribosomal protein L34



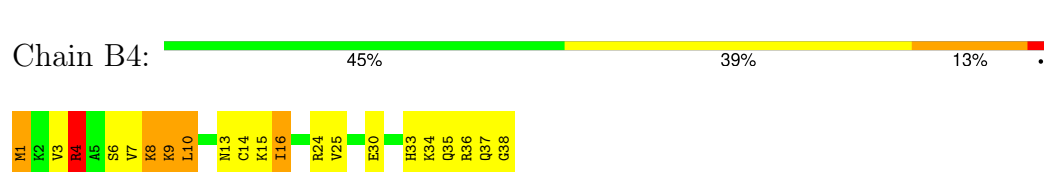
- Molecule 53: 50S ribosomal protein L35



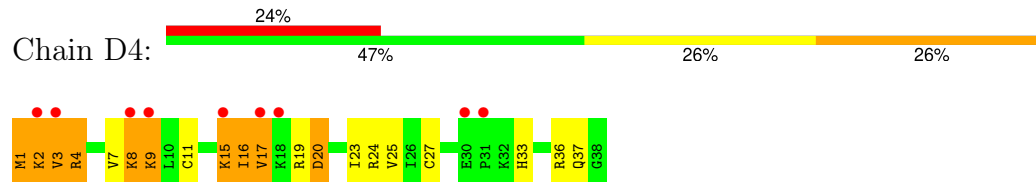
- Molecule 53: 50S ribosomal protein L35



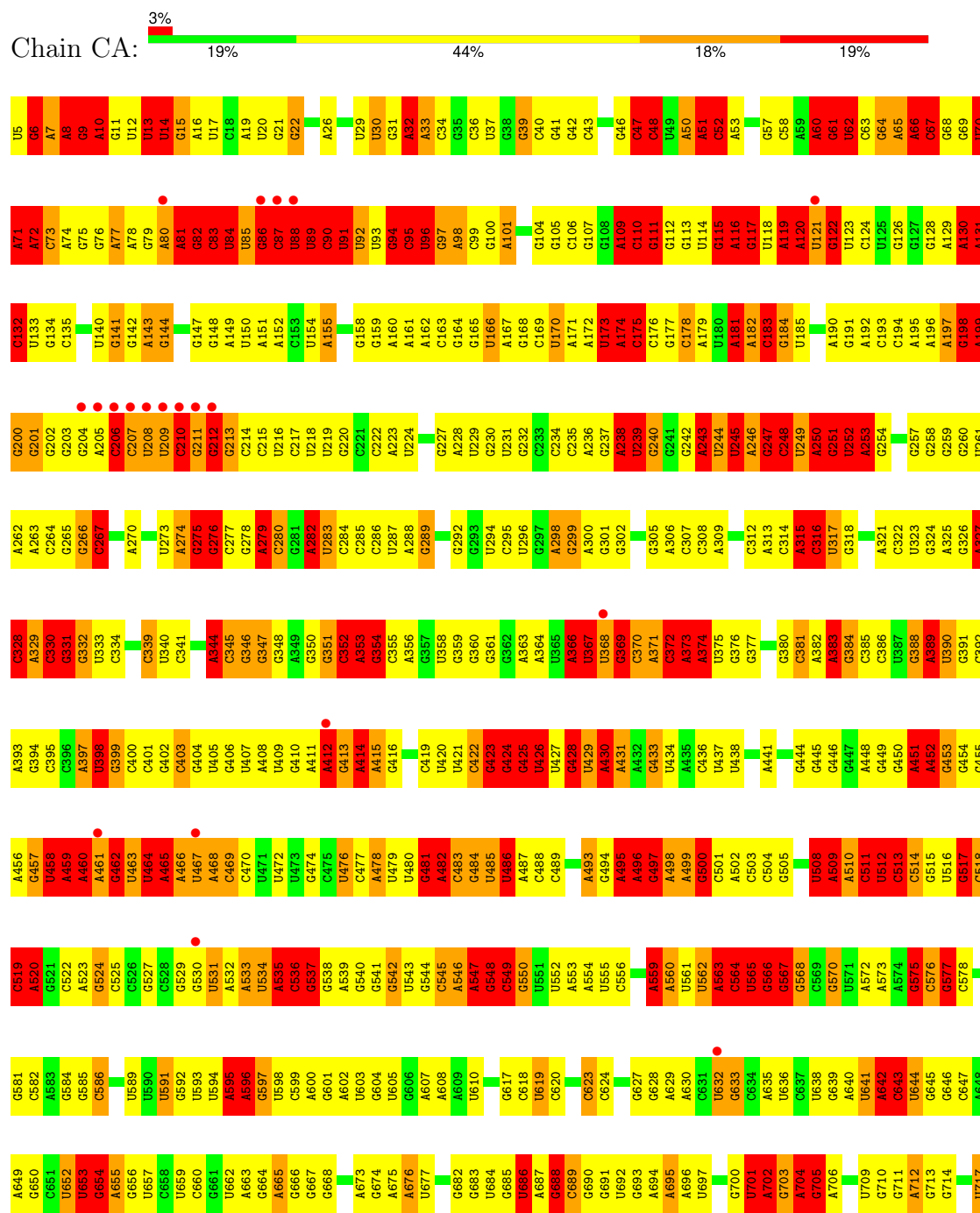
- Molecule 54: 50S ribosomal protein L36

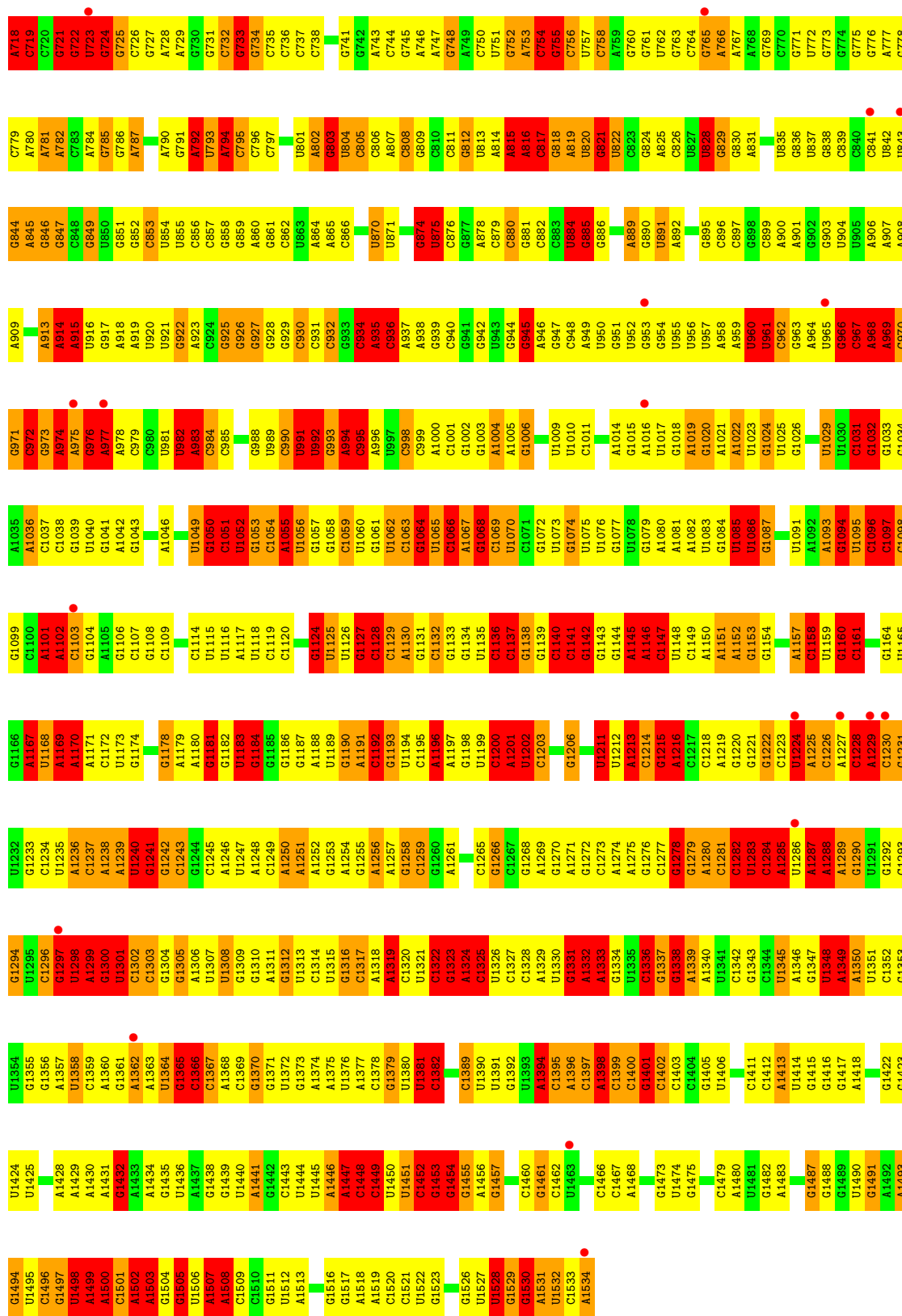


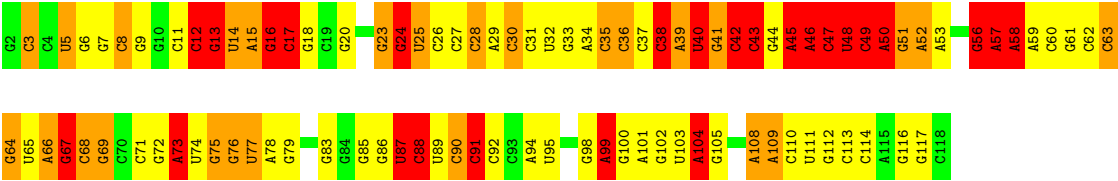
• Molecule 54: 50S ribosomal protein L36



• Molecule 55: 16S rRNA







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.72Å 435.07Å 628.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.71 – 3.81 75.71 – 3.81	Depositor EDS
% Data completeness (in resolution range)	78.6 (75.71-3.81) 78.6 (75.71-3.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.253 0.218 , 0.261	Depositor DCC
R_{free} test set	8842 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	99.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	285420	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AB	0.27	0/1735	0.48	0/2338
1	CB	0.28	0/1735	0.52	0/2338
2	AC	0.28	0/1651	0.50	0/2225
2	CC	0.29	0/1651	0.48	0/2225
3	AD	0.29	0/1665	0.48	0/2227
3	CD	0.36	0/1665	0.53	0/2227
4	AE	0.35	0/1118	0.64	1/1504 (0.1%)
4	CE	0.34	0/1118	0.55	0/1504
5	AF	0.27	0/835	0.49	0/1128
5	CF	0.26	0/835	0.48	0/1128
6	AG	0.26	0/1195	0.45	0/1602
6	CG	0.30	0/1187	0.51	0/1591
7	AH	0.31	0/989	0.49	0/1326
7	CH	0.30	0/989	0.50	0/1326
8	AI	0.26	0/1034	0.46	0/1375
8	CI	0.26	0/1034	0.46	0/1375
9	AJ	0.26	0/796	0.49	0/1077
9	CJ	0.26	0/796	0.50	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.30	0/893	0.52	0/1205
11	AL	0.34	0/969	0.60	0/1300
11	CL	0.30	0/969	0.56	0/1300
12	AM	0.27	0/892	0.54	1/1193 (0.1%)
12	CM	0.36	0/884	1.04	4/1181 (0.3%)
13	AN	0.25	0/785	0.45	0/1043
13	CN	0.26	0/780	0.45	0/1036
14	AO	0.25	0/722	0.45	0/964
14	CO	0.26	0/722	0.47	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.49	0/870
16	AQ	0.32	0/657	0.57	0/881
16	CQ	0.31	0/657	0.49	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.25	0/462	0.46	0/621
17	CR	0.31	0/462	0.49	0/621
18	AS	0.25	0/652	0.44	0/877
18	CS	0.25	0/652	0.46	0/877
19	AT	0.30	0/671	0.51	0/888
19	CT	0.27	0/671	0.46	0/888
20	AU	0.28	0/430	0.53	0/570
20	CU	0.33	0/430	0.57	0/570
21	AA	0.57	0/36834	1.45	646/57462 (1.1%)
22	AV	0.56	0/401	1.20	2/622 (0.3%)
22	CV	0.55	0/401	1.18	1/622 (0.2%)
23	AW	0.76	0/138	1.54	3/212 (1.4%)
23	CW	0.79	0/138	1.93	4/212 (1.9%)
24	BA	0.77	12/68626 (0.0%)	1.70	1788/107056 (1.7%)
24	DA	0.57	3/68314 (0.0%)	1.49	1376/106569 (1.3%)
25	BB	0.71	0/2828	1.59	62/4410 (1.4%)
26	BC	0.47	0/2121	0.73	1/2852 (0.0%)
26	DC	0.35	0/2121	0.58	0/2852
27	BD	0.52	0/1586	0.81	1/2134 (0.0%)
27	DD	0.32	0/1586	0.60	0/2134
28	BE	0.45	0/1571	0.67	0/2113
28	DE	0.33	0/1571	0.53	0/2113
29	BF	0.44	1/1434 (0.1%)	0.62	1/1926 (0.1%)
29	DF	0.45	3/1444 (0.2%)	0.79	5/1937 (0.3%)
30	BG	0.38	0/1343	0.64	0/1816
30	DG	0.28	0/1343	0.50	0/1816
31	BH	0.48	1/1122 (0.1%)	0.62	1/1515 (0.1%)
31	DH	0.39	0/1122	0.54	0/1515
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.24	0/1046	0.44	0/1410
33	BJ	0.56	0/1152	0.77	1/1551 (0.1%)
33	DJ	0.37	0/1152	0.62	0/1551
34	BK	0.53	0/947	0.82	1/1268 (0.1%)
34	DK	0.35	0/947	0.61	0/1268
35	BL	0.47	0/1054	0.76	1/1403 (0.1%)
35	DL	0.34	0/1054	0.58	0/1403
36	BM	0.50	0/1093	0.70	0/1460
36	DM	0.45	0/1093	0.63	0/1460
37	BN	0.48	0/973	0.73	1/1301 (0.1%)
37	DN	0.32	0/973	0.56	0/1301
38	BO	0.41	0/902	0.61	0/1209
38	DO	0.44	0/902	0.71	2/1209 (0.2%)
39	BP	0.48	0/929	0.74	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DP	0.33	0/929	0.52	0/1242
40	BQ	0.58	0/960	0.74	0/1278
40	DQ	0.36	0/960	0.54	0/1278
41	BR	0.57	0/829	0.77	0/1107
41	DR	0.38	0/829	0.58	0/1107
42	BS	0.54	0/864	0.78	0/1156
42	DS	0.30	0/864	0.56	0/1156
43	BT	0.44	0/744	0.67	0/994
43	DT	0.27	0/744	0.51	0/994
44	BU	0.42	0/787	0.71	1/1051 (0.1%)
44	DU	0.35	0/787	0.56	1/1051 (0.1%)
45	BV	0.47	0/766	0.68	0/1025
45	DV	0.68	3/766 (0.4%)	0.81	3/1025 (0.3%)
46	BW	0.54	0/603	0.84	0/797
46	DW	0.34	0/603	0.55	0/797
47	BX	0.41	0/635	0.68	1/848 (0.1%)
47	DX	0.32	0/635	0.55	0/848
48	BY	0.42	0/510	0.67	0/677
48	DY	0.28	0/510	0.49	0/677
49	BZ	0.47	0/453	0.73	0/605
49	DZ	0.32	0/453	0.58	0/605
50	B0	0.40	0/450	0.70	0/599
50	D0	0.31	0/450	0.55	0/599
51	B1	0.40	0/416	0.59	0/554
51	D1	0.31	0/416	0.49	0/554
52	B2	0.48	0/380	0.80	0/498
52	D2	0.31	0/380	0.53	0/498
53	B3	0.46	0/513	0.67	0/676
53	D3	0.36	0/513	0.57	0/676
54	B4	0.50	0/303	0.80	0/397
54	D4	0.41	0/303	0.60	0/397
55	CA	0.55	1/36762 (0.0%)	1.45	694/57350 (1.2%)
56	DB	0.68	4/2803 (0.1%)	1.79	112/4371 (2.6%)
All	All	0.57	28/307815 (0.0%)	1.37	4715/460233 (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
27	BD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	DF	0	1
36	DM	0	1
All	All	0	4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-11.34	1.31	1.37
45	DV	31	TYR	CE1-CZ	10.97	1.52	1.38
24	DA	1060	U	C2-N3	7.54	1.43	1.37
24	BA	1142	A	C8-N7	7.36	1.36	1.31
24	BA	2857	G	N3-C4	7.16	1.40	1.35

The worst 5 of 4715 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	CM	2	ARG	NE-CZ-NH1	-22.49	109.06	120.30
24	BA	2447	G	C6-N1-C2	-18.42	114.05	125.10
12	CM	2	ARG	NE-CZ-NH2	17.95	129.28	120.30
24	BA	1330	C	N1-C1'-C2'	-17.28	91.53	114.00
56	DB	104	A	C8-N9-C4	-16.28	99.29	105.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	10	GLY	Peptide
27	BD	9	VAL	Peptide
29	DF	78	ILE	Peptide
36	DM	135	VAL	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	269	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CB	1704	0	1732	208	0
2	AC	1624	0	1699	139	0
2	CC	1624	0	1699	159	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	143	0
4	AE	1105	0	1148	242	0
4	CE	1105	0	1148	122	0
5	AF	817	0	808	78	0
5	CF	817	0	808	79	0
6	AG	1181	0	1240	98	0
6	CG	1174	0	1230	151	0
7	AH	979	0	1034	118	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	116	0
8	CI	1022	0	1070	141	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	124	0
10	AK	877	0	887	85	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	102	0
12	AM	883	0	944	71	0
12	CM	876	0	937	137	0
13	AN	774	0	827	80	0
13	CN	769	0	822	89	0
14	AO	714	0	737	54	0
14	CO	714	0	737	40	0
15	AP	649	0	666	55	0
15	CP	638	0	656	65	0
16	AQ	648	0	691	82	0
16	CQ	648	0	691	47	0
17	AR	455	0	478	42	0
17	CR	455	0	478	40	0
18	AS	637	0	665	51	0
18	CS	637	0	665	78	0
19	AT	665	0	714	59	0
19	CT	665	0	714	47	0
20	AU	425	0	449	68	0
20	CU	425	0	449	76	0
21	AA	32895	0	16553	1701	0
22	AV	360	0	185	10	0
22	CV	360	0	185	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AW	125	0	63	4	0
23	CW	125	0	63	6	0
24	BA	61274	0	30819	3143	0
24	DA	60995	0	30677	3530	0
25	BB	2529	0	1281	108	0
26	BC	2082	0	2157	200	0
26	DC	2082	0	2157	211	0
27	BD	1565	0	1616	189	0
27	DD	1565	0	1616	165	0
28	BE	1552	0	1619	150	0
28	DE	1552	0	1619	167	0
29	BF	1410	0	1447	123	0
29	DF	1420	0	1460	197	0
30	BG	1323	0	1374	163	0
30	DG	1323	0	1374	147	0
31	BH	1111	0	1148	109	0
31	DH	1111	0	1148	106	0
32	BI	1032	0	1088	110	0
32	DI	1032	0	1088	67	0
33	BJ	1129	0	1162	158	0
33	DJ	1129	0	1162	118	0
34	BK	938	0	1012	113	0
34	DK	938	0	1012	112	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	142	0
36	BM	1074	0	1157	111	0
36	DM	1074	0	1157	109	0
37	BN	960	0	1000	99	0
37	DN	960	0	1000	115	0
38	BO	892	0	923	67	0
38	DO	892	0	923	155	0
39	BP	917	0	965	134	0
39	DP	917	0	965	106	0
40	BQ	947	0	1022	130	0
40	DQ	947	0	1022	129	0
41	BR	816	0	839	88	0
41	DR	816	0	839	97	0
42	BS	857	0	922	69	0
42	DS	857	0	922	69	0
43	BT	738	0	807	108	0
43	DT	738	0	807	93	0
44	BU	779	0	834	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DU	779	0	834	107	0
45	BV	753	0	780	53	0
45	DV	753	0	780	118	0
46	BW	596	0	610	179	0
46	DW	596	0	610	120	0
47	BX	625	0	655	69	0
47	DX	625	0	655	73	0
48	BY	509	0	543	67	0
48	DY	509	0	543	62	0
49	BZ	449	0	491	46	0
49	DZ	449	0	491	38	0
50	B0	444	0	461	32	0
50	D0	444	0	461	52	0
51	B1	409	0	440	37	0
51	D1	409	0	440	33	0
52	B2	377	0	418	32	0
52	D2	377	0	418	33	0
53	B3	504	0	574	46	0
53	D3	504	0	574	50	0
54	B4	302	0	340	32	0
54	D4	302	0	340	24	0
55	CA	32831	0	16521	1808	0
56	DB	2507	0	1270	203	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	DA	134	0	0	0	0
57	DB	1	0	0	0	0
57	DC	1	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	195	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	1	0
59	AN	5	0	0	0	0
59	AT	3	0	0	0	0
59	AU	1	0	0	0	0
59	B2	2	0	0	0	0
59	B3	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B4	2	0	0	0	0
59	BA	615	0	0	31	0
59	BB	19	0	0	0	0
59	BC	7	0	0	1	0
59	BD	2	0	0	3	0
59	BE	1	0	0	1	0
59	BL	4	0	0	1	0
59	BN	2	0	0	0	0
59	BQ	1	0	0	0	0
59	BT	1	0	0	1	0
59	BV	1	0	0	1	0
59	CA	196	0	0	4	0
59	CE	3	0	0	1	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	598	0	0	14	0
59	DB	4	0	0	0	0
59	DC	14	0	0	2	0
59	DD	4	0	0	0	0
59	DE	2	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	5	0	0	0	0
59	DN	2	0	0	0	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	285420	0	191332	18973	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 40.

The worst 5 of 18973 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)
24:DA:1439:A:C2	24:DA:1552:A:C6	2.21	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DA:1439:A:N1	24:DA:1552:A:C5	2.03	1.26
24:DA:1439:A:C2	24:DA:1552:A:C5	2.25	1.25
38:DO:100:HIS:CE1	56:DB:48:U:O2'	1.89	1.25
38:DO:30:ARG:HB2	38:DO:30:ARG:NH1	1.53	1.21

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	216/241 (90%)	128 (59%)	60 (28%)	28 (13%)	0	4
1	CB	216/241 (90%)	145 (67%)	49 (23%)	22 (10%)	0	8
2	AC	204/233 (88%)	139 (68%)	51 (25%)	14 (7%)	1	14
2	CC	204/233 (88%)	146 (72%)	41 (20%)	17 (8%)	0	11
3	AD	203/206 (98%)	126 (62%)	52 (26%)	25 (12%)	0	5
3	CD	203/206 (98%)	141 (70%)	40 (20%)	22 (11%)	0	7
4	AE	148/167 (89%)	100 (68%)	31 (21%)	17 (12%)	0	5
4	CE	148/167 (89%)	98 (66%)	37 (25%)	13 (9%)	0	10
5	AF	98/135 (73%)	62 (63%)	25 (26%)	11 (11%)	0	6
5	CF	98/135 (73%)	65 (66%)	21 (21%)	12 (12%)	0	5
6	AG	149/179 (83%)	109 (73%)	29 (20%)	11 (7%)	1	13
6	CG	148/179 (83%)	80 (54%)	44 (30%)	24 (16%)	0	3
7	AH	127/130 (98%)	97 (76%)	22 (17%)	8 (6%)	1	16
7	CH	127/130 (98%)	96 (76%)	24 (19%)	7 (6%)	1	18
8	AI	125/130 (96%)	80 (64%)	34 (27%)	11 (9%)	0	10
8	CI	125/130 (96%)	86 (69%)	33 (26%)	6 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	96/103 (93%)	69 (72%)	12 (12%)	15 (16%)	0	3
9	CJ	96/103 (93%)	61 (64%)	20 (21%)	15 (16%)	0	3
10	AK	115/129 (89%)	86 (75%)	22 (19%)	7 (6%)	1	16
10	CK	115/129 (89%)	74 (64%)	31 (27%)	10 (9%)	0	10
11	AL	121/124 (98%)	80 (66%)	24 (20%)	17 (14%)	0	3
11	CL	121/124 (98%)	86 (71%)	25 (21%)	10 (8%)	0	11
12	AM	112/118 (95%)	87 (78%)	16 (14%)	9 (8%)	1	12
12	CM	111/118 (94%)	65 (59%)	30 (27%)	16 (14%)	0	3
13	AN	92/101 (91%)	58 (63%)	25 (27%)	9 (10%)	0	8
13	CN	91/101 (90%)	59 (65%)	24 (26%)	8 (9%)	0	10
14	AO	86/89 (97%)	64 (74%)	17 (20%)	5 (6%)	1	17
14	CO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	11	42
15	AP	80/82 (98%)	54 (68%)	15 (19%)	11 (14%)	0	3
15	CP	78/82 (95%)	56 (72%)	14 (18%)	8 (10%)	0	7
16	AQ	78/84 (93%)	48 (62%)	21 (27%)	9 (12%)	0	5
16	CQ	78/84 (93%)	59 (76%)	13 (17%)	6 (8%)	1	13
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	2	23
17	CR	53/75 (71%)	44 (83%)	6 (11%)	3 (6%)	1	17
18	AS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	1	18
18	CS	77/92 (84%)	54 (70%)	19 (25%)	4 (5%)	1	18
19	AT	83/87 (95%)	55 (66%)	21 (25%)	7 (8%)	0	11
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	3	24
20	AU	49/71 (69%)	22 (45%)	18 (37%)	9 (18%)	0	2
20	CU	49/71 (69%)	20 (41%)	17 (35%)	12 (24%)	0	1
26	BC	269/273 (98%)	184 (68%)	59 (22%)	26 (10%)	0	9
26	DC	269/273 (98%)	181 (67%)	60 (22%)	28 (10%)	0	7
27	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	3
27	DD	207/209 (99%)	132 (64%)	45 (22%)	30 (14%)	0	3
28	BE	199/201 (99%)	151 (76%)	24 (12%)	24 (12%)	0	5
28	DE	199/201 (99%)	130 (65%)	43 (22%)	26 (13%)	0	3
29	BF	175/179 (98%)	133 (76%)	25 (14%)	17 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	176/179 (98%)	97 (55%)	45 (26%)	34 (19%)	0	2
30	BG	174/177 (98%)	112 (64%)	35 (20%)	27 (16%)	0	3
30	DG	174/177 (98%)	105 (60%)	41 (24%)	28 (16%)	0	3
31	BH	147/149 (99%)	62 (42%)	54 (37%)	31 (21%)	0	1
31	DH	147/149 (99%)	76 (52%)	50 (34%)	21 (14%)	0	3
32	BI	139/142 (98%)	84 (60%)	44 (32%)	11 (8%)	1	12
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	3
33	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	0	8
33	DJ	140/142 (99%)	95 (68%)	33 (24%)	12 (9%)	0	10
34	BK	120/123 (98%)	84 (70%)	18 (15%)	18 (15%)	0	3
34	DK	120/123 (98%)	80 (67%)	21 (18%)	19 (16%)	0	3
35	BL	141/144 (98%)	101 (72%)	28 (20%)	12 (8%)	0	11
35	DL	141/144 (98%)	83 (59%)	37 (26%)	21 (15%)	0	3
36	BM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	6
36	DM	134/136 (98%)	92 (69%)	25 (19%)	17 (13%)	0	4
37	BN	118/127 (93%)	87 (74%)	21 (18%)	10 (8%)	0	11
37	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0	8
38	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	12
38	DO	114/117 (97%)	76 (67%)	29 (25%)	9 (8%)	1	12
39	BP	112/115 (97%)	71 (63%)	22 (20%)	19 (17%)	0	3
39	DP	112/115 (97%)	67 (60%)	28 (25%)	17 (15%)	0	3
40	BQ	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	12
40	DQ	115/118 (98%)	79 (69%)	26 (23%)	10 (9%)	0	10
41	BR	101/103 (98%)	79 (78%)	14 (14%)	8 (8%)	1	12
41	DR	101/103 (98%)	72 (71%)	19 (19%)	10 (10%)	0	8
42	BS	108/110 (98%)	76 (70%)	27 (25%)	5 (5%)	2	20
42	DS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	0	11
43	BT	91/100 (91%)	53 (58%)	23 (25%)	15 (16%)	0	3
43	DT	91/100 (91%)	48 (53%)	28 (31%)	15 (16%)	0	3
44	BU	100/104 (96%)	71 (71%)	13 (13%)	16 (16%)	0	3
44	DU	100/104 (96%)	51 (51%)	28 (28%)	21 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	5	32
45	DV	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	1	13
46	BW	77/85 (91%)	29 (38%)	22 (29%)	26 (34%)	0	0
46	DW	77/85 (91%)	32 (42%)	27 (35%)	18 (23%)	0	1
47	BX	75/78 (96%)	59 (79%)	13 (17%)	3 (4%)	2	22
47	DX	75/78 (96%)	48 (64%)	21 (28%)	6 (8%)	1	12
48	BY	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	3
48	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	11
49	BZ	56/59 (95%)	39 (70%)	13 (23%)	4 (7%)	1	14
49	DZ	56/59 (95%)	31 (55%)	18 (32%)	7 (12%)	0	4
50	B0	54/57 (95%)	39 (72%)	9 (17%)	6 (11%)	0	6
50	D0	54/57 (95%)	40 (74%)	8 (15%)	6 (11%)	0	6
51	B1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	0	11
51	D1	48/55 (87%)	35 (73%)	9 (19%)	4 (8%)	0	11
52	B2	44/46 (96%)	35 (80%)	8 (18%)	1 (2%)	5	31
52	D2	44/46 (96%)	32 (73%)	7 (16%)	5 (11%)	0	6
53	B3	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	3	26
53	D3	62/65 (95%)	39 (63%)	17 (27%)	6 (10%)	0	9
54	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	0	11
54	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	3
All	All	11238/11970 (94%)	7499 (67%)	2485 (22%)	1254 (11%)	0	6

5 of 1254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	40	ILE
1	AB	71	THR
1	AB	72	LYS

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/199 (90%)	147 (82%)	33 (18%)	1	9
1	CB	180/199 (90%)	157 (87%)	23 (13%)	3	18
2	AC	170/190 (90%)	148 (87%)	22 (13%)	3	18
2	CC	170/190 (90%)	153 (90%)	17 (10%)	6	25
3	AD	172/173 (99%)	144 (84%)	28 (16%)	2	13
3	CD	172/173 (99%)	146 (85%)	26 (15%)	2	14
4	AE	113/126 (90%)	90 (80%)	23 (20%)	1	6
4	CE	113/126 (90%)	97 (86%)	16 (14%)	2	17
5	AF	87/116 (75%)	77 (88%)	10 (12%)	4	21
5	CF	87/116 (75%)	78 (90%)	9 (10%)	6	24
6	AG	124/147 (84%)	116 (94%)	8 (6%)	14	40
6	CG	123/147 (84%)	97 (79%)	26 (21%)	1	6
7	AH	104/105 (99%)	92 (88%)	12 (12%)	4	21
7	CH	104/105 (99%)	87 (84%)	17 (16%)	2	13
8	AI	105/107 (98%)	88 (84%)	17 (16%)	2	13
8	CI	105/107 (98%)	91 (87%)	14 (13%)	3	18
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	2	13
9	CJ	86/90 (96%)	74 (86%)	12 (14%)	3	17
10	AK	90/99 (91%)	81 (90%)	9 (10%)	6	25
10	CK	90/99 (91%)	73 (81%)	17 (19%)	1	8
11	AL	103/104 (99%)	85 (82%)	18 (18%)	1	11
11	CL	103/104 (99%)	85 (82%)	18 (18%)	1	11
12	AM	92/96 (96%)	87 (95%)	5 (5%)	18	45
12	CM	91/96 (95%)	75 (82%)	16 (18%)	1	10
13	AN	79/84 (94%)	74 (94%)	5 (6%)	15	41
13	CN	79/84 (94%)	67 (85%)	12 (15%)	2	14
14	AO	76/77 (99%)	69 (91%)	7 (9%)	7	28
14	CO	76/77 (99%)	71 (93%)	5 (7%)	14	39
15	AP	65/65 (100%)	59 (91%)	6 (9%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CP	65/65 (100%)	59 (91%)	6 (9%)	7	28
16	AQ	74/78 (95%)	57 (77%)	17 (23%)	0	4
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	3	18
17	AR	48/65 (74%)	47 (98%)	1 (2%)	48	67
17	CR	48/65 (74%)	45 (94%)	3 (6%)	15	41
18	AS	70/79 (89%)	62 (89%)	8 (11%)	4	21
18	CS	70/79 (89%)	59 (84%)	11 (16%)	2	14
19	AT	65/66 (98%)	56 (86%)	9 (14%)	3	17
19	CT	65/66 (98%)	58 (89%)	7 (11%)	5	23
20	AU	44/61 (72%)	36 (82%)	8 (18%)	1	9
20	CU	44/61 (72%)	33 (75%)	11 (25%)	0	3
26	BC	216/218 (99%)	177 (82%)	39 (18%)	1	9
26	DC	216/218 (99%)	191 (88%)	25 (12%)	4	21
27	BD	164/164 (100%)	133 (81%)	31 (19%)	1	8
27	DD	164/164 (100%)	144 (88%)	20 (12%)	4	20
28	BE	165/165 (100%)	128 (78%)	37 (22%)	1	5
28	DE	165/165 (100%)	150 (91%)	15 (9%)	7	29
29	BF	148/150 (99%)	129 (87%)	19 (13%)	3	18
29	DF	149/150 (99%)	121 (81%)	28 (19%)	1	9
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	6
30	DG	137/138 (99%)	120 (88%)	17 (12%)	4	19
31	BH	114/114 (100%)	98 (86%)	16 (14%)	3	17
31	DH	114/114 (100%)	97 (85%)	17 (15%)	2	15
32	BI	109/110 (99%)	92 (84%)	17 (16%)	2	14
32	DI	109/110 (99%)	102 (94%)	7 (6%)	14	40
33	BJ	116/116 (100%)	91 (78%)	25 (22%)	1	5
33	DJ	116/116 (100%)	105 (90%)	11 (10%)	7	27
34	BK	103/104 (99%)	82 (80%)	21 (20%)	1	6
34	DK	103/104 (99%)	85 (82%)	18 (18%)	1	11
35	BL	102/103 (99%)	77 (76%)	25 (24%)	0	4
35	DL	102/103 (99%)	87 (85%)	15 (15%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BM	109/109 (100%)	89 (82%)	20 (18%)	1	9
36	DM	109/109 (100%)	96 (88%)	13 (12%)	4	20
37	BN	100/103 (97%)	78 (78%)	22 (22%)	1	5
37	DN	100/103 (97%)	87 (87%)	13 (13%)	3	18
38	BO	86/87 (99%)	69 (80%)	17 (20%)	1	7
38	DO	86/87 (99%)	76 (88%)	10 (12%)	4	21
39	BP	99/100 (99%)	77 (78%)	22 (22%)	1	5
39	DP	99/100 (99%)	91 (92%)	8 (8%)	9	33
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	1	10
40	DQ	89/90 (99%)	78 (88%)	11 (12%)	4	19
41	BR	84/84 (100%)	68 (81%)	16 (19%)	1	8
41	DR	84/84 (100%)	72 (86%)	12 (14%)	2	16
42	BS	93/93 (100%)	76 (82%)	17 (18%)	1	9
42	DS	93/93 (100%)	80 (86%)	13 (14%)	3	17
43	BT	80/84 (95%)	63 (79%)	17 (21%)	1	6
43	DT	80/84 (95%)	75 (94%)	5 (6%)	15	41
44	BU	83/85 (98%)	73 (88%)	10 (12%)	4	20
44	DU	83/85 (98%)	72 (87%)	11 (13%)	3	18
45	BV	78/78 (100%)	64 (82%)	14 (18%)	1	10
45	DV	78/78 (100%)	65 (83%)	13 (17%)	2	12
46	BW	59/63 (94%)	39 (66%)	20 (34%)	0	1
46	DW	59/63 (94%)	43 (73%)	16 (27%)	0	2
47	BX	67/68 (98%)	56 (84%)	11 (16%)	2	12
47	DX	67/68 (98%)	58 (87%)	9 (13%)	3	18
48	BY	55/55 (100%)	41 (74%)	14 (26%)	0	3
48	DY	55/55 (100%)	51 (93%)	4 (7%)	11	36
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	2
49	DZ	48/49 (98%)	39 (81%)	9 (19%)	1	9
50	B0	47/48 (98%)	43 (92%)	4 (8%)	8	32
50	D0	47/48 (98%)	41 (87%)	6 (13%)	3	18
51	B1	45/49 (92%)	35 (78%)	10 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	D1	45/49 (92%)	41 (91%)	4 (9%)	8	30
52	B2	38/38 (100%)	32 (84%)	6 (16%)	2	14
52	D2	38/38 (100%)	34 (90%)	4 (10%)	5	24
53	B3	51/52 (98%)	45 (88%)	6 (12%)	4	20
53	D3	51/52 (98%)	42 (82%)	9 (18%)	1	10
54	B4	34/34 (100%)	29 (85%)	5 (15%)	2	15
54	D4	34/34 (100%)	29 (85%)	5 (15%)	2	15
All	All	9331/9756 (96%)	7927 (85%)	1404 (15%)	2	15

5 of 1404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	CI	125	GLN
30	DG	19	ASN
10	CK	115	ILE
8	CI	115	VAL
19	CT	47	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
26	DC	52	HIS
40	DQ	71	ASN
26	DC	199	HIS
32	DI	93	ASN
44	DU	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	474 (30%)	255 (16%)
22	AV	16/17 (94%)	0	0
22	CV	16/17 (94%)	1 (6%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	2 (40%)	1 (20%)
24	BA	2850/2903 (98%)	958 (33%)	492 (17%)
24	DA	2838/2903 (97%)	1000 (35%)	519 (18%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	BB	117/118 (99%)	33 (28%)	19 (16%)
55	CA	1530/1530 (100%)	519 (33%)	252 (16%)
56	DB	116/117 (99%)	42 (36%)	18 (15%)
All	All	9025/9150 (98%)	3032 (33%)	1557 (17%)

5 of 3032 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 1557 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	CA	913	A
24	DA	655	A
55	CA	1085	U
55	CA	889	A
24	DA	103	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	218/241 (90%)	1.47	57 (26%) 2 4	206, 268, 283, 298	0
1	CB	218/241 (90%)	0.77	18 (8%) 19 18	146, 174, 199, 216	0
2	AC	206/233 (88%)	-0.09	1 (0%) 87 74	106, 135, 169, 198	0
2	CC	206/233 (88%)	0.01	3 (1%) 71 55	111, 140, 177, 195	0
3	AD	205/206 (99%)	0.30	11 (5%) 32 28	102, 139, 185, 204	0
3	CD	205/206 (99%)	0.20	6 (2%) 54 41	86, 109, 140, 157	0
4	AE	150/167 (89%)	2.64	85 (56%) 0 1	102, 214, 237, 255	0
4	CE	150/167 (89%)	1.05	27 (18%) 4 8	86, 134, 166, 209	0
5	AF	100/135 (74%)	0.34	7 (7%) 24 22	140, 166, 186, 192	0
5	CF	100/135 (74%)	0.39	4 (4%) 43 35	140, 170, 200, 208	0
6	AG	151/179 (84%)	0.17	5 (3%) 49 39	128, 157, 186, 202	0
6	CG	150/179 (83%)	1.01	29 (19%) 4 7	115, 165, 204, 219	0
7	AH	129/130 (99%)	-0.00	4 (3%) 51 40	102, 134, 158, 182	0
7	CH	129/130 (99%)	0.40	5 (3%) 44 35	106, 135, 159, 174	0
8	AI	127/130 (97%)	0.48	7 (5%) 32 27	108, 158, 190, 210	0
8	CI	127/130 (97%)	0.73	16 (12%) 9 13	114, 174, 206, 221	0
9	AJ	98/103 (95%)	0.31	5 (5%) 34 29	105, 150, 194, 211	0
9	CJ	98/103 (95%)	0.61	11 (11%) 11 14	113, 165, 210, 220	0
10	AK	117/129 (90%)	-0.10	0 100 100	100, 149, 183, 200	0
10	CK	117/129 (90%)	0.42	7 (5%) 29 25	89, 133, 167, 192	0
11	AL	123/124 (99%)	0.17	7 (5%) 30 26	75, 95, 132, 157	0
11	CL	123/124 (99%)	0.12	4 (3%) 49 39	83, 101, 132, 151	0
12	AM	114/118 (96%)	0.24	5 (4%) 39 33	122, 182, 213, 232	0
12	CM	113/118 (95%)	0.68	8 (7%) 23 22	133, 193, 225, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	0.30	2 (2%) 63 48	111, 142, 184, 210	0
13	CN	95/101 (94%)	0.97	15 (15%) 6 9	117, 149, 199, 207	0
14	AO	88/89 (98%)	-0.14	1 (1%) 77 62	105, 133, 163, 199	0
14	CO	88/89 (98%)	0.16	1 (1%) 77 62	113, 141, 174, 197	0
15	AP	82/82 (100%)	0.51	8 (9%) 14 15	95, 127, 165, 208	0
15	CP	80/82 (97%)	0.55	6 (7%) 22 21	98, 122, 156, 189	0
16	AQ	80/84 (95%)	0.13	2 (2%) 58 45	69, 100, 142, 159	0
16	CQ	80/84 (95%)	-0.02	1 (1%) 74 58	72, 111, 142, 159	0
17	AR	55/75 (73%)	0.04	1 (1%) 67 51	129, 148, 180, 190	0
17	CR	55/75 (73%)	0.14	2 (3%) 46 37	131, 150, 170, 182	0
18	AS	79/92 (85%)	0.52	5 (6%) 27 24	140, 176, 210, 235	0
18	CS	79/92 (85%)	0.45	4 (5%) 34 29	151, 182, 215, 230	0
19	AT	85/87 (97%)	0.12	1 (1%) 76 59	89, 121, 149, 180	0
19	CT	85/87 (97%)	0.41	7 (8%) 19 18	115, 153, 185, 206	0
20	AU	51/71 (71%)	0.84	9 (17%) 4 8	98, 145, 201, 208	0
20	CU	51/71 (71%)	0.96	9 (17%) 4 8	104, 139, 173, 193	0
21	AA	1533/1533 (100%)	-0.21	24 (1%) 70 53	65, 123, 208, 301	0
22	AV	17/17 (100%)	-0.57	0 100 100	102, 112, 149, 197	0
22	CV	17/17 (100%)	-0.24	0 100 100	99, 104, 145, 179	0
23	AW	6/6 (100%)	0.15	0 100 100	100, 109, 120, 155	0
23	CW	6/6 (100%)	0.23	0 100 100	98, 105, 123, 130	0
24	BA	2854/2903 (98%)	-0.32	45 (1%) 70 53	36, 66, 188, 342	0
24	DA	2841/2903 (97%)	0.38	90 (3%) 50 39	79, 132, 236, 340	0
25	BB	118/118 (100%)	-0.27	0 100 100	52, 81, 113, 162	0
26	BC	271/273 (99%)	0.33	11 (4%) 42 34	44, 80, 122, 159	0
26	DC	271/273 (99%)	0.98	31 (11%) 11 14	89, 133, 164, 189	0
27	BD	209/209 (100%)	-0.01	2 (0%) 79 64	37, 59, 105, 146	0
27	DD	209/209 (100%)	0.81	22 (10%) 13 14	83, 131, 164, 186	0
28	BE	201/201 (100%)	-0.04	3 (1%) 71 55	38, 84, 131, 164	0
28	DE	201/201 (100%)	0.81	27 (13%) 8 12	95, 171, 212, 250	0
29	BF	177/179 (98%)	0.67	13 (7%) 22 21	90, 148, 201, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DF	178/179 (99%)	1.73	59 (33%) 1 3	250, 278, 301, 305	0
30	BG	176/177 (99%)	0.01	4 (2%) 61 46	66, 90, 135, 160	0
30	DG	176/177 (99%)	0.56	11 (6%) 27 24	120, 148, 177, 204	0
31	BH	149/149 (100%)	0.86	25 (16%) 5 8	89, 262, 290, 299	0
31	DH	149/149 (100%)	1.48	41 (27%) 2 4	156, 244, 279, 286	0
32	BI	141/142 (99%)	0.73	10 (7%) 23 22	237, 306, 364, 376	0
32	DI	141/142 (99%)	0.80	8 (5%) 30 26	277, 331, 367, 378	0
33	BJ	142/142 (100%)	-0.13	2 (1%) 73 57	41, 57, 102, 157	0
33	DJ	142/142 (100%)	0.58	11 (7%) 21 19	92, 115, 142, 181	0
34	BK	122/123 (99%)	-0.03	4 (3%) 49 39	41, 56, 110, 177	0
34	DK	122/123 (99%)	0.47	6 (4%) 36 30	93, 115, 144, 173	0
35	BL	143/144 (99%)	0.04	1 (0%) 84 70	38, 77, 119, 160	0
35	DL	143/144 (99%)	1.38	36 (25%) 2 4	93, 155, 197, 209	0
36	BM	136/136 (100%)	0.01	1 (0%) 84 70	41, 67, 114, 152	0
36	DM	136/136 (100%)	0.33	2 (1%) 71 55	80, 107, 142, 164	0
37	BN	120/127 (94%)	-0.00	1 (0%) 82 68	46, 63, 84, 138	0
37	DN	120/127 (94%)	1.17	27 (22%) 3 5	122, 154, 180, 217	0
38	BO	116/117 (99%)	0.02	2 (1%) 69 52	73, 84, 124, 149	0
38	DO	116/117 (99%)	1.94	46 (39%) 1 2	165, 197, 217, 225	0
39	BP	114/115 (99%)	-0.16	0 100 100	49, 67, 123, 152	0
39	DP	114/115 (99%)	0.82	9 (7%) 20 19	117, 137, 163, 182	0
40	BQ	117/118 (99%)	-0.22	0 100 100	40, 58, 100, 127	0
40	DQ	117/118 (99%)	0.92	18 (15%) 6 10	97, 119, 143, 172	0
41	BR	103/103 (100%)	0.15	3 (2%) 54 41	39, 70, 116, 158	0
41	DR	103/103 (100%)	1.16	19 (18%) 4 7	96, 133, 157, 164	0
42	BS	110/110 (100%)	-0.03	1 (0%) 81 66	41, 58, 95, 161	0
42	DS	110/110 (100%)	0.90	13 (11%) 10 13	98, 141, 173, 188	0
43	BT	93/100 (93%)	0.70	12 (12%) 9 12	56, 95, 135, 165	0
43	DT	93/100 (93%)	1.67	32 (34%) 1 3	144, 196, 226, 237	0
44	BU	102/104 (98%)	0.48	8 (7%) 20 19	77, 105, 139, 194	0
44	DU	102/104 (98%)	1.60	28 (27%) 2 4	174, 208, 248, 279	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BV	94/94 (100%)	0.10	2 (2%) 63 48	60, 81, 115, 143	0
45	DV	94/94 (100%)	1.81	34 (36%) 1 2	125, 188, 226, 239	0
46	BW	79/85 (92%)	0.75	9 (11%) 11 14	50, 75, 131, 168	0
46	DW	79/85 (92%)	1.02	12 (15%) 6 10	88, 134, 164, 184	0
47	BX	77/78 (98%)	0.08	0 100 100	50, 84, 126, 147	0
47	DX	77/78 (98%)	1.56	24 (31%) 1 3	110, 157, 187, 203	0
48	BY	63/63 (100%)	0.79	11 (17%) 5 8	87, 109, 154, 163	0
48	DY	63/63 (100%)	0.98	9 (14%) 7 11	196, 218, 251, 257	0
49	BZ	58/59 (98%)	0.02	0 100 100	49, 63, 106, 145	0
49	DZ	58/59 (98%)	0.57	3 (5%) 34 29	97, 116, 142, 155	0
50	B0	56/57 (98%)	-0.09	0 100 100	40, 63, 119, 143	0
50	D0	56/57 (98%)	0.69	4 (7%) 23 22	93, 152, 190, 202	0
51	B1	50/55 (90%)	-0.17	1 (2%) 64 49	63, 91, 117, 156	0
51	D1	50/55 (90%)	0.65	7 (14%) 7 11	113, 142, 173, 179	0
52	B2	46/46 (100%)	0.08	2 (4%) 40 33	50, 61, 80, 165	0
52	D2	46/46 (100%)	1.66	17 (36%) 1 2	118, 137, 161, 174	0
53	B3	64/65 (98%)	-0.17	0 100 100	45, 63, 98, 133	0
53	D3	64/65 (98%)	1.48	17 (26%) 2 4	105, 123, 146, 174	0
54	B4	38/38 (100%)	0.16	0 100 100	54, 68, 100, 118	0
54	D4	38/38 (100%)	1.43	9 (23%) 2 5	95, 117, 138, 142	0
55	CA	1530/1530 (100%)	0.12	39 (2%) 58 45	77, 126, 214, 305	0
56	DB	117/117 (100%)	0.04	0 100 100	87, 166, 194, 210	0
All	All	20477/21120 (96%)	0.32	1314 (6%) 27 24	36, 125, 246, 378	0

The worst 5 of 1314 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	BY	63	ALA	11.7
29	DF	153	ILE	10.9
29	DF	129	MET	10.9
4	AE	114	LEU	10.1
38	DO	28	VAL	10.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3062	1/1	-0.29	0.65	85,85,85,85	0
57	MG	AA	1619	1/1	-0.12	0.32	136,136,136,136	0
57	MG	DA	3076	1/1	-0.02	0.68	109,109,109,109	0
57	MG	CA	1624	1/1	0.18	0.49	79,79,79,79	0
57	MG	DA	3134	1/1	0.19	0.55	126,126,126,126	0
57	MG	DA	3065	1/1	0.27	0.61	84,84,84,84	0
57	MG	BA	3015	1/1	0.34	0.53	38,38,38,38	0
57	MG	DA	3071	1/1	0.36	0.38	94,94,94,94	0
57	MG	DA	3016	1/1	0.37	0.57	96,96,96,96	0
57	MG	DA	3131	1/1	0.40	0.41	103,103,103,103	0
57	MG	DA	3060	1/1	0.40	0.29	96,96,96,96	0
57	MG	BA	3058	1/1	0.44	0.37	44,44,44,44	0
57	MG	DA	3004	1/1	0.51	0.42	150,150,150,150	0
57	MG	DA	3110	1/1	0.51	0.52	82,82,82,82	0
57	MG	DC	301	1/1	0.52	0.20	103,103,103,103	0
57	MG	CA	1612	1/1	0.53	0.31	86,86,86,86	0
57	MG	DA	3133	1/1	0.53	0.30	115,115,115,115	0
57	MG	DA	3040	1/1	0.53	0.37	102,102,102,102	0
57	MG	CA	1617	1/1	0.55	0.25	130,130,130,130	0
57	MG	DA	3093	1/1	0.55	0.28	93,93,93,93	0
57	MG	DA	3077	1/1	0.59	0.36	86,86,86,86	0
57	MG	DA	3084	1/1	0.63	0.16	157,157,157,157	0
57	MG	BB	201	1/1	0.63	0.30	105,105,105,105	0
57	MG	DA	3075	1/1	0.63	0.10	255,255,255,255	0
57	MG	CA	1629	1/1	0.65	0.25	111,111,111,111	0
57	MG	BA	3075	1/1	0.66	0.37	40,40,40,40	0
57	MG	DA	3021	1/1	0.66	0.27	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3112	1/1	0.67	0.25	115,115,115,115	0
57	MG	AA	1607	1/1	0.68	0.22	88,88,88,88	0
57	MG	DA	3064	1/1	0.68	0.30	87,87,87,87	0
57	MG	DA	3086	1/1	0.68	0.18	148,148,148,148	0
57	MG	BA	3135	1/1	0.69	0.36	43,43,43,43	0
57	MG	DA	3047	1/1	0.70	0.15	148,148,148,148	0
57	MG	BA	3077	1/1	0.70	0.24	45,45,45,45	0
57	MG	AA	1636	1/1	0.70	0.18	120,120,120,120	0
57	MG	DA	3090	1/1	0.70	0.21	92,92,92,92	0
57	MG	CA	1625	1/1	0.70	0.21	86,86,86,86	0
57	MG	DA	3100	1/1	0.71	0.21	149,149,149,149	0
57	MG	DB	201	1/1	0.71	0.18	108,108,108,108	0
57	MG	BA	3133	1/1	0.72	0.45	53,53,53,53	0
57	MG	DA	3051	1/1	0.73	0.10	177,177,177,177	0
57	MG	DA	3007	1/1	0.74	0.12	192,192,192,192	0
57	MG	DA	3128	1/1	0.74	0.26	100,100,100,100	0
57	MG	CA	1602	1/1	0.74	0.22	106,106,106,106	0
57	MG	DA	3011	1/1	0.75	0.35	110,110,110,110	0
57	MG	DA	3107	1/1	0.75	0.16	130,130,130,130	0
57	MG	BA	3132	1/1	0.75	0.41	42,42,42,42	0
57	MG	DA	3054	1/1	0.76	0.26	88,88,88,88	0
57	MG	BA	3070	1/1	0.76	0.13	140,140,140,140	0
57	MG	DA	3020	1/1	0.77	0.18	153,153,153,153	0
57	MG	DA	3041	1/1	0.77	0.14	113,113,113,113	0
57	MG	BA	3112	1/1	0.77	0.12	46,46,46,46	0
57	MG	DA	3066	1/1	0.77	0.21	92,92,92,92	0
57	MG	DA	3126	1/1	0.77	0.17	99,99,99,99	0
57	MG	BA	3131	1/1	0.78	0.51	48,48,48,48	0
57	MG	CA	1615	1/1	0.78	0.20	118,118,118,118	0
57	MG	DA	3006	1/1	0.78	0.11	149,149,149,149	0
57	MG	BA	3014	1/1	0.79	0.32	38,38,38,38	0
57	MG	BA	3061	1/1	0.79	0.36	39,39,39,39	0
57	MG	DA	3019	1/1	0.79	0.11	150,150,150,150	0
57	MG	DA	3015	1/1	0.80	0.19	88,88,88,88	0
57	MG	DA	3109	1/1	0.80	0.13	92,92,92,92	0
57	MG	BA	3085	1/1	0.80	0.42	42,42,42,42	0
57	MG	CA	1613	1/1	0.80	0.14	79,79,79,79	0
57	MG	BA	3115	1/1	0.80	0.27	49,49,49,49	0
57	MG	DA	3099	1/1	0.81	0.39	98,98,98,98	0
57	MG	BA	3037	1/1	0.81	0.35	42,42,42,42	0
57	MG	DA	3059	1/1	0.81	0.26	88,88,88,88	0
57	MG	CA	1607	1/1	0.81	0.14	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3014	1/1	0.81	0.17	90,90,90,90	0
57	MG	CA	1619	1/1	0.81	0.24	119,119,119,119	0
57	MG	BA	3062	1/1	0.82	0.43	38,38,38,38	0
57	MG	DA	3003	1/1	0.82	0.13	94,94,94,94	0
57	MG	AA	1641	1/1	0.82	0.25	89,89,89,89	0
57	MG	CA	1634	1/1	0.82	0.16	97,97,97,97	0
57	MG	DA	3108	1/1	0.82	0.19	82,82,82,82	0
57	MG	DA	3027	1/1	0.82	0.14	87,87,87,87	0
57	MG	DA	3032	1/1	0.82	0.19	87,87,87,87	0
57	MG	BA	3124	1/1	0.83	0.39	41,41,41,41	0
57	MG	DA	3017	1/1	0.83	0.20	102,102,102,102	0
57	MG	DA	3088	1/1	0.83	0.14	101,101,101,101	0
57	MG	DA	3120	1/1	0.84	0.24	96,96,96,96	0
57	MG	DA	3085	1/1	0.84	0.09	190,190,190,190	0
57	MG	BA	3060	1/1	0.84	0.29	39,39,39,39	0
57	MG	AA	1620	1/1	0.84	0.11	144,144,144,144	0
57	MG	DA	3028	1/1	0.84	0.38	103,103,103,103	0
57	MG	DA	3080	1/1	0.84	0.29	84,84,84,84	0
57	MG	CA	1636	1/1	0.84	0.32	88,88,88,88	0
57	MG	DA	3124	1/1	0.85	0.12	133,133,133,133	0
57	MG	DA	3045	1/1	0.85	0.12	141,141,141,141	0
57	MG	BA	3102	1/1	0.85	0.32	40,40,40,40	0
57	MG	DA	3048	1/1	0.85	0.15	131,131,131,131	0
57	MG	CA	1614	1/1	0.85	0.13	114,114,114,114	0
57	MG	BA	3084	1/1	0.85	0.36	49,49,49,49	0
57	MG	AA	1626	1/1	0.85	0.12	107,107,107,107	0
57	MG	AA	1637	1/1	0.86	0.12	87,87,87,87	0
57	MG	BA	3056	1/1	0.86	0.27	45,45,45,45	0
57	MG	DA	3009	1/1	0.86	0.10	121,121,121,121	0
57	MG	AA	1631	1/1	0.86	0.19	98,98,98,98	0
57	MG	DA	3012	1/1	0.86	0.25	96,96,96,96	0
57	MG	CA	1603	1/1	0.86	0.23	92,92,92,92	0
57	MG	CA	1606	1/1	0.86	0.09	85,85,85,85	0
57	MG	DA	3029	1/1	0.86	0.13	108,108,108,108	0
57	MG	AA	1628	1/1	0.87	0.13	107,107,107,107	0
57	MG	BA	3007	1/1	0.87	0.16	90,90,90,90	0
57	MG	DA	3042	1/1	0.87	0.09	101,101,101,101	0
57	MG	DA	3002	1/1	0.87	0.14	125,125,125,125	0
57	MG	BA	3118	1/1	0.87	0.23	42,42,42,42	0
57	MG	BA	3123	1/1	0.87	0.11	63,63,63,63	0
57	MG	DA	3094	1/1	0.87	0.10	126,126,126,126	0
57	MG	BA	3098	1/1	0.87	0.42	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3026	1/1	0.87	0.31	41,41,41,41	0
57	MG	DA	3058	1/1	0.87	0.11	96,96,96,96	0
57	MG	DA	3035	1/1	0.87	0.12	88,88,88,88	0
57	MG	CA	1616	1/1	0.88	0.10	136,136,136,136	0
57	MG	BB	202	1/1	0.88	0.12	114,114,114,114	0
57	MG	AA	1625	1/1	0.88	0.12	90,90,90,90	0
57	MG	DA	3030	1/1	0.88	0.23	101,101,101,101	0
57	MG	CA	1622	1/1	0.88	0.08	138,138,138,138	0
57	MG	AA	1606	1/1	0.88	0.10	96,96,96,96	0
57	MG	CA	1639	1/1	0.89	0.07	165,165,165,165	0
57	MG	BA	3095	1/1	0.89	0.15	75,75,75,75	0
57	MG	DA	3001	1/1	0.89	0.13	115,115,115,115	0
57	MG	BA	3046	1/1	0.89	0.10	63,63,63,63	0
57	MG	DA	3061	1/1	0.89	0.22	84,84,84,84	0
57	MG	DA	3096	1/1	0.89	0.14	120,120,120,120	0
57	MG	DA	3031	1/1	0.89	0.20	98,98,98,98	0
57	MG	DA	3129	1/1	0.89	0.18	83,83,83,83	0
57	MG	DA	3081	1/1	0.89	0.09	87,87,87,87	0
57	MG	DA	3101	1/1	0.89	0.13	82,82,82,82	0
57	MG	CA	1628	1/1	0.89	0.25	79,79,79,79	0
57	MG	CA	1638	1/1	0.89	0.09	141,141,141,141	0
57	MG	BA	3071	1/1	0.90	0.28	38,38,38,38	0
57	MG	DA	3023	1/1	0.90	0.21	101,101,101,101	0
57	MG	CA	1627	1/1	0.90	0.10	106,106,106,106	0
57	MG	DA	3043	1/1	0.90	0.18	107,107,107,107	0
57	MG	AA	1604	1/1	0.90	0.07	126,126,126,126	0
57	MG	BA	3001	1/1	0.90	0.20	45,45,45,45	0
57	MG	DA	3089	1/1	0.90	0.09	110,110,110,110	0
57	MG	DJ	201	1/1	0.90	0.20	101,101,101,101	0
57	MG	DA	3070	1/1	0.90	0.09	94,94,94,94	0
57	MG	DA	3050	1/1	0.90	0.12	148,148,148,148	0
57	MG	DA	3074	1/1	0.90	0.09	98,98,98,98	0
57	MG	DA	3008	1/1	0.90	0.06	177,177,177,177	0
57	MG	BA	3004	1/1	0.90	0.17	69,69,69,69	0
57	MG	DA	3010	1/1	0.90	0.10	108,108,108,108	0
57	MG	CA	1601	1/1	0.91	0.10	142,142,142,142	0
57	MG	DA	3122	1/1	0.91	0.09	142,142,142,142	0
57	MG	BA	3045	1/1	0.91	0.17	62,62,62,62	0
57	MG	BA	3030	1/1	0.91	0.36	41,41,41,41	0
57	MG	BA	3025	1/1	0.91	0.09	41,41,41,41	0
57	MG	BA	3099	1/1	0.91	0.13	41,41,41,41	0
57	MG	DA	3130	1/1	0.91	0.37	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3005	1/1	0.91	0.09	157,157,157,157	0
57	MG	DA	3095	1/1	0.91	0.12	159,159,159,159	0
57	MG	CA	1609	1/1	0.91	0.10	96,96,96,96	0
57	MG	DA	3116	1/1	0.91	0.14	98,98,98,98	0
57	MG	BA	3047	1/1	0.92	0.09	63,63,63,63	0
57	MG	AA	1632	1/1	0.92	0.10	95,95,95,95	0
57	MG	DA	3078	1/1	0.92	0.20	79,79,79,79	0
57	MG	BA	3119	1/1	0.92	0.28	52,52,52,52	0
57	MG	CA	1640	1/1	0.92	0.27	87,87,87,87	0
57	MG	DA	3082	1/1	0.92	0.19	83,83,83,83	0
57	MG	DA	3049	1/1	0.92	0.14	150,150,150,150	0
57	MG	BA	3121	1/1	0.92	0.12	45,45,45,45	0
57	MG	AA	1610	1/1	0.92	0.07	125,125,125,125	0
57	MG	AA	1627	1/1	0.92	0.22	109,109,109,109	0
57	MG	BA	3107	1/1	0.92	0.11	49,49,49,49	0
57	MG	BA	3091	1/1	0.92	0.08	69,69,69,69	0
57	MG	BA	3092	1/1	0.93	0.08	108,108,108,108	0
57	MG	BA	3035	1/1	0.93	0.20	55,55,55,55	0
57	MG	BA	3074	1/1	0.93	0.11	38,38,38,38	0
57	MG	CA	1604	1/1	0.93	0.06	106,106,106,106	0
57	MG	CA	1626	1/1	0.93	0.08	110,110,110,110	0
57	MG	BA	3005	1/1	0.93	0.14	73,73,73,73	0
57	MG	DA	3115	1/1	0.93	0.14	84,84,84,84	0
57	MG	BA	3126	1/1	0.93	0.13	57,57,57,57	0
57	MG	AA	1630	1/1	0.93	0.10	79,79,79,79	0
57	MG	CA	1631	1/1	0.93	0.10	91,91,91,91	0
57	MG	CA	1610	1/1	0.93	0.06	129,129,129,129	0
57	MG	BA	3080	1/1	0.93	0.07	74,74,74,74	0
57	MG	CA	1637	1/1	0.93	0.14	83,83,83,83	0
57	MG	BA	3011	1/1	0.93	0.33	44,44,44,44	0
57	MG	BA	3113	1/1	0.93	0.15	38,38,38,38	0
57	MG	BA	3136	1/1	0.93	0.32	47,47,47,47	0
57	MG	DA	3097	1/1	0.93	0.11	119,119,119,119	0
57	MG	AA	1618	1/1	0.93	0.08	104,104,104,104	0
57	MG	BA	3055	1/1	0.93	0.16	44,44,44,44	0
57	MG	AA	1624	1/1	0.94	0.12	94,94,94,94	0
57	MG	BA	3109	1/1	0.94	0.11	42,42,42,42	0
57	MG	BA	3111	1/1	0.94	0.10	38,38,38,38	0
57	MG	DA	3111	1/1	0.94	0.10	164,164,164,164	0
57	MG	DA	3024	1/1	0.94	0.09	90,90,90,90	0
57	MG	DA	3026	1/1	0.94	0.09	88,88,88,88	0
57	MG	DA	3067	1/1	0.94	0.07	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1623	1/1	0.94	0.09	89,89,89,89	0
57	MG	DA	3013	1/1	0.94	0.09	93,93,93,93	0
57	MG	DA	3072	1/1	0.94	0.07	84,84,84,84	0
57	MG	BA	3076	1/1	0.94	0.09	47,47,47,47	0
57	MG	AA	1638	1/1	0.94	0.08	81,81,81,81	0
57	MG	BA	3019	1/1	0.94	0.07	70,70,70,70	0
57	MG	DA	3098	1/1	0.94	0.09	87,87,87,87	0
57	MG	AA	1617	1/1	0.94	0.07	123,123,123,123	0
57	MG	DA	3132	1/1	0.94	0.06	94,94,94,94	0
57	MG	DA	3034	1/1	0.94	0.14	89,89,89,89	0
57	MG	AA	1614	1/1	0.94	0.08	113,113,113,113	0
57	MG	DA	3038	1/1	0.94	0.14	108,108,108,108	0
57	MG	CA	1642	1/1	0.95	0.07	102,102,102,102	0
57	MG	BA	3114	1/1	0.95	0.08	73,73,73,73	0
57	MG	BA	3089	1/1	0.95	0.14	50,50,50,50	0
57	MG	DA	3103	1/1	0.95	0.10	91,91,91,91	0
57	MG	DA	3018	1/1	0.95	0.07	106,106,106,106	0
57	MG	BA	3090	1/1	0.95	0.07	47,47,47,47	0
57	MG	AA	1621	1/1	0.95	0.10	67,67,67,67	0
57	MG	AA	1633	1/1	0.95	0.07	107,107,107,107	0
57	MG	BA	3094	1/1	0.95	0.09	75,75,75,75	0
57	MG	BA	3002	1/1	0.95	0.27	47,47,47,47	0
57	MG	DA	3025	1/1	0.95	0.12	105,105,105,105	0
57	MG	BA	3003	1/1	0.95	0.06	73,73,73,73	0
57	MG	DA	3119	1/1	0.95	0.11	138,138,138,138	0
57	MG	DA	3052	1/1	0.95	0.08	118,118,118,118	0
57	MG	DA	3121	1/1	0.95	0.13	97,97,97,97	0
57	MG	BA	3024	1/1	0.95	0.08	42,42,42,42	0
57	MG	CA	1632	1/1	0.95	0.05	125,125,125,125	0
57	MG	AA	1608	1/1	0.95	0.10	82,82,82,82	0
57	MG	AA	1616	1/1	0.95	0.06	126,126,126,126	0
57	MG	BA	3059	1/1	0.95	0.14	50,50,50,50	0
57	MG	BA	3081	1/1	0.95	0.19	40,40,40,40	0
57	MG	BA	3006	1/1	0.95	0.06	88,88,88,88	0
57	MG	AA	1611	1/1	0.95	0.07	91,91,91,91	0
57	MG	DA	3036	1/1	0.95	0.08	84,84,84,84	0
57	MG	DA	3037	1/1	0.95	0.08	83,83,83,83	0
57	MG	DA	3069	1/1	0.95	0.09	86,86,86,86	0
57	MG	BA	3065	1/1	0.96	0.12	38,38,38,38	0
57	MG	DA	3044	1/1	0.96	0.05	116,116,116,116	0
57	MG	AA	1603	1/1	0.96	0.07	76,76,76,76	0
57	MG	DA	3073	1/1	0.96	0.18	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3104	1/1	0.96	0.10	107,107,107,107	0
57	MG	DA	3106	1/1	0.96	0.06	92,92,92,92	0
57	MG	DA	3046	1/1	0.96	0.09	142,142,142,142	0
57	MG	BA	3048	1/1	0.96	0.07	74,74,74,74	0
57	MG	BA	3093	1/1	0.96	0.16	84,84,84,84	0
57	MG	BA	3049	1/1	0.96	0.09	45,45,45,45	0
57	MG	CA	1608	1/1	0.96	0.11	86,86,86,86	0
57	MG	CA	1630	1/1	0.96	0.24	79,79,79,79	0
57	MG	DA	3113	1/1	0.96	0.09	86,86,86,86	0
57	MG	DA	3114	1/1	0.96	0.07	98,98,98,98	0
57	MG	BA	3052	1/1	0.96	0.09	38,38,38,38	0
57	MG	AA	1601	1/1	0.96	0.05	111,111,111,111	0
57	MG	DA	3117	1/1	0.96	0.10	90,90,90,90	0
57	MG	DA	3055	1/1	0.96	0.07	85,85,85,85	0
57	MG	AA	1629	1/1	0.96	0.12	129,129,129,129	0
57	MG	BA	3079	1/1	0.96	0.06	89,89,89,89	0
57	MG	DA	3087	1/1	0.96	0.07	88,88,88,88	0
57	MG	AA	1642	1/1	0.96	0.07	74,74,74,74	0
57	MG	DA	3125	1/1	0.96	0.09	90,90,90,90	0
57	MG	BA	3042	1/1	0.96	0.09	56,56,56,56	0
57	MG	DA	3127	1/1	0.96	0.13	104,104,104,104	0
57	MG	BA	3044	1/1	0.96	0.07	71,71,71,71	0
57	MG	DA	3091	1/1	0.96	0.06	93,93,93,93	0
57	MG	AA	1643	1/1	0.96	0.06	81,81,81,81	0
57	MG	CA	1618	1/1	0.96	0.09	108,108,108,108	0
57	MG	BA	3088	1/1	0.96	0.07	58,58,58,58	0
57	MG	BB	204	1/1	0.96	0.10	57,57,57,57	0
57	MG	DA	3068	1/1	0.96	0.09	86,86,86,86	0
57	MG	AA	1605	1/1	0.96	0.06	103,103,103,103	0
57	MG	BA	3029	1/1	0.97	0.12	38,38,38,38	0
57	MG	DA	3092	1/1	0.97	0.09	102,102,102,102	0
57	MG	DA	3053	1/1	0.97	0.10	101,101,101,101	0
57	MG	CA	1620	1/1	0.97	0.12	93,93,93,93	0
57	MG	DA	3039	1/1	0.97	0.12	104,104,104,104	0
57	MG	DA	3057	1/1	0.97	0.07	92,92,92,92	0
57	MG	AA	1640	1/1	0.97	0.06	132,132,132,132	0
57	MG	BA	3134	1/1	0.97	0.07	38,38,38,38	0
57	MG	BA	3032	1/1	0.97	0.06	40,40,40,40	0
57	MG	AA	1602	1/1	0.97	0.16	79,79,79,79	0
57	MG	CA	1611	1/1	0.97	0.06	93,93,93,93	0
57	MG	DA	3102	1/1	0.97	0.07	84,84,84,84	0
57	MG	DA	3063	1/1	0.97	0.10	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3083	1/1	0.97	0.10	121,121,121,121	0
57	MG	BA	3097	1/1	0.97	0.06	49,49,49,49	0
57	MG	AA	1635	1/1	0.97	0.05	114,114,114,114	0
57	MG	BA	3086	1/1	0.97	0.08	43,43,43,43	0
57	MG	AA	1615	1/1	0.97	0.05	117,117,117,117	0
57	MG	AA	1623	1/1	0.97	0.08	108,108,108,108	0
57	MG	AA	1609	1/1	0.97	0.07	91,91,91,91	0
57	MG	BA	3028	1/1	0.97	0.19	39,39,39,39	0
57	MG	DA	3105	1/1	0.98	0.09	91,91,91,91	0
57	MG	BA	3069	1/1	0.98	0.04	52,52,52,52	0
57	MG	BA	3122	1/1	0.98	0.05	40,40,40,40	0
57	MG	DA	3022	1/1	0.98	0.14	105,105,105,105	0
57	MG	BA	3010	1/1	0.98	0.05	46,46,46,46	0
57	MG	AA	1639	1/1	0.98	0.05	119,119,119,119	0
57	MG	BA	3051	1/1	0.98	0.11	39,39,39,39	0
57	MG	BA	3038	1/1	0.98	0.06	42,42,42,42	0
57	MG	BA	3053	1/1	0.98	0.09	41,41,41,41	0
57	MG	DA	3056	1/1	0.98	0.08	101,101,101,101	0
57	MG	BA	3039	1/1	0.98	0.07	40,40,40,40	0
57	MG	BA	3101	1/1	0.98	0.06	38,38,38,38	0
57	MG	BA	3040	1/1	0.98	0.04	41,41,41,41	0
57	MG	DA	3118	1/1	0.98	0.15	99,99,99,99	0
57	MG	BA	3105	1/1	0.98	0.07	38,38,38,38	0
57	MG	AA	1612	1/1	0.98	0.05	82,82,82,82	0
57	MG	BA	3043	1/1	0.98	0.07	56,56,56,56	0
57	MG	BB	203	1/1	0.98	0.05	57,57,57,57	0
57	MG	BA	3110	1/1	0.98	0.08	50,50,50,50	0
57	MG	BD	301	1/1	0.98	0.11	39,39,39,39	0
57	MG	AA	1634	1/1	0.98	0.06	102,102,102,102	0
57	MG	AA	1613	1/1	0.98	0.05	74,74,74,74	0
57	MG	BA	3009	1/1	0.98	0.06	46,46,46,46	0
57	MG	BA	3063	1/1	0.98	0.10	37,37,37,37	0
57	MG	BA	3064	1/1	0.98	0.04	38,38,38,38	0
57	MG	BA	3034	1/1	0.98	0.05	40,40,40,40	0
57	MG	CA	1633	1/1	0.98	0.09	101,101,101,101	0
57	MG	BA	3067	1/1	0.98	0.07	40,40,40,40	0
57	MG	CA	1635	1/1	0.98	0.04	114,114,114,114	0
57	MG	BA	3120	1/1	0.98	0.05	41,41,41,41	0
58	ZN	B4	101	1/1	0.98	0.04	79,79,79,79	0
57	MG	BA	3106	1/1	0.99	0.05	40,40,40,40	0
57	MG	BA	3013	1/1	0.99	0.06	38,38,38,38	0
57	MG	BA	3108	1/1	0.99	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3082	1/1	0.99	0.05	38,38,38,38	0
57	MG	BA	3083	1/1	0.99	0.06	43,43,43,43	0
57	MG	BA	3036	1/1	0.99	0.03	47,47,47,47	0
57	MG	CA	1605	1/1	0.99	0.14	89,89,89,89	0
57	MG	DA	3033	1/1	0.99	0.08	94,94,94,94	0
57	MG	BA	3016	1/1	0.99	0.25	39,39,39,39	0
57	MG	BA	3050	1/1	0.99	0.04	40,40,40,40	0
57	MG	BA	3087	1/1	0.99	0.03	45,45,45,45	0
57	MG	BA	3066	1/1	0.99	0.04	43,43,43,43	0
57	MG	BA	3116	1/1	0.99	0.07	38,38,38,38	0
57	MG	BA	3117	1/1	0.99	0.06	56,56,56,56	0
57	MG	BA	3017	1/1	0.99	0.03	39,39,39,39	0
57	MG	BA	3027	1/1	0.99	0.07	41,41,41,41	0
57	MG	BA	3018	1/1	0.99	0.04	67,67,67,67	0
57	MG	DA	3079	1/1	0.99	0.11	90,90,90,90	0
57	MG	BA	3041	1/1	0.99	0.12	43,43,43,43	0
57	MG	BA	3072	1/1	0.99	0.18	38,38,38,38	0
57	MG	BA	3073	1/1	0.99	0.04	43,43,43,43	0
57	MG	AA	1622	1/1	0.99	0.08	85,85,85,85	0
57	MG	BA	3125	1/1	0.99	0.07	40,40,40,40	0
57	MG	BA	3096	1/1	0.99	0.09	45,45,45,45	0
57	MG	DA	3123	1/1	0.99	0.06	93,93,93,93	0
57	MG	CA	1621	1/1	0.99	0.07	85,85,85,85	0
57	MG	BA	3127	1/1	0.99	0.08	40,40,40,40	0
57	MG	BA	3128	1/1	0.99	0.06	52,52,52,52	0
57	MG	BA	3130	1/1	0.99	0.09	49,49,49,49	0
57	MG	BA	3057	1/1	0.99	0.22	42,42,42,42	0
57	MG	BA	3020	1/1	0.99	0.04	46,46,46,46	0
57	MG	BA	3021	1/1	0.99	0.08	42,42,42,42	0
57	MG	BA	3100	1/1	0.99	0.03	59,59,59,59	0
57	MG	BA	3078	1/1	0.99	0.07	86,86,86,86	0
57	MG	BA	3033	1/1	0.99	0.05	40,40,40,40	0
57	MG	BA	3103	1/1	0.99	0.07	64,64,64,64	0
57	MG	BA	3104	1/1	0.99	0.09	38,38,38,38	0
57	MG	BA	3022	1/1	0.99	0.05	38,38,38,38	0
58	ZN	D4	101	1/1	0.99	0.09	79,79,79,79	0
57	MG	BA	3023	1/1	1.00	0.04	41,41,41,41	0
57	MG	BA	3054	1/1	1.00	0.06	44,44,44,44	0
57	MG	BA	3008	1/1	1.00	0.05	43,43,43,43	0
57	MG	CA	1641	1/1	1.00	0.08	91,91,91,91	0
57	MG	BA	3031	1/1	1.00	0.04	42,42,42,42	0
57	MG	BA	3012	1/1	1.00	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3068	1/1	1.00	0.09	52,52,52,52	0
57	MG	BA	3129	1/1	1.00	0.02	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.