



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 06:40 pm BST

PDB ID : 4V9D  
Title : Structures of the bacterial ribosome in classical and hybrid states of tRNA binding  
Authors : Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.  
Deposited on : 2012-07-31  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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



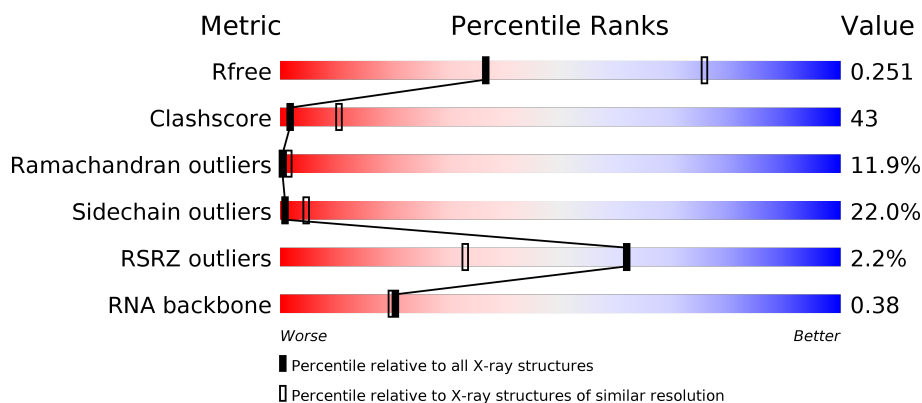
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

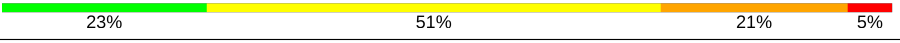

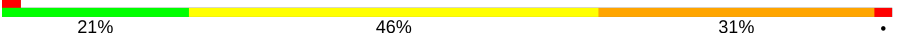
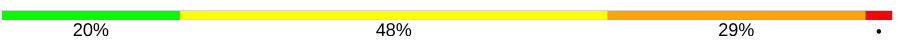


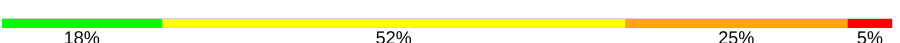
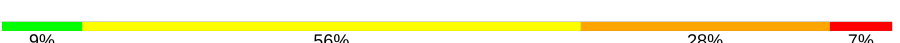
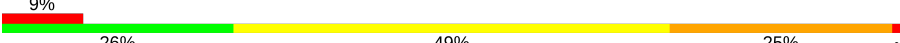


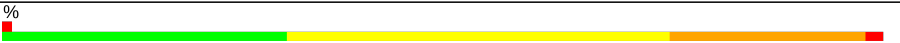
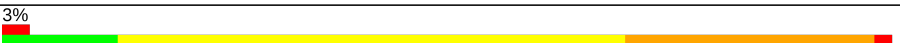
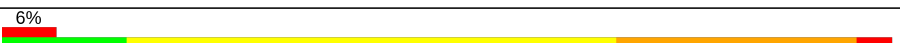
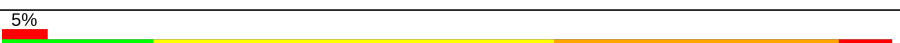

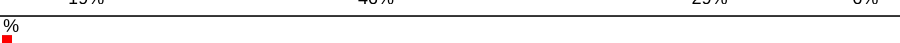
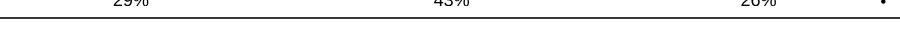
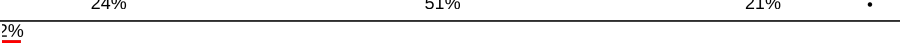

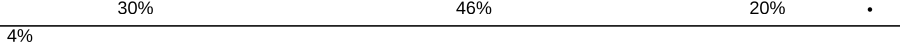
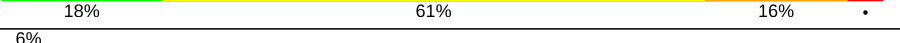

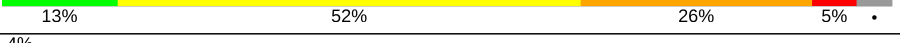

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div>14%</div> <div>54%</div> <div>28%</div> <div>.</div> </div>
1	BA	1539	<div> <div>13%</div> <div>55%</div> <div>28%</div> <div>.</div> </div>
2	AB	218	<div> <div>6%</div> <div>10%</div> <div>45%</div> <div>36%</div> <div>9%</div> </div>
2	BB	218	<div> <div>6%</div> <div>15%</div> <div>51%</div> <div>26%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	150	
5	BE	150	
6	AF	100	
6	BF	100	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	98	
10	BJ	98	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	85	
20	BT	85	
21	AU	51	
21	BU	51	
22	AV	76	
22	BV	76	
23	AX	16	
23	BX	16	
24	AY	183	
25	CA	2903	
25	DA	2903	
26	CB	119	
27	CC	271	
27	DC	271	
28	CD	209	
28	DD	209	

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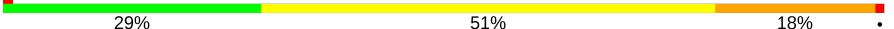

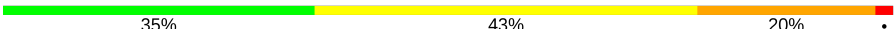
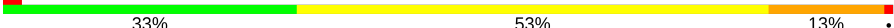
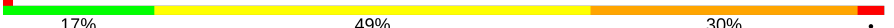


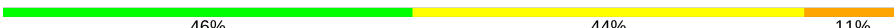
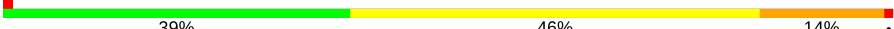



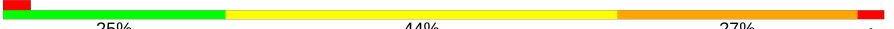




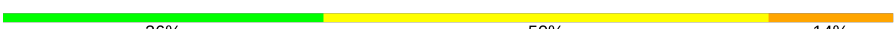
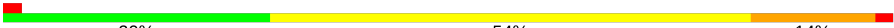

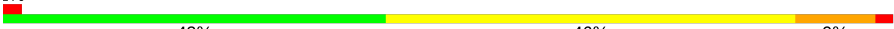


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Mol	Chain	Length	Quality of chain
29	CE	201	
29	DE	201	
30	CF	177	
30	DF	177	
31	CG	176	
31	DG	176	
32	CH	149	
32	DH	149	
33	CI	141	
33	DI	141	
34	CJ	142	
34	DJ	142	
35	CK	122	
35	DK	122	
36	CL	143	
36	DL	143	
37	CM	136	
37	DM	136	
38	CN	120	
38	DN	120	
39	CO	116	
39	DO	116	
40	CP	114	
40	DP	114	
41	CQ	117	

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Mol	Chain	Length	Quality of chain
41	DQ	117	
42	CR	103	
42	DR	103	
43	CS	110	
43	DS	110	
44	CT	93	
44	DT	93	
45	CU	102	
45	DU	102	
46	CV	94	
46	DV	94	
47	CW	76	
48	CX	77	
48	DX	77	
49	CY	63	
49	DY	63	
50	CZ	58	
50	DZ	58	
51	C0	56	
51	D0	56	
52	C1	50	
52	D1	50	
53	C2	46	
53	D2	46	
54	C3	64	

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Mol	Chain	Length	Quality of chain
54	D3	64	
55	C4	38	
55	D4	38	
56	DB	118	
57	DW	75	

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
58	MG	DA	3098	-	-	-	X



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	BA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	BB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

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

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

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	BF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	BU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	BV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	BX	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	2	GLY	-	EXPRESSION TAG	UNP P0A805

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
25	DA	2896	Total	C	N	O	P	0	0	0
			62173	27735	11441	20101	2896			

- Molecule 26 is a RNA chain called 5S rRNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CB	119	Total	C	N	O	P	0	0	0
			2548	1135	466	829	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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



- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
35	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.



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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
38	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
44	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				
45	DU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CW	76	Total	C	N	O	S	0	0	0
			575	356	117	101	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.



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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	C1	50	Total	C	N	O	0	0	0
			410	263	75	72			
52	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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

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

- Molecule 57 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DW	75	Total	C	N	O	S	0	0	0
			564	350	113	100	1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	56	Total	Mg	0	0
			56	56		
58	CA	194	Total	Mg	0	0
			194	194		
58	DQ	1	Total	Mg	0	0
			1	1		
58	CB	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DL	1	Total 1	Mg 1	0	0
58	AA	72	Total 72	Mg 72	0	0
58	CQ	1	Total 1	Mg 1	0	0
58	DA	166	Total 166	Mg 166	0	0
58	DB	3	Total 3	Mg 3	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D4	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	197	Total 197	O 197	0	0
60	AN	4	Total 4	O 4	0	0
60	AT	1	Total 1	O 1	0	0
60	AU	1	Total 1	O 1	0	0
60	BA	190	Total 190	O 190	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	5	Total 5	O 5	0	0
60	BT	1	Total 1	O 1	0	0
60	BU	1	Total 1	O 1	0	0
60	CA	625	Total 625	O 625	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CB	13	Total 13	O 13	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	2	Total 2	O 2	0	0
60	CE	2	Total 2	O 2	0	0
60	CF	1	Total 1	O 1	0	0
60	CJ	1	Total 1	O 1	0	0
60	CL	6	Total 6	O 6	0	0
60	CN	4	Total 4	O 4	0	0
60	CS	1	Total 1	O 1	0	0
60	CV	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	622	Total 622	O 622	0	0
60	DB	14	Total 14	O 14	0	0
60	DC	4	Total 4	O 4	0	0
60	DD	5	Total 5	O 5	0	0
60	DE	2	Total 2	O 2	0	0
60	DJ	1	Total 1	O 1	0	0
60	DL	4	Total 4	O 4	0	0
60	DN	1	Total 1	O 1	0	0

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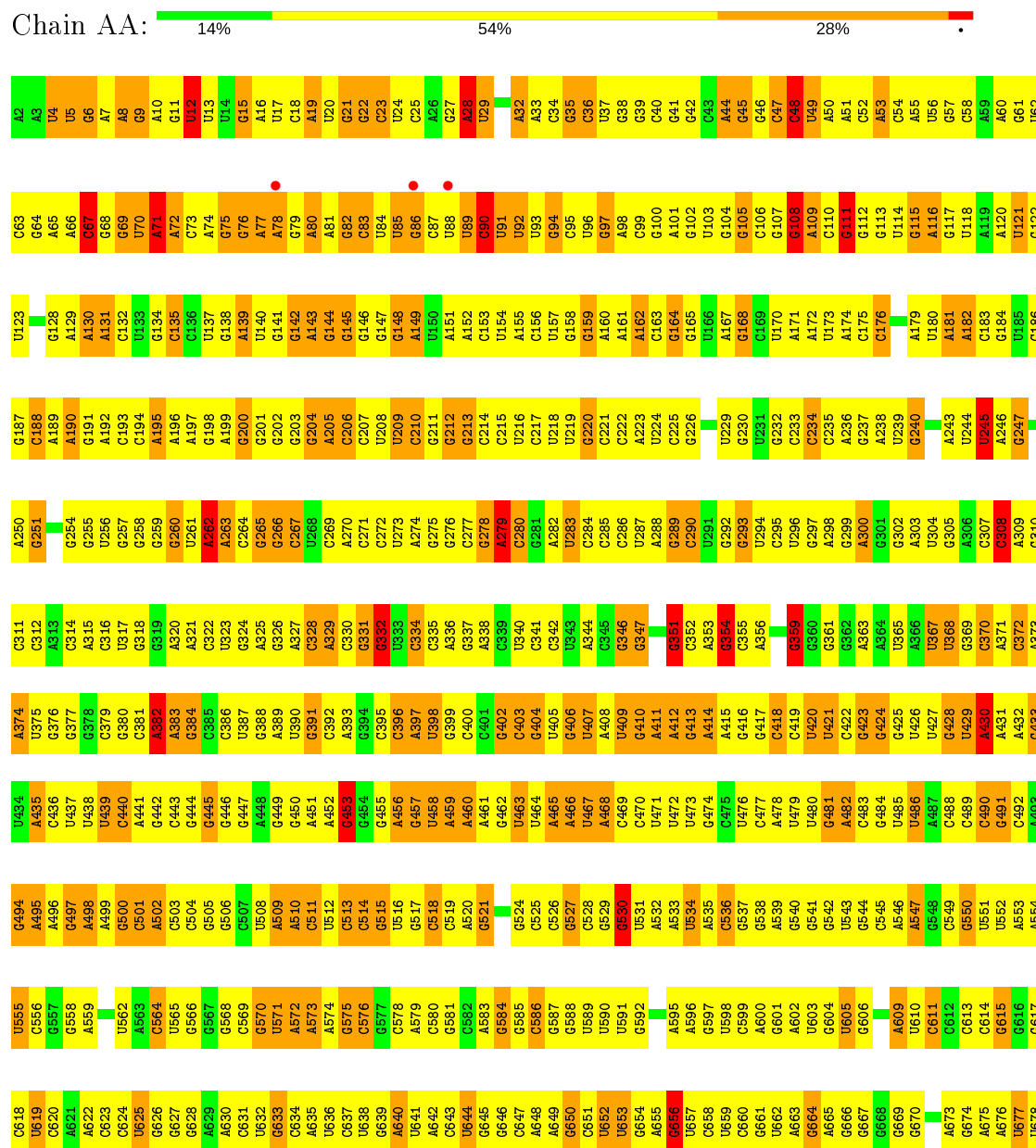
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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60	D3	2	Total 2	O 2	0	0
60	D4	1	Total 1	O 1	0	0



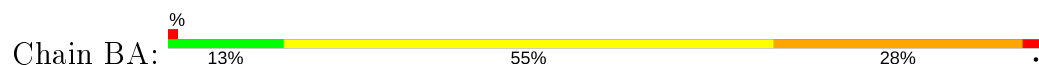
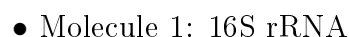
### 3 Residue-property plots

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

#### • Molecule 1: 16S rRNA



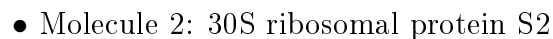






G939	G940	G941	G942	G943	G944	A949	U950	G951	U952	G953	G954	G955	G956	U957	G958	G959	U960	G961	G962	G963	A964	U965	G966	G967	A968	A969	C970	G971	C972	G973	A974	A975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	A1000	C1001	G1002	G1003	A1004																																																		
G877	A878	C879	C880	G881	C882	C883	U884	G885	A889	G890	U891	A892	C893	G894	G895	C896	C897	U898	G899	U899	G900	G901	G902	G903	U904	U905	U906	U907	A908	A909	C910	U911	G912	A913	U914	G915	U916	A917	U918	C919	C920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	C931	C932	G933	U934	C935	A936	A937	A938																																																				
A815	A816	C817	C818	A819	U820	G821	U822	C823	G824	A825	C826	U827	U828	G829	G830	A831	A832	C833	U834	U835	G836	U837	C840	G841	U842	U843	G844	A845	A846	G847	C848	G849	G850	G851	G852	G853	U854	U855	C856	C857	G858	G859	A860	G861	C862	U863	A864	A865	A866	G867	C868	G869	U870	U871	G872	A873	U874	U875	C876																																																				
C67	G68	G69	U70	U71	A72	C73	A74	G75	G76	A77	G78	G79	A80	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95	U96	G97	A98	C99	G100	A101	G102	U103	G104	G105	C106	G107	G108	A109	C110	G111	G112	G113	U114	G115	A116	G117	A120	G121	U122	G123	G126	G127	A128	A129																																																					
A130	A131	C132	U133	G134	C135	C136	U137	G138	G141	A142	A143	G144	G145	G146	G147	G148	A149	U150	A151	G152	C153	U154	A155	C156	U157	U158	G159	C160	U161	A162	C163	G164	U165	U166	A167	G168	C169	U170	A171	C172	U173	A174	C175	G176	G177	G178	A179	U180	A181	A182	C183	G184	U185	C186	G187	C188	A189	A190																																																					
G191	A192	C193	C194	A195	A196	A197	G198	A199	G200	G201	G202	G203	G204	A205	C206	C207	U208	U209	C210	G211	G212	G213	C214	C215	U216	U219	G220	C221	G222	A223	G226	U229	G230	G231	G232	C233	C234	C235	A236	G237	G240	G241	G242	A243	C244	U245	U246	A247	C248	U249	A250	G251	U252	A253	G254	C255	G256	G257	G258	C259	G260	U261	C264	G265	G266	C267	U268	C269	A270	C271	C272	C273	U274	G275	G276	C277	G278	C279	C280	G281	A282	U283	C284	C285	C286	G289	C290	U291	G292	G293	U294	C295	U296	C297	G298	A300	A303	U304	G305	A306	C307	C308	A309	G310	C311	C312	A313	C316	U317	G318	G319
C381	A382	A383	G384	C385	C386	U387	G388	A389	U390	C391	C392	A393	G394	C395	A396	U397	U398	C399	C400	C401	G402	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	A414	A415	G416	G417	C418	U419	G420	C421	C422	A423	G424	C425	U426	U427	G428	U429	A430	C431	A432	G433	U434	A435	C436	U437	U438	U439	C440																																																				
G443	G444	G445	G446	G447	A448	A449	G450	A451	A452	G453	A454	G455	A456	A457	U458	A459	A460	A461	A462	U463	U464	A465	A466	U467	A468	A469	C470	U471	U472	U473	G474	U475	U476	C477	A478	U479	U480	G481	A482	C483	G484	U485	U486	A487	C488	C489	U490	A491	C492	A493	G494	A495	A496	G497	A498	A499	G500	C501																																																					
A502	C503	U504	G505	G506	C507	A510	C511	U512	C513	U516	G517	C518	C519	C522	A523	G524	C525	C526	G527	A528	A529	A530	U531	A532	A533	U534	A535	C536	G537	G538	A539	G540	G541	G542	U543	G544	C545	A546	A547	G548	C549	G550	U551	U552	A553	A554	U555	C556	G557	G558	A559	A560	U561	U562	A563	C564	U565																																																						
G566	G567	U568	C569	U570	U571	A572	A573	A574	C575	G576	G577	C578	A579	C580	G581	C582	G583	C584	G585	C586	U587	G588	U589	U590	U591	G592	U593	A594	U595	G596	A600	G601	A602	U603	G604	U605	G606	A607	A608	U609	C610	C611	C612	G613	G614	G615	G616	G617	C618	U619	C620	A621	G622	C623	G624	U625	A626	G627																																																					
G628	A629	A630	C631	U632	G633	C634	A635	G636	C637	U638	G639	A640	U641	A642	C643	U644	G645	G646	C647	A648	A649	G650	C651	G652	U653	U654	A655	G656	U657	C658	U659	C660	G661	U662	A663	G664	A665	G666	G669	G670	G671	U672	A673	G674	A675	A676	U677	U678	C679	C680	A681	G682	C683	U684	G685	U686	G687	G688																																																					
C689	G690	U691	G692	G693	A694	A695	C699	G700	U701	A702	G703	A704	U705	A706	U707	G708	U709	G710	G711	G712	A713	G714	A715	A716	U717	A718	A719	C720	U721	G722	U723	G724	G725	C726	G727	A728	A729	U730	G731	A732	U733	A734	C735	C736	U737	C738	C739	U740	C741	G742	A743	C744	G745	U746	A747	U748	C749	C750																																																					
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A815	A816	C817	C818	A819	U820	G821	U822	C823	G824	A825	C826	U827	U828	G829	G830	A831	A832	C833	U834	U835	G836	U837	C840	G841	U842	U843	G844	A845	A846	G847	C848	G849	G850	G851	G852	G853	U854	U855	C856	C857	G858	G859	A860	G861	C862	U863	A864	A865	A866	G867	C868	G869	U870	U871	G872	A873	U874	U875	C876																																																				
C877	A878	C879	C880	G881	C882	C883	U884	G885	A889	G890	U891	A892	C893	G894	G895	C896	C897	U898	G899	U899	G900	G901	G902	G903	U904	U905	U906	U907	A908	A909	C910	U911	G912	A913	U914	G915	U916	A917	U918	C919	C920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	C931	C932	G933	U934	C935	A936	A937	A938																																																				
U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	A1000	C1001	G1002	G1003	A1004																																														



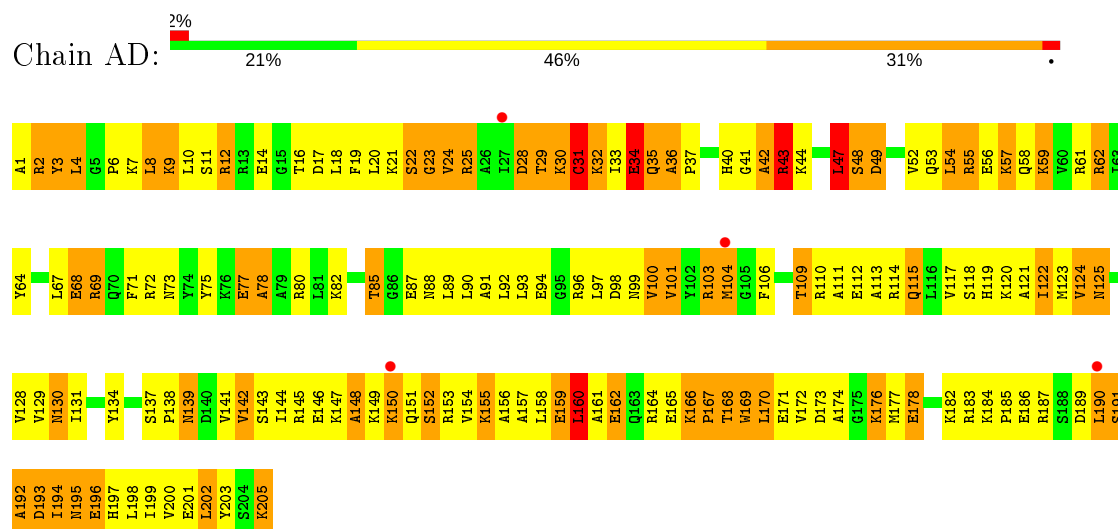




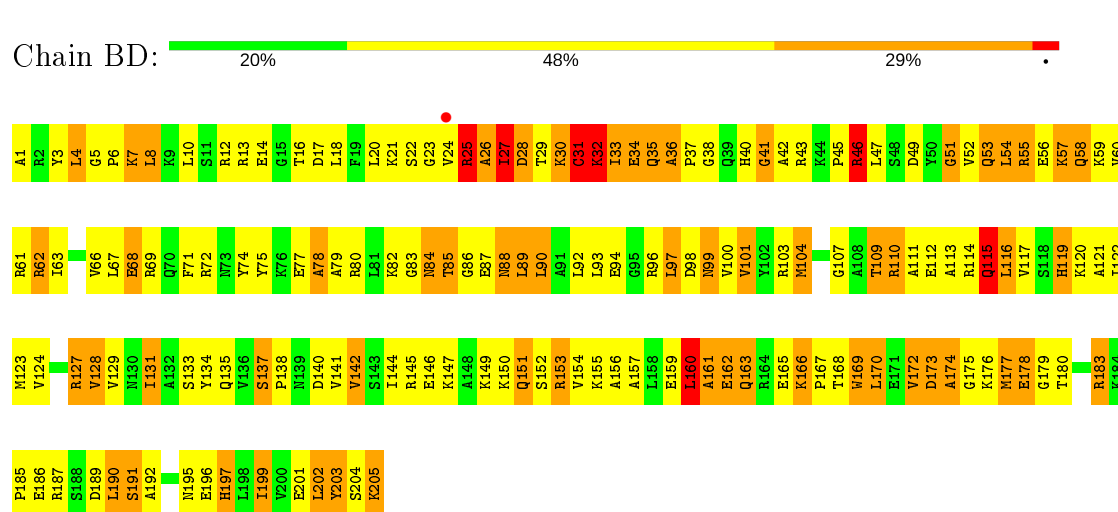




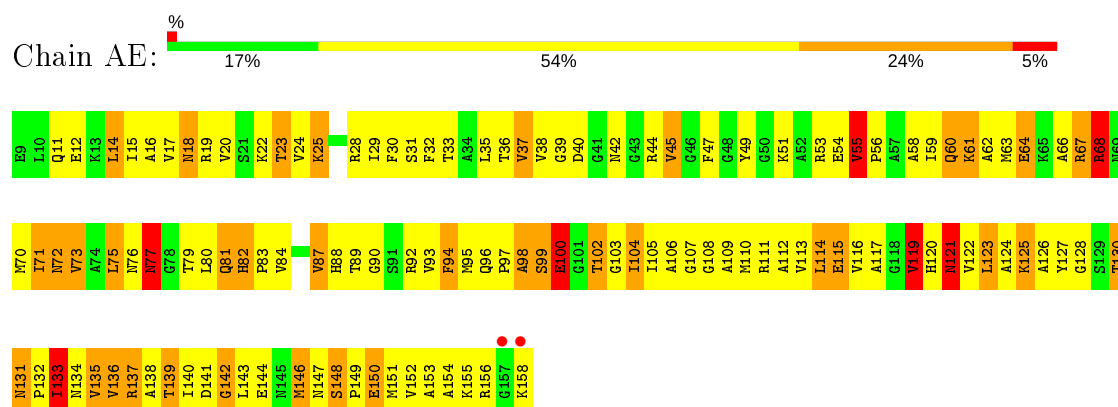
- Molecule 4: 30S ribosomal protein S4



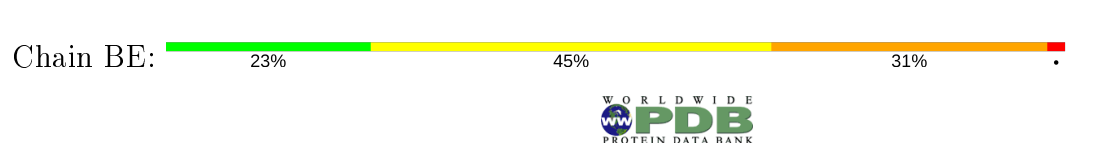
- Molecule 4: 30S ribosomal protein S4



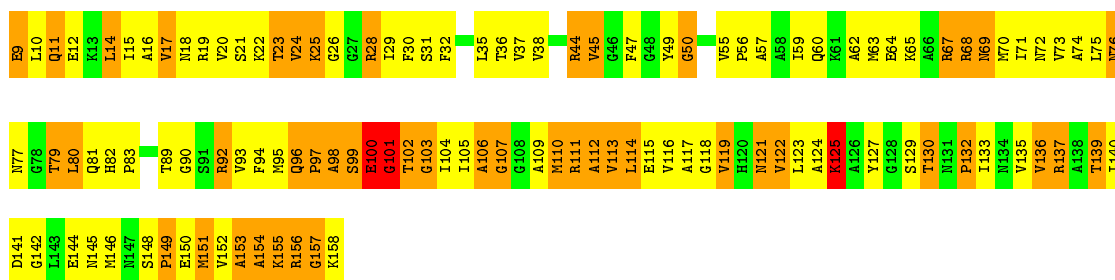
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

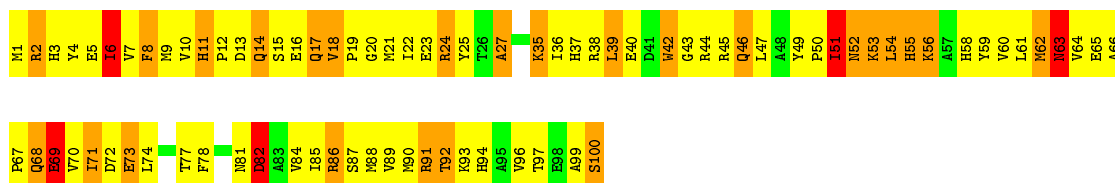






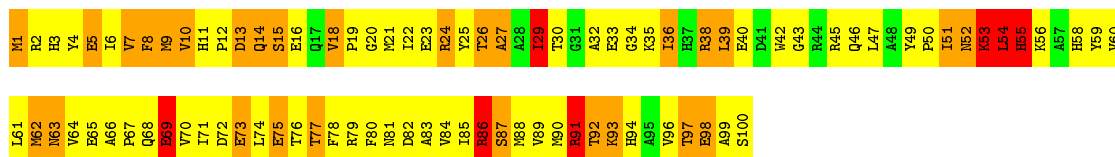
- Molecule 6: 30S ribosomal protein S6

Chain AF: 18% 52% 25% 5%



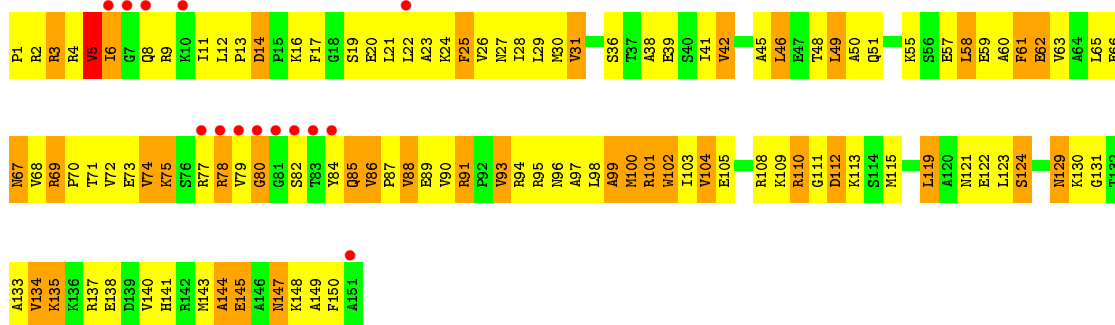
- Molecule 6: 30S ribosomal protein S6

Chain BF: 9% 56% 28% 7%



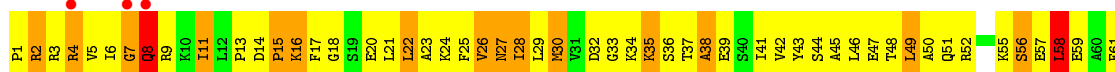
- Molecule 7: 30S ribosomal protein S7

Chain AG: 9% 26% 49% 25%

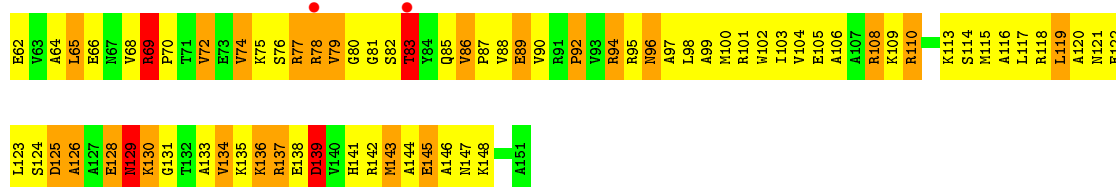


- Molecule 7: 30S ribosomal protein S7

Chain BG: 3% 16% 55% 25%

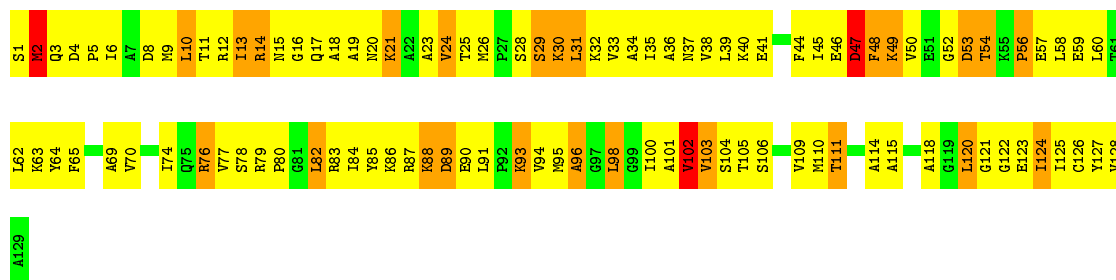






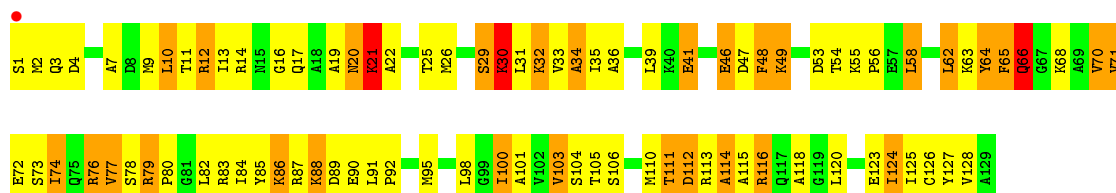
• Molecule 8: 30S ribosomal protein S8

Chain AH: 21% 58% 19%



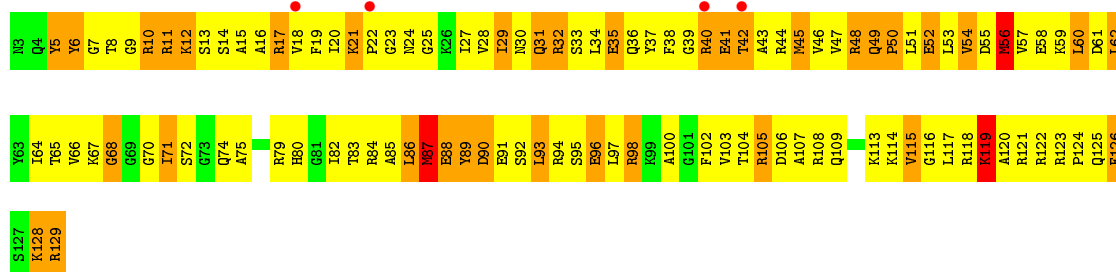
• Molecule 8: 30S ribosomal protein S8

Chain BH: 32% 43% 22%



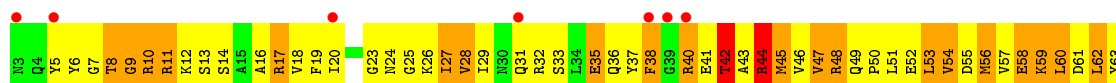
• Molecule 9: 30S ribosomal protein S9

Chain AI: 3% 13% 57% 28%

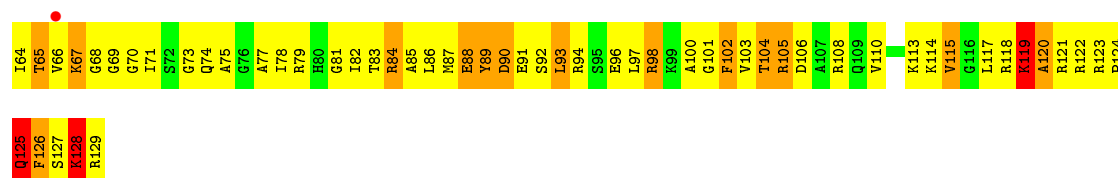


• Molecule 9: 30S ribosomal protein S9

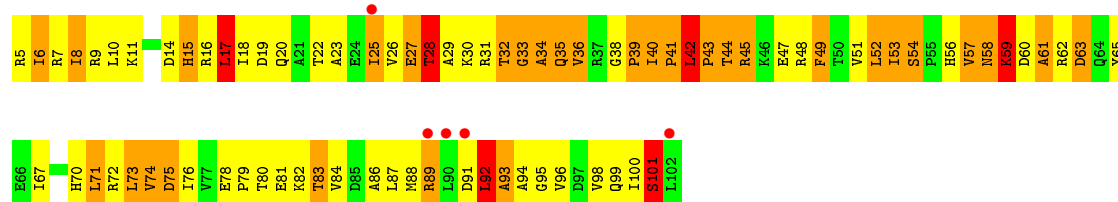
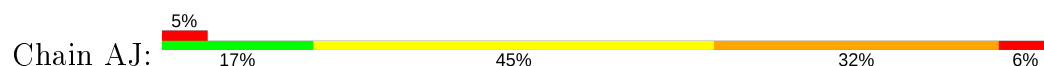
Chain BI: 6% 14% 55% 27%



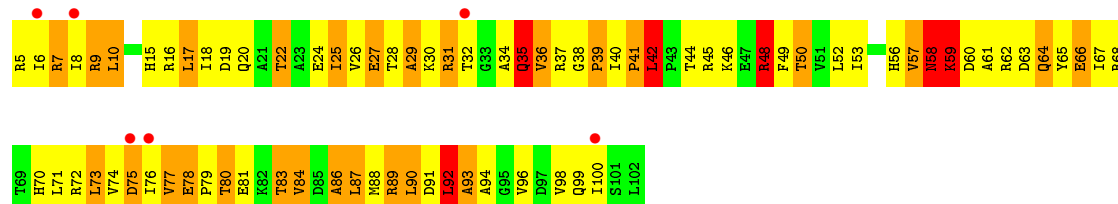
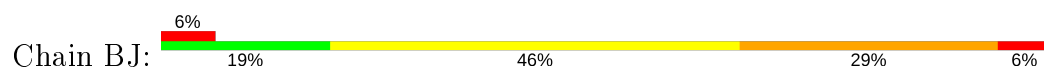




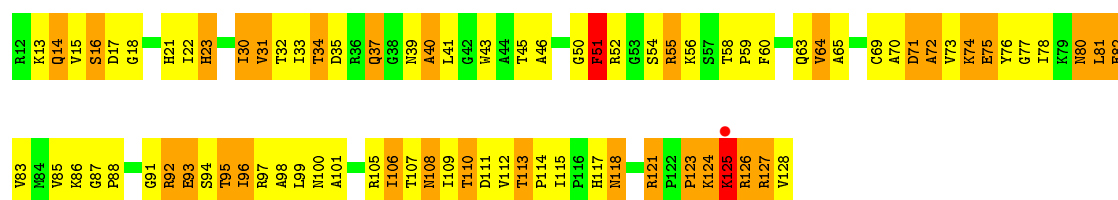
- Molecule 10: 30S ribosomal protein S10



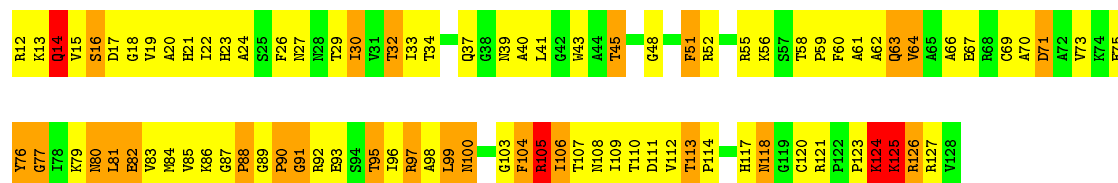
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

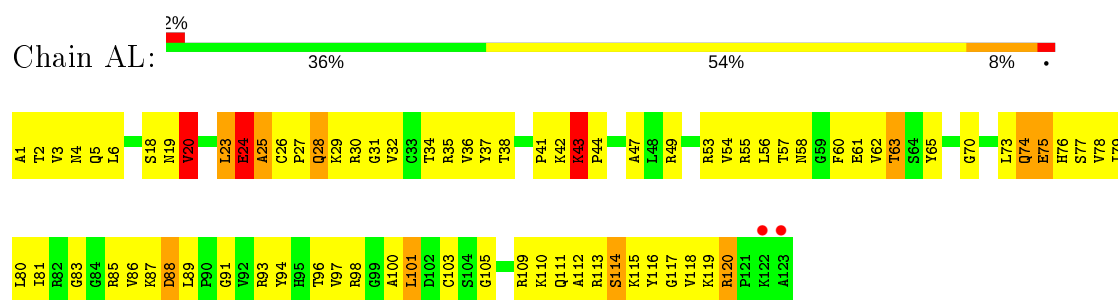


- Molecule 11: 30S ribosomal protein S11

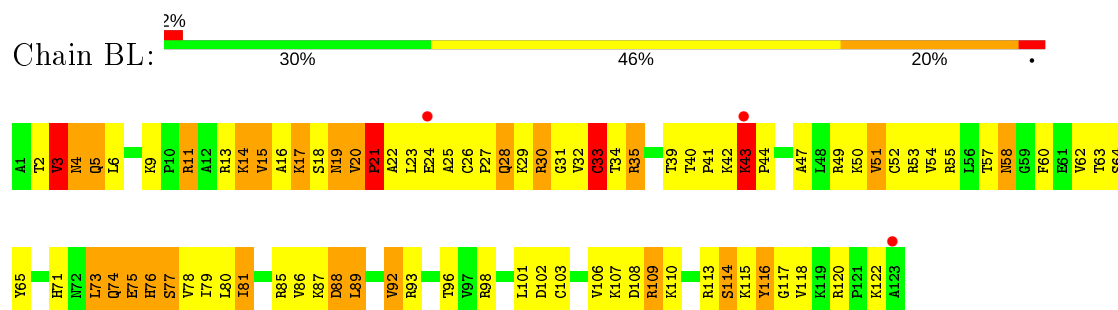


- Molecule 12: 30S ribosomal protein S12

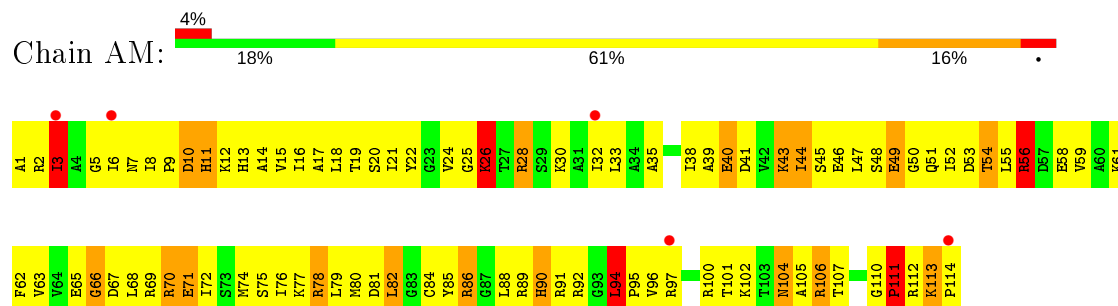




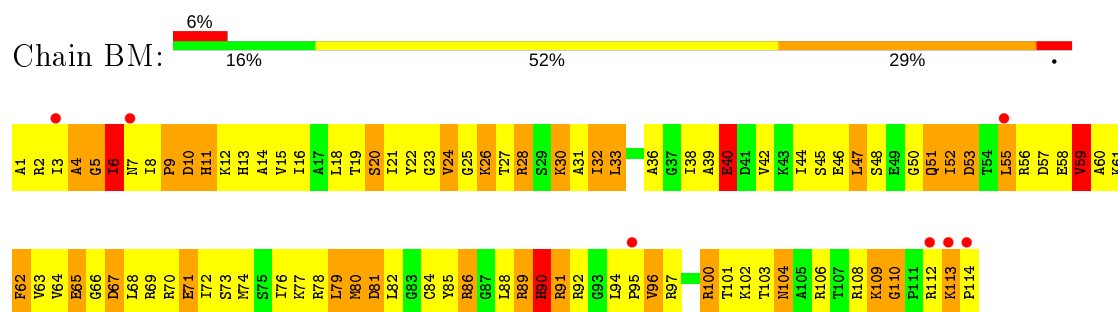
• Molecule 12: 30S ribosomal protein S12



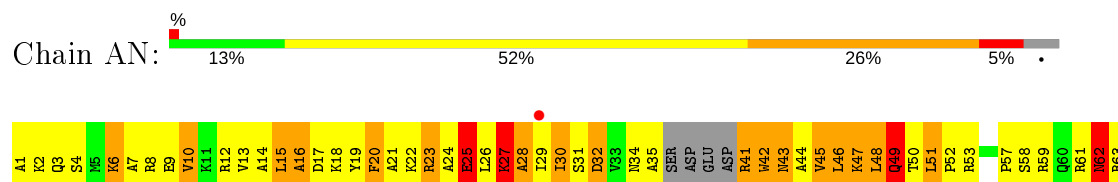
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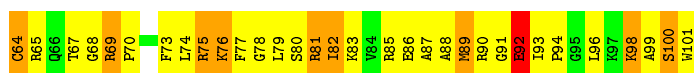
• Molecule 13: 30S ribosomal protein S13



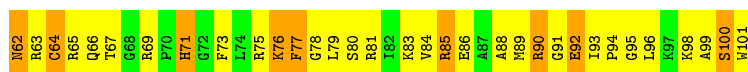
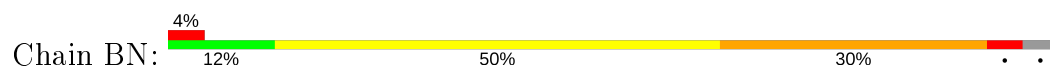
• Molecule 14: 30S ribosomal protein S14



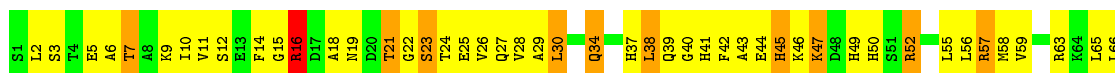




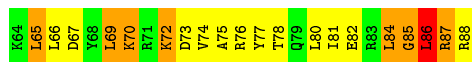
- Molecule 14: 30S ribosomal protein S14



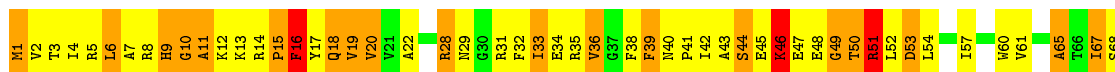
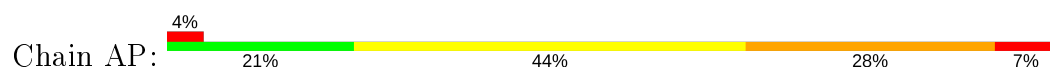
- Molecule 15: 30S ribosomal protein S15



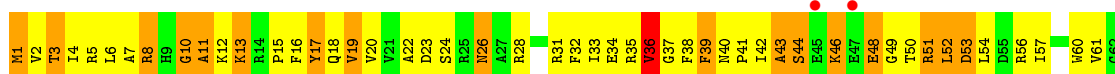
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



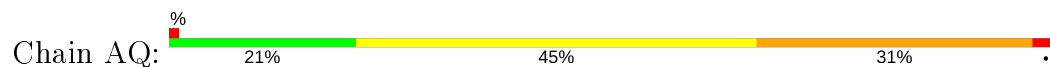
- Molecule 16: 30S ribosomal protein S16



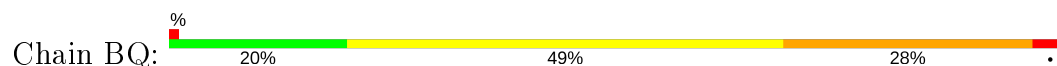




- Molecule 17: 30S ribosomal protein S17



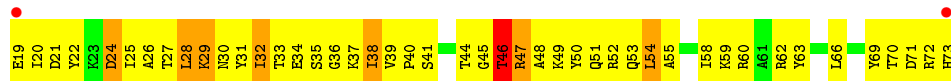
- Molecule 17: 30S ribosomal protein S17



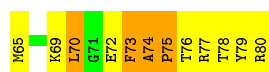
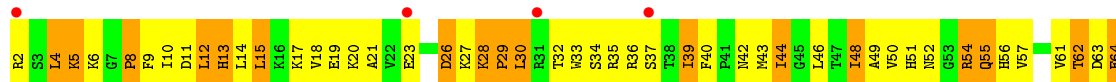
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

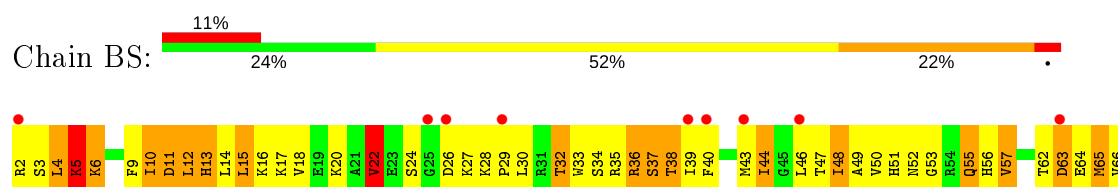


- Molecule 19: 30S ribosomal protein S19

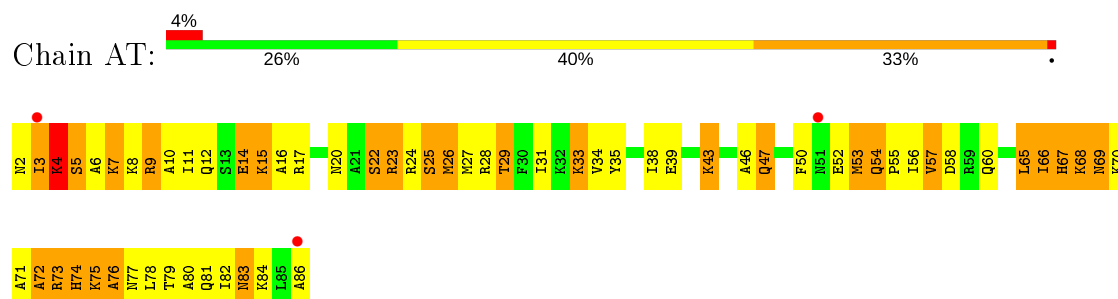


- Molecule 19: 30S ribosomal protein S19

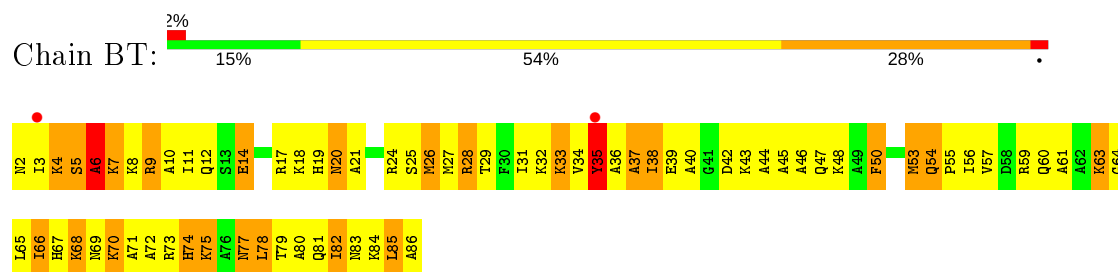




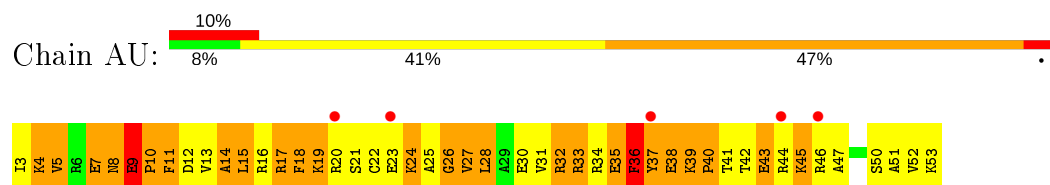
- Molecule 20: 30S ribosomal protein S20



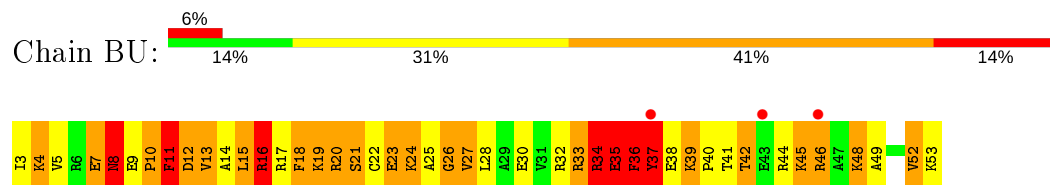
- Molecule 20: 30S ribosomal protein S20



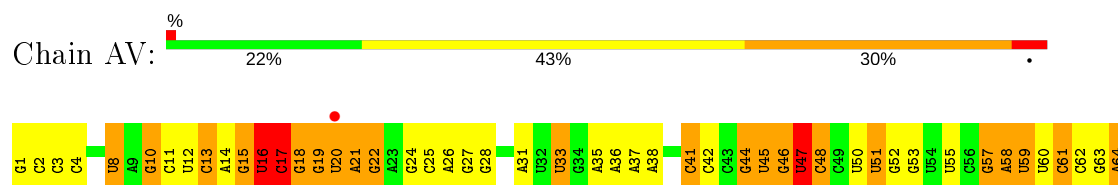
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: phenylalanine specific transfer RNA

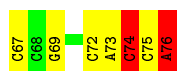






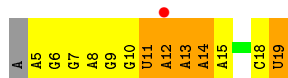
- Molecule 22: phenylalanine specific transfer RNA

Chain BV: 28% 54% 14%



- Molecule 23: messenger RNA

Chain AX: 6% 13% 50% 31% 6%



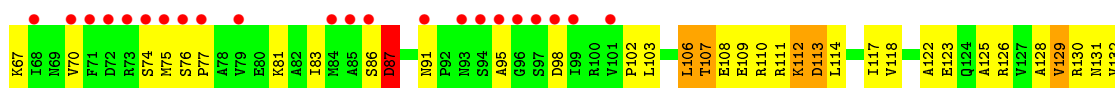
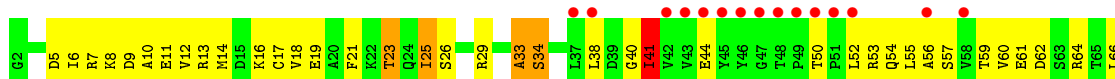
- Molecule 23: messenger RNA

Chain BX: 6% 6% 69% 25%



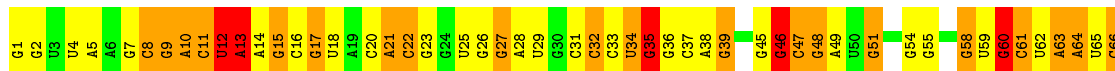
- Molecule 24: ribosome recycling factor

Chain AY: 21% 44% 45% 9%



- Molecule 25: 23S rRNA

Chain CA: 18% 44% 30% 7%









WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

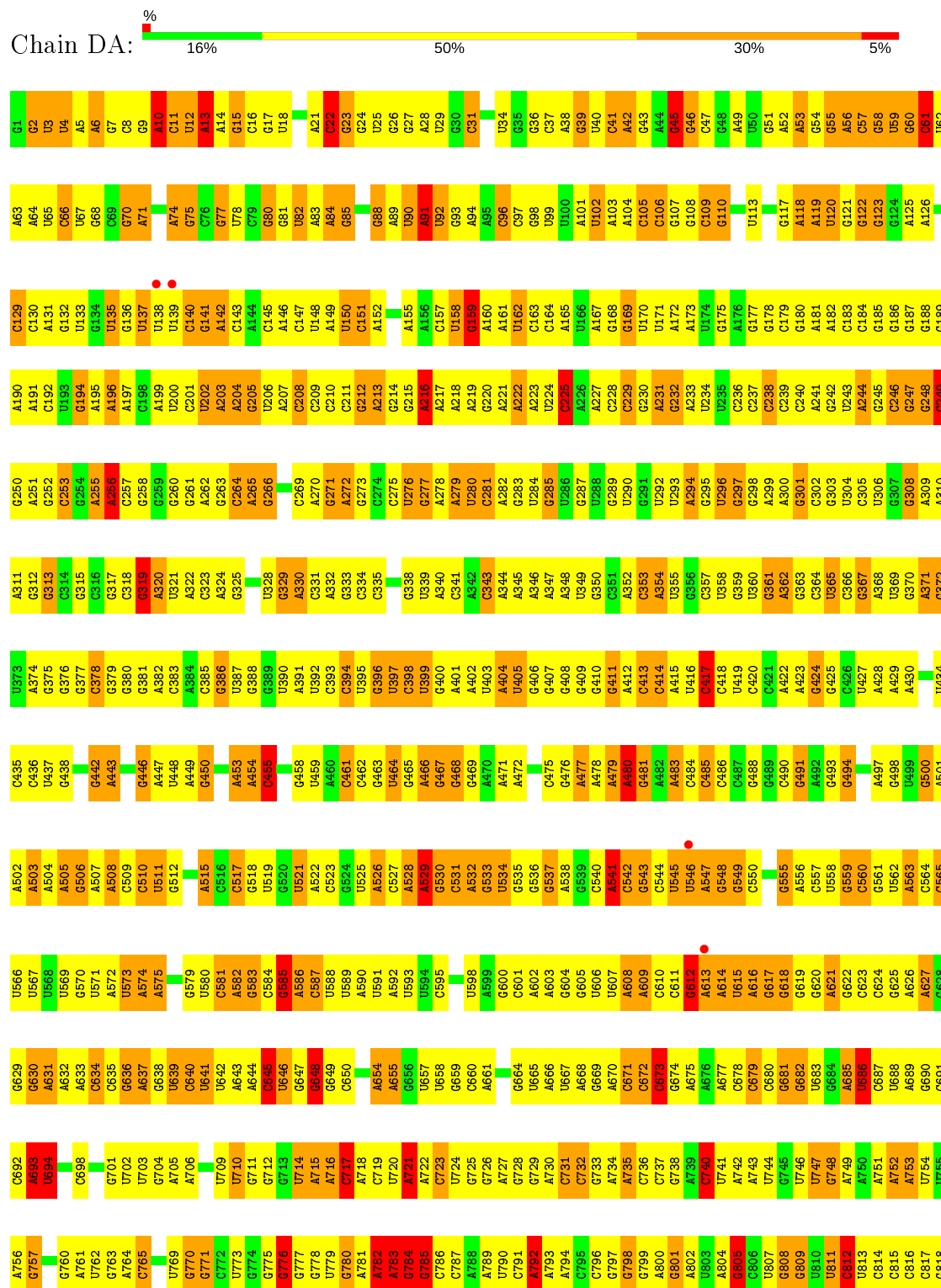


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• Molecule 25: 23S rRNA



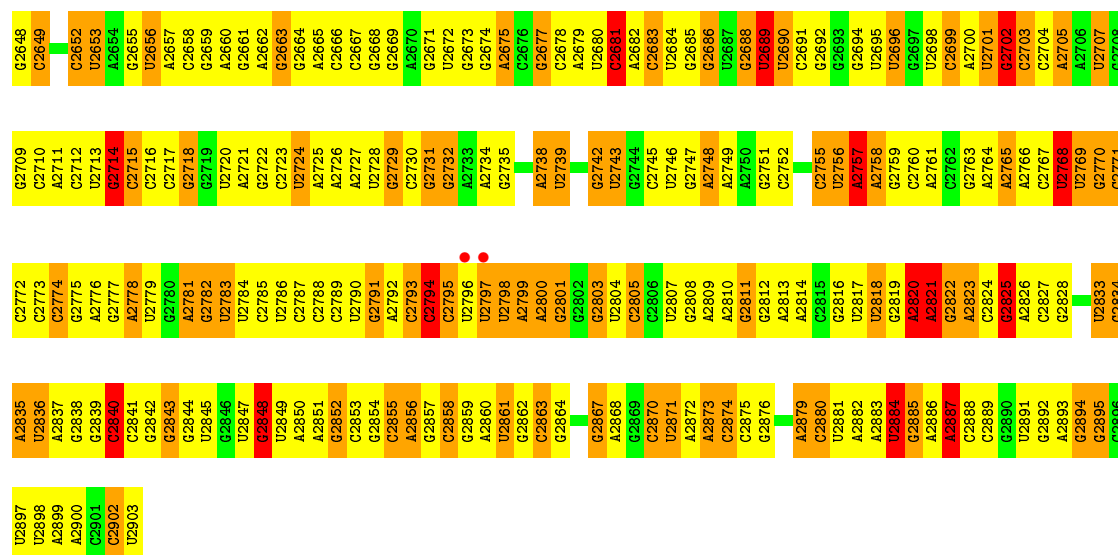


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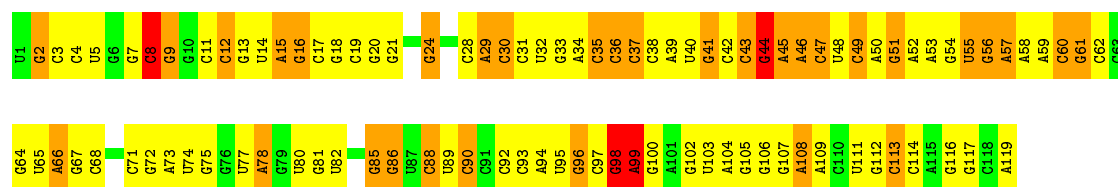
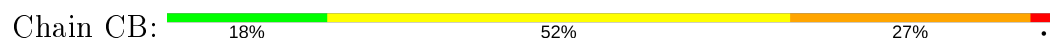


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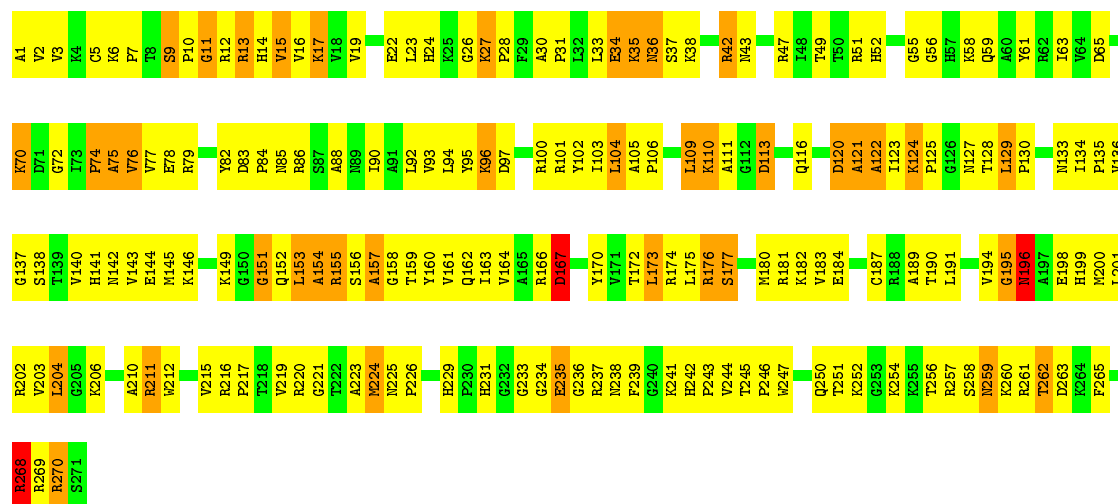




- Molecule 26: 5S rRNA



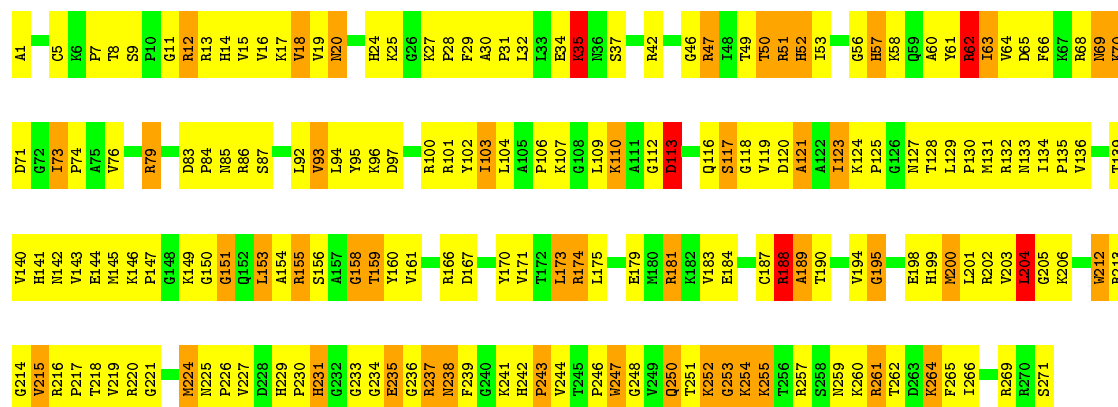
- Molecule 27: 50S ribosomal protein L2



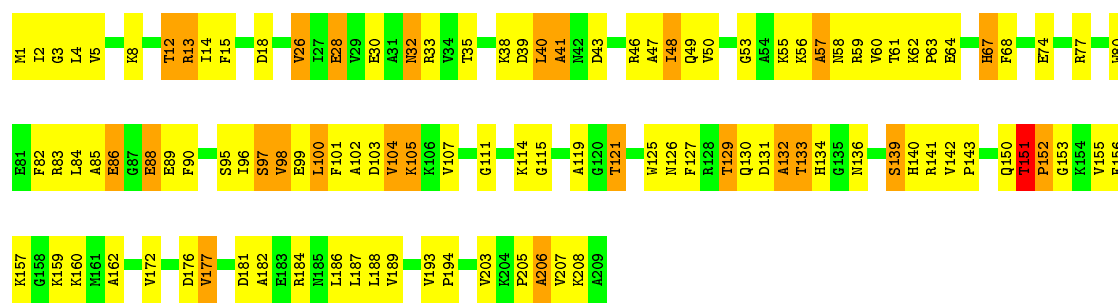
- Molecule 27: 50S ribosomal protein L2



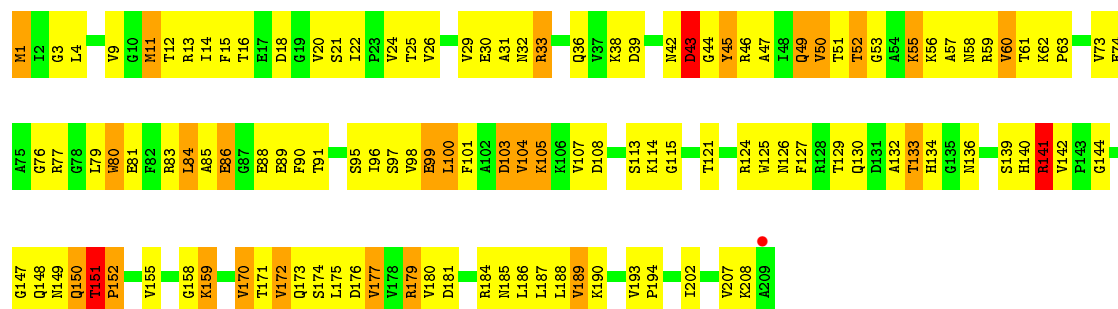




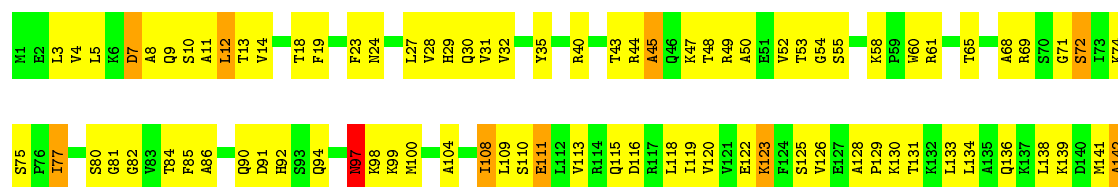
• Molecule 28: 50S ribosomal protein L3



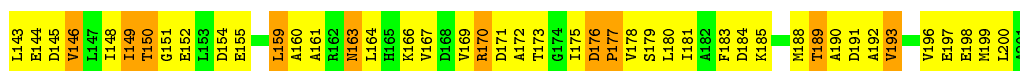
• Molecule 28: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L4

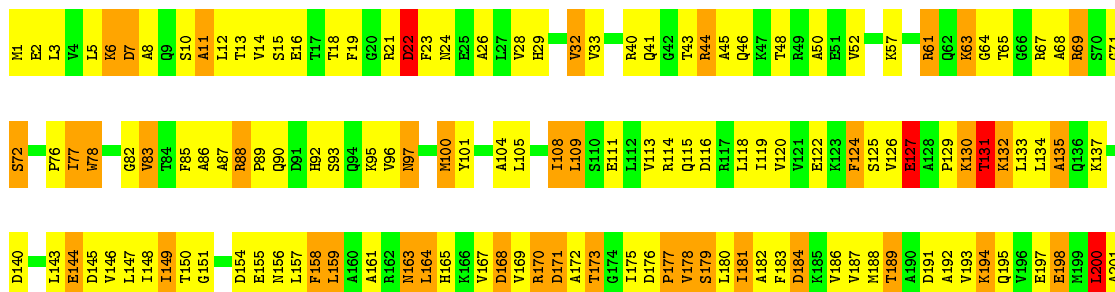






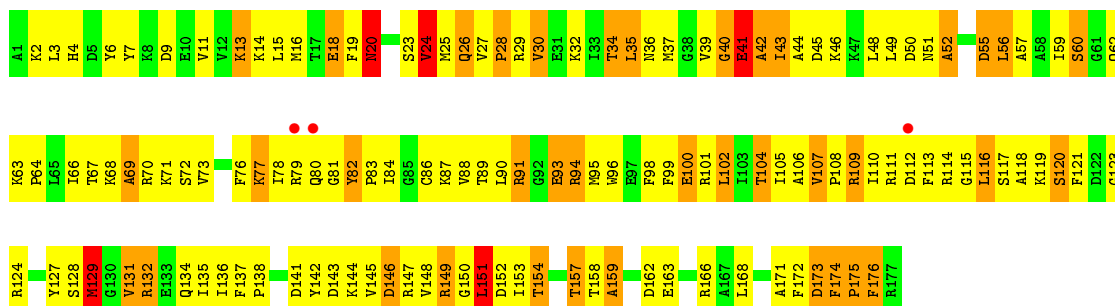
• Molecule 29: 50S ribosomal protein L4

Chain DE: 32% 47% 19%



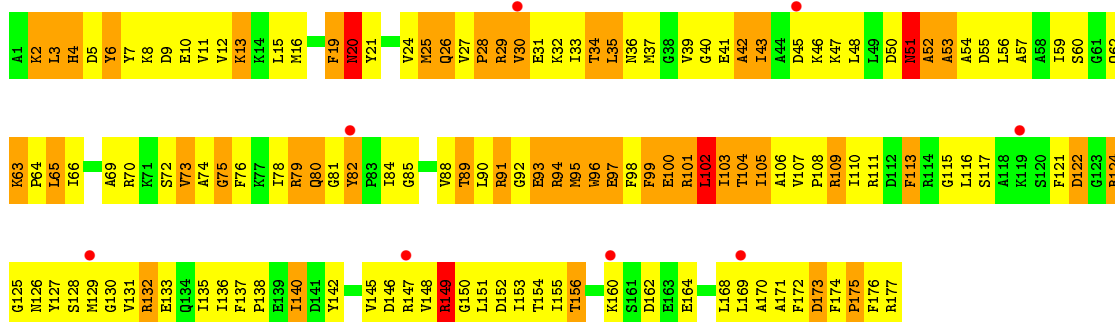
• Molecule 30: 50S ribosomal protein L5

Chain CF: 2% 23% 53% 21%



• Molecule 30: 50S ribosomal protein L5

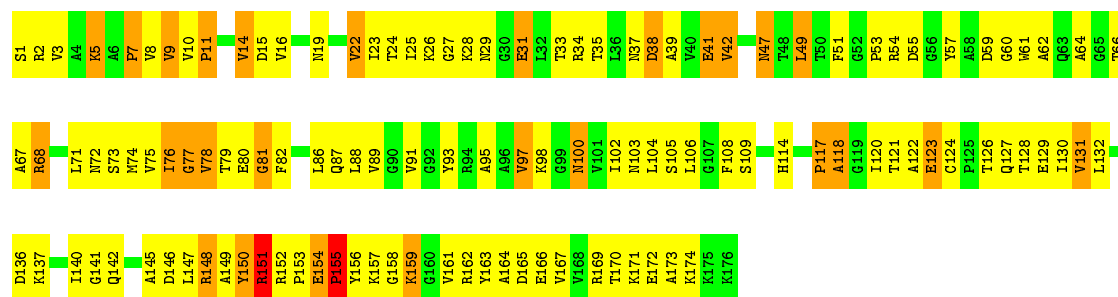
Chain DF: 5% 21% 51% 26%



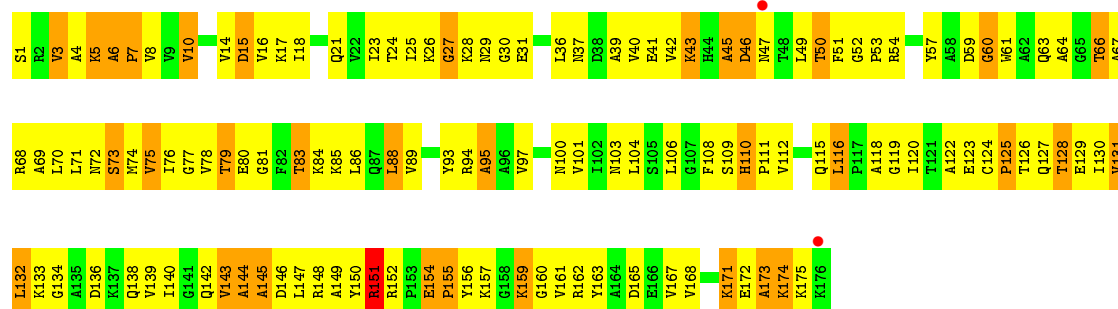
• Molecule 31: 50S ribosomal protein L6

Chain CG: 31% 53% 15%

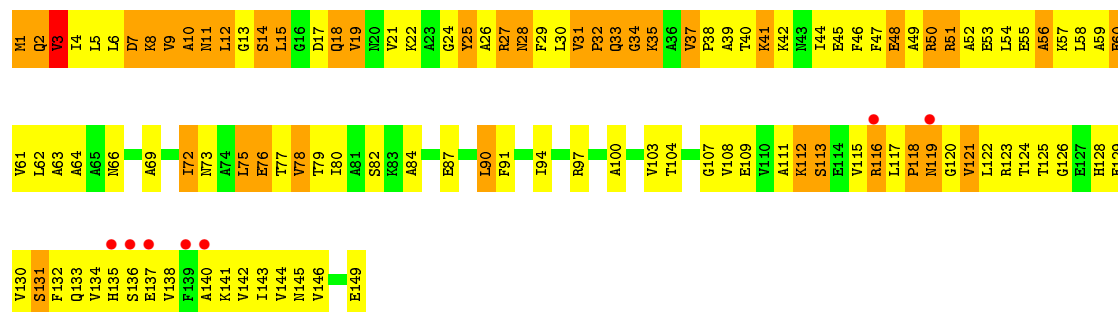




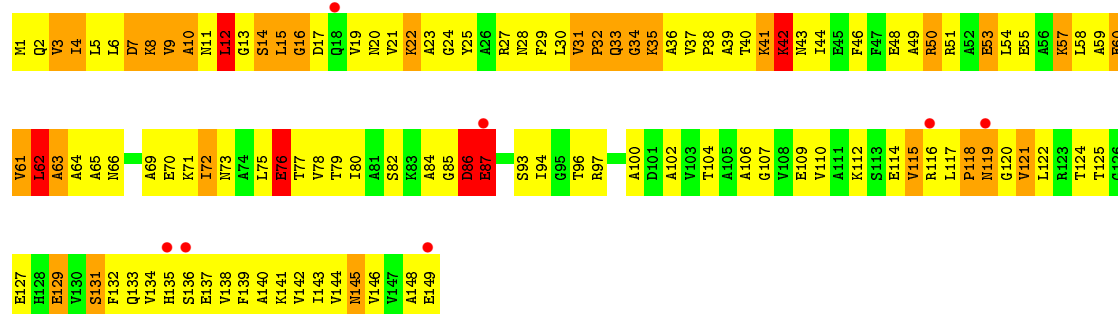
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

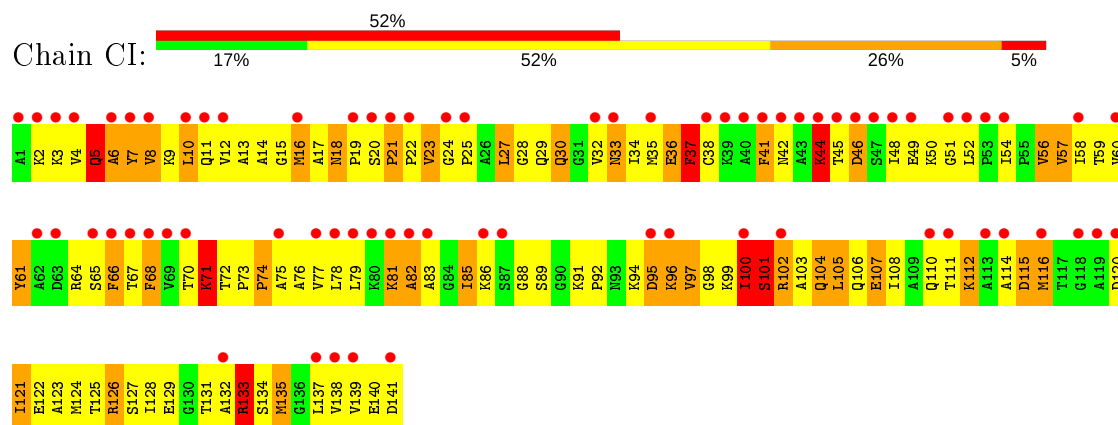


• Molecule 32: 50S ribosomal protein L9

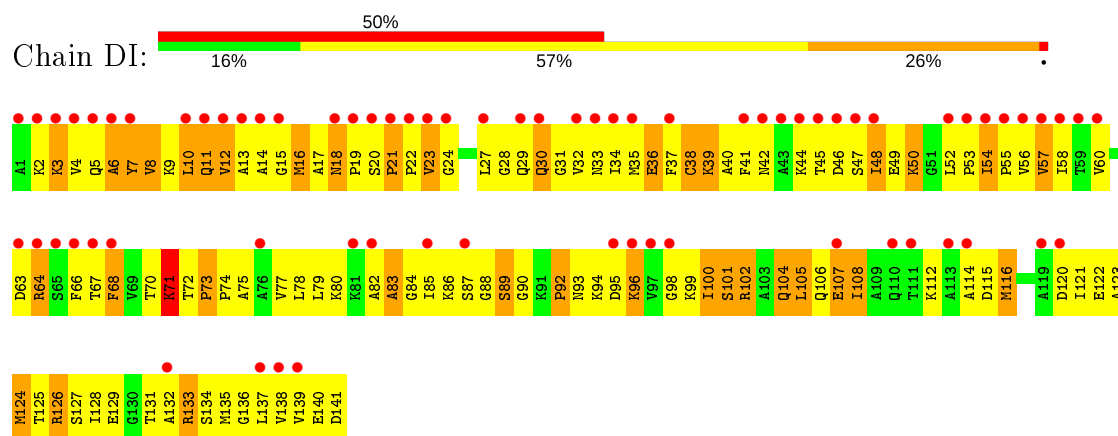




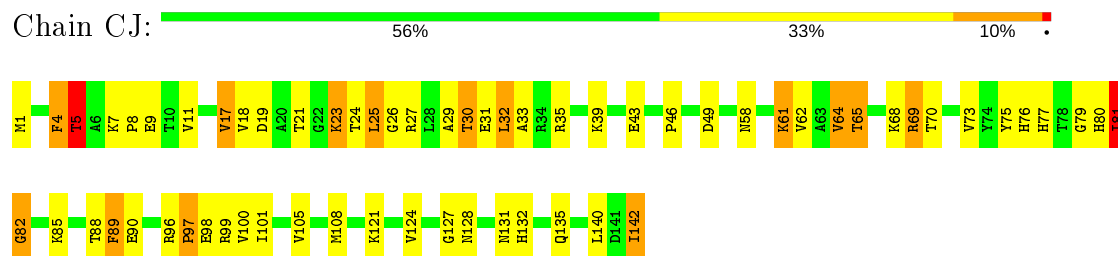
• Molecule 33: 50S ribosomal protein L11



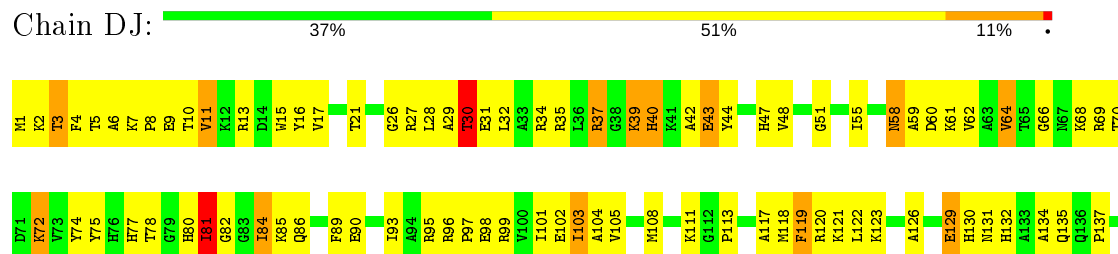
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13

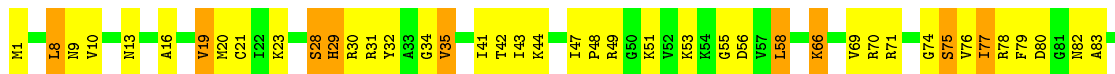






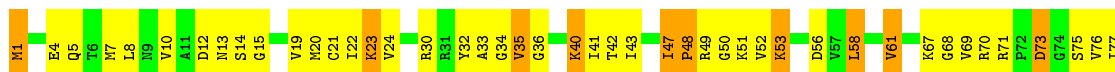
- Molecule 35: 50S ribosomal protein L14

Chain CK: 43% 40% 16% .



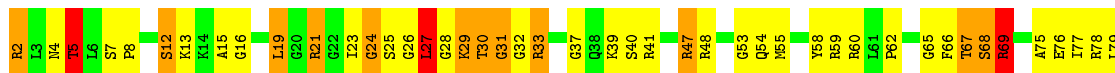
- Molecule 35: 50S ribosomal protein L14

Chain DK: 40% 43% 17% .



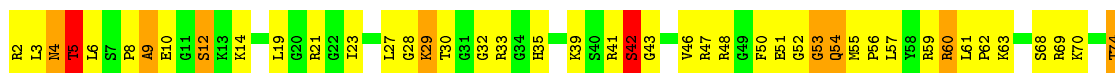
- Molecule 36: 50S ribosomal protein L15

Chain CL: 34% 46% 17% .



- Molecule 36: 50S ribosomal protein L15

Chain DL: 2% 27% 55% 14% .



- Molecule 37: 50S ribosomal protein L16

Chain CM: 42% 40% 16% .

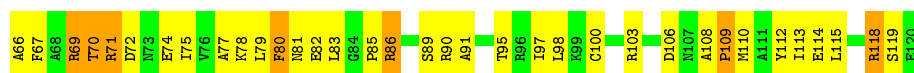




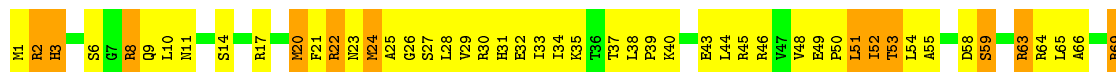
- Molecule 37: 50S ribosomal protein L16



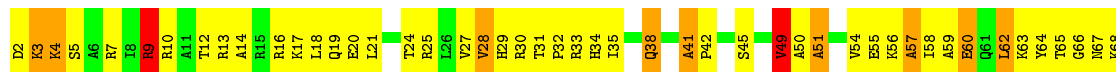
- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

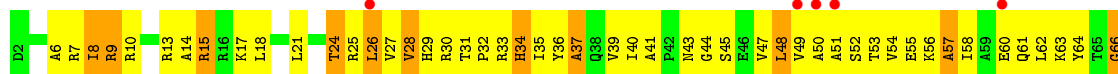


- Molecule 39: 50S ribosomal protein L18

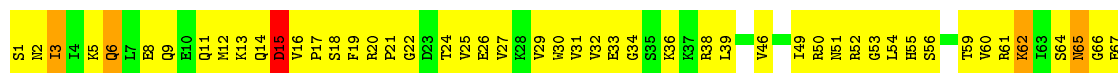


- Molecule 39: 50S ribosomal protein L18

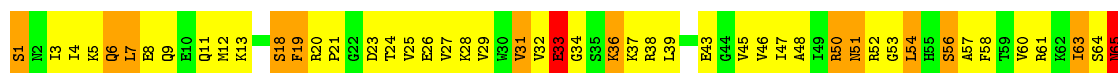




- Molecule 40: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20

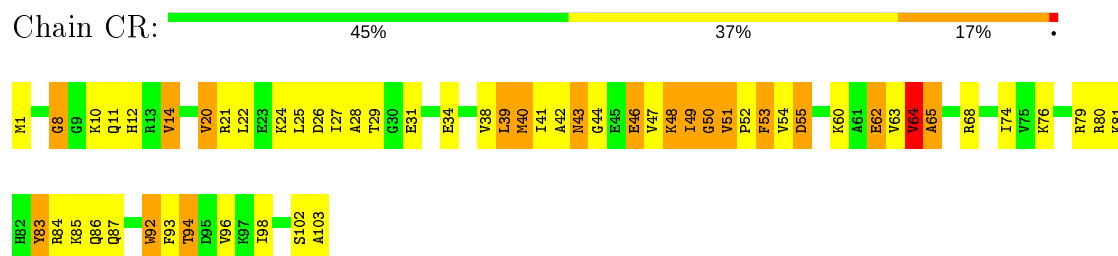


- Molecule 41: 50S ribosomal protein L20

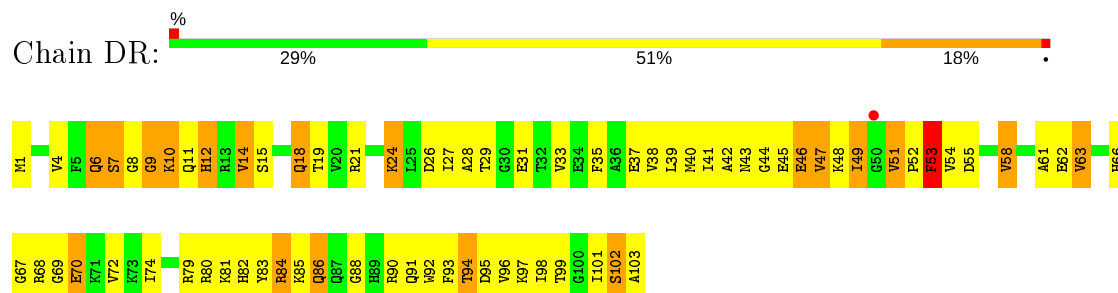




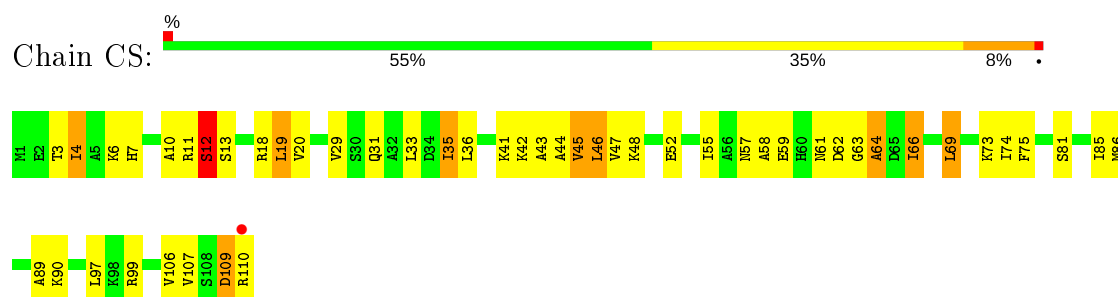
- Molecule 42: 50S ribosomal protein L21



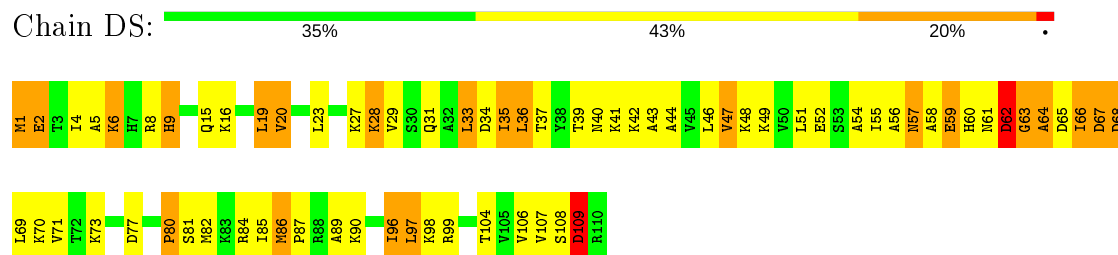
- Molecule 42: 50S ribosomal protein L21



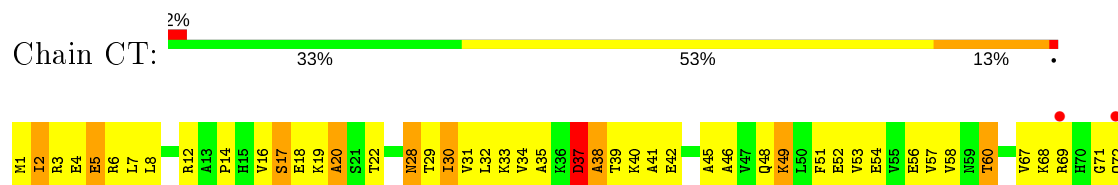
- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22



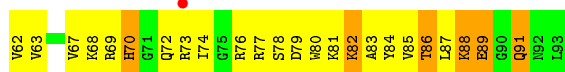
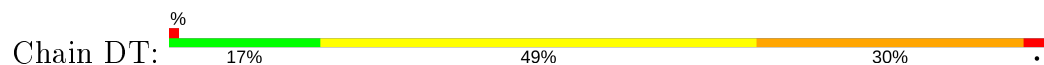
- Molecule 44: 50S ribosomal protein L23



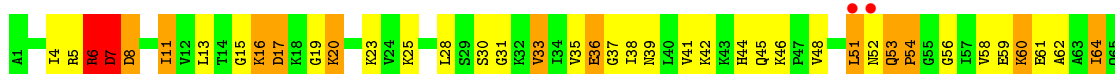




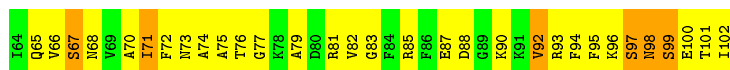
• Molecule 44: 50S ribosomal protein L23



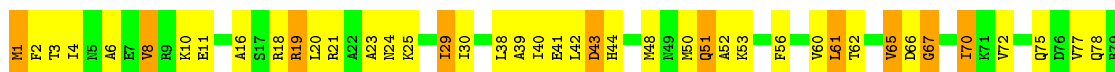
• Molecule 45: 50S ribosomal protein L24



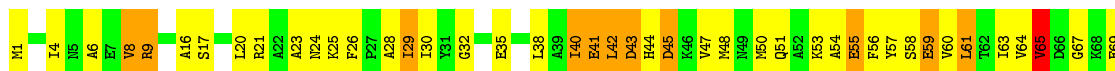
• Molecule 45: 50S ribosomal protein L24



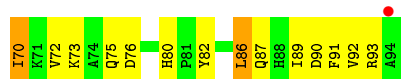
• Molecule 46: 50S ribosomal protein L25



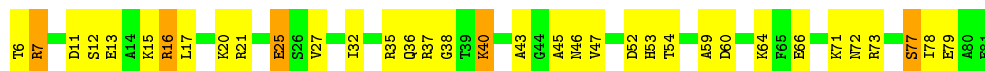
• Molecule 46: 50S ribosomal protein L25



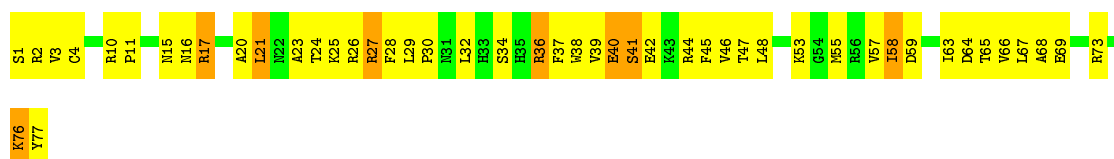




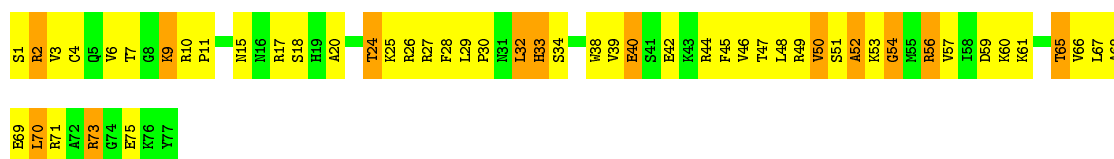
- Molecule 47: 50S ribosomal protein L27



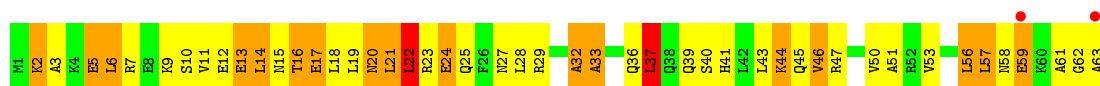
- Molecule 48: 50S ribosomal protein L28



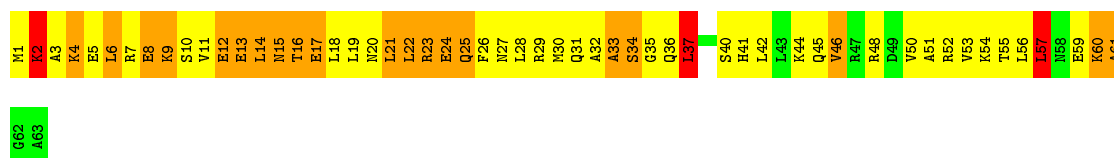
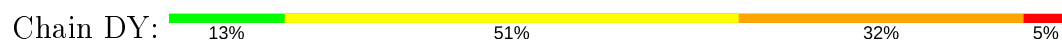
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



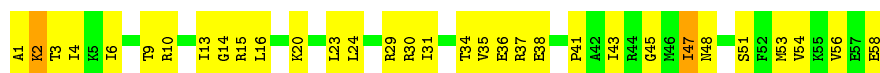
- Molecule 49: 50S ribosomal protein L29



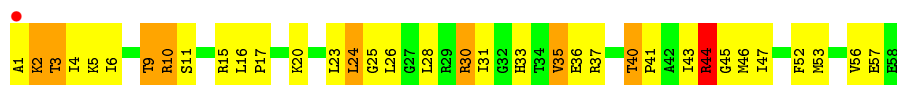
- Molecule 50: 50S ribosomal protein L30







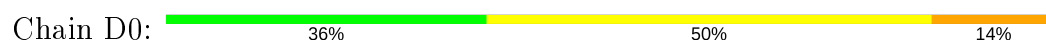
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



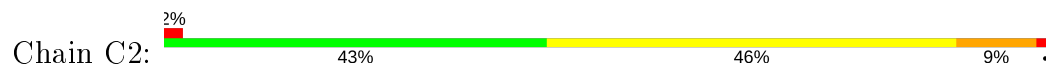
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34







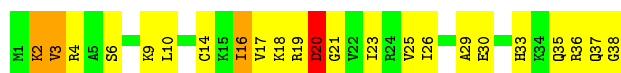
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



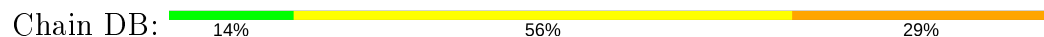
- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 5S rRNA



- Molecule 57: 50S ribosomal protein L27





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.67Å 438.07Å 613.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 69.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 83.5 (69.21-3.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.202 , 0.260 0.196 , 0.251	Depositor DCC
$R_{free}$ test set	19022 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 22.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	292354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	AA	0.87	8/36944 (0.0%)	1.28	318/57632 (0.6%)
1	BA	0.86	8/36966 (0.0%)	1.30	335/57666 (0.6%)
2	AB	0.60	0/1736	0.79	0/2338
2	BB	0.54	0/1736	0.72	0/2338
3	AC	0.56	0/1652	0.72	0/2225
3	BC	0.51	0/1652	0.72	1/2225 (0.0%)
4	AD	0.59	0/1665	0.74	1/2227 (0.0%)
4	BD	0.65	0/1665	0.80	1/2227 (0.0%)
5	AE	0.62	0/1119	0.85	0/1504
5	BE	0.62	0/1119	0.85	0/1504
6	AF	0.65	0/836	0.82	1/1128 (0.1%)
6	BF	0.55	0/836	0.80	1/1128 (0.1%)
7	AG	0.50	0/1196	0.67	0/1602
7	BG	0.48	0/1196	0.67	0/1602
8	AH	0.60	0/989	0.77	0/1326
8	BH	0.58	0/989	0.74	0/1326
9	AI	0.48	0/1034	0.71	0/1375
9	BI	0.53	0/1034	0.75	0/1375
10	AJ	0.57	0/797	0.74	0/1077
10	BJ	0.52	0/797	0.76	1/1077 (0.1%)
11	AK	0.67	0/893	0.82	0/1205
11	BK	0.59	0/893	0.75	0/1205
12	AL	0.61	0/969	0.81	0/1300
12	BL	0.72	0/969	0.92	0/1300
13	AM	0.52	0/893	0.74	0/1193
13	BM	0.50	0/893	0.71	0/1193
14	AN	0.55	0/785	0.76	0/1043
14	BN	0.51	0/785	0.65	0/1043
15	AO	0.55	0/722	0.73	0/964
15	BO	0.53	0/722	0.73	0/964
16	AP	0.54	0/659	0.82	1/884 (0.1%)
16	BP	0.61	0/659	0.79	1/884 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.57	0/658	0.74	0/881
17	BQ	0.62	0/658	0.76	0/881
18	AR	0.61	0/463	0.69	0/621
18	BR	0.54	0/463	0.68	0/621
19	AS	0.48	0/653	0.73	0/877
19	BS	0.55	0/653	0.67	0/877
20	AT	0.54	0/671	0.69	0/888
20	BT	0.57	0/671	0.73	0/888
21	AU	0.93	0/431	0.96	0/570
21	BU	0.78	0/431	0.85	0/570
22	AV	0.76	1/1813 (0.1%)	1.22	14/2823 (0.5%)
22	BV	0.74	1/1813 (0.1%)	1.22	10/2823 (0.4%)
23	AX	0.86	0/363	1.11	0/564
23	BX	0.73	0/388	1.09	0/603
24	AY	0.65	0/1430	0.74	0/1924
25	CA	1.60	600/69659 (0.9%)	1.67	2062/108672 (1.9%)
25	DA	1.07	82/69633 (0.1%)	1.48	1284/108629 (1.2%)
26	CB	1.33	5/2847 (0.2%)	1.58	77/4440 (1.7%)
27	CC	0.80	0/2122	0.90	1/2852 (0.0%)
27	DC	0.68	1/2122 (0.0%)	0.86	1/2852 (0.0%)
28	CD	0.96	0/1586	0.92	1/2134 (0.0%)
28	DD	0.70	0/1586	0.87	2/2134 (0.1%)
29	CE	0.91	0/1571	0.89	1/2113 (0.0%)
29	DE	0.67	0/1571	0.81	0/2113
30	CF	0.64	0/1435	0.74	0/1926
30	DF	0.51	0/1435	0.67	0/1926
31	CG	0.75	0/1343	0.85	1/1816 (0.1%)
31	DG	0.51	0/1343	0.69	0/1816
32	CH	0.68	1/1121 (0.1%)	0.77	0/1515
32	DH	0.66	1/1121 (0.1%)	0.80	1/1515 (0.1%)
33	CI	0.72	0/1046	0.74	0/1410
33	DI	0.67	0/1046	0.72	0/1410
34	CJ	1.01	0/1152	0.84	1/1551 (0.1%)
34	DJ	0.77	0/1152	0.82	0/1551
35	CK	0.91	3/948 (0.3%)	0.94	1/1268 (0.1%)
35	DK	0.68	0/948	0.84	0/1268
36	CL	0.94	0/1054	1.01	0/1403
36	DL	0.65	0/1054	0.85	0/1403
37	CM	0.94	0/1093	0.96	0/1460
37	DM	0.64	0/1093	0.80	0/1460
38	CN	0.91	0/974	0.96	1/1301 (0.1%)
38	DN	0.67	0/974	0.82	0/1301
39	CO	0.76	0/902	0.87	1/1209 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DO	0.50	0/902	0.66	0/1209
40	CP	0.89	0/929	0.88	1/1242 (0.1%)
40	DP	0.71	0/929	0.82	0/1242
41	CQ	1.14	0/960	0.96	1/1278 (0.1%)
41	DQ	0.80	0/960	0.79	0/1278
42	CR	1.01	1/829 (0.1%)	0.98	0/1107
42	DR	0.79	0/829	0.90	1/1107 (0.1%)
43	CS	1.08	1/864 (0.1%)	0.97	1/1156 (0.1%)
43	DS	0.71	0/864	0.89	1/1156 (0.1%)
44	CT	0.82	0/745	0.86	0/994
44	DT	0.59	0/745	0.74	0/994
45	CU	0.91	0/788	0.90	0/1051
45	DU	0.66	0/788	0.76	0/1051
46	CV	0.79	0/766	0.81	0/1025
46	DV	0.53	0/766	0.69	0/1025
47	CW	1.02	0/582	0.97	0/769
48	CX	0.78	0/635	0.84	0/848
48	DX	0.61	0/635	0.77	0/848
49	CY	0.76	0/510	0.96	1/677 (0.1%)
49	DY	0.56	0/510	0.77	0/677
50	CZ	1.04	0/453	0.94	0/605
50	DZ	0.58	0/453	0.78	0/605
51	C0	0.95	0/450	0.98	2/599 (0.3%)
51	D0	0.71	0/450	0.89	1/599 (0.2%)
52	C1	0.74	0/417	0.76	0/554
52	D1	0.50	0/417	0.66	0/554
53	C2	1.03	0/380	0.99	2/498 (0.4%)
53	D2	0.70	0/380	0.84	0/498
54	C3	0.94	0/513	0.85	0/676
54	D3	0.60	0/513	0.78	1/676 (0.1%)
55	C4	0.92	0/303	0.99	0/397
55	D4	0.68	0/303	0.76	0/397
56	DB	0.75	0/2828	1.23	18/4410 (0.4%)
57	DW	0.60	0/571	0.72	0/755
All	All	1.08	713/315257 (0.2%)	1.34	4150/471496 (0.9%)

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
4	AD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	BD	0	1
5	AE	0	1
5	BE	0	2
6	BF	0	1
9	AI	0	1
11	AK	0	1
11	BK	0	2
12	BL	0	2
13	AM	0	1
14	AN	0	1
20	BT	0	1
21	AU	0	2
21	BU	0	1
27	CC	0	1
27	DC	0	1
28	CD	0	2
28	DD	0	1
32	DH	0	2
33	CI	0	1
34	DJ	0	1
39	DO	0	1
42	CR	0	1
45	CU	0	1
50	CZ	0	1
All	All	0	31

The worst 5 of 713 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CA	1142	A	N9-C4	-18.22	1.26	1.37
25	CA	984	A	N9-C4	-13.29	1.29	1.37
25	DA	984	A	N9-C4	-10.51	1.31	1.37
25	CA	984	A	C5-C6	-10.44	1.31	1.41
25	CA	528	A	N7-C5	-10.29	1.33	1.39

The worst 5 of 4150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	984	A	C2-N3-C4	-18.86	101.17	110.60
25	CA	2250	G	N3-C4-C5	17.23	137.22	128.60
25	CA	1638	C	N1-C2-O2	-16.64	108.92	118.90
25	CA	1142	A	C2-N3-C4	-16.61	102.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	1142	A	N3-C4-C5	16.11	138.07	126.80

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	47	LEU	Peptide
5	AE	100	GLU	Peptide
9	AI	5	TYR	Peptide
11	AK	125	LYS	Peptide
13	AM	111	PRO	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	AA	32995	0	16607	2052	0
1	BA	33015	0	16617	2194	0
2	AB	1705	0	1732	374	0
2	BB	1705	0	1732	298	0
3	AC	1625	0	1699	235	0
3	BC	1625	0	1699	237	0
4	AD	1643	0	1710	291	0
4	BD	1643	0	1710	228	0
5	AE	1106	0	1148	214	0
5	BE	1106	0	1148	211	0
6	AF	818	0	808	116	0
6	BF	818	0	808	156	0
7	AG	1182	0	1240	116	0
7	BG	1182	0	1240	166	0
8	AH	979	0	1034	161	0
8	BH	979	0	1034	119	0
9	AI	1022	0	1070	189	0
9	BI	1022	0	1070	186	0
10	AJ	787	0	828	178	0
10	BJ	787	0	828	142	0
11	AK	877	0	887	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BK	877	0	887	136	0
12	AL	955	0	1019	94	0
12	BL	955	0	1019	118	0
13	AM	884	0	944	163	0
13	BM	884	0	944	144	0
14	AN	774	0	827	130	0
14	BN	774	0	827	131	0
15	AO	714	0	737	61	0
15	BO	714	0	737	87	0
16	AP	649	0	666	106	0
16	BP	649	0	666	87	0
17	AQ	649	0	691	118	0
17	BQ	649	0	691	103	0
18	AR	456	0	478	46	0
18	BR	456	0	478	57	0
19	AS	638	0	665	88	0
19	BS	638	0	665	96	0
20	AT	665	0	714	84	0
20	BT	665	0	714	129	0
21	AU	426	0	449	139	0
21	BU	426	0	449	119	0
22	AV	1623	0	821	88	0
22	BV	1623	0	821	47	0
23	AX	324	0	162	19	0
23	BX	346	0	173	24	0
24	AY	1419	0	1467	97	0
25	CA	62195	0	31271	2445	0
25	DA	62173	0	31270	3398	0
26	CB	2548	0	1292	98	0
27	CC	2083	0	2157	227	0
27	DC	2083	0	2157	213	0
28	CD	1565	0	1616	129	0
28	DD	1565	0	1616	114	0
29	CE	1552	0	1619	143	0
29	DE	1552	0	1619	163	0
30	CF	1411	0	1447	202	0
30	DF	1411	0	1447	197	0
31	CG	1323	0	1374	146	0
31	DG	1323	0	1374	177	0
32	CH	1110	0	1148	145	0
32	DH	1110	0	1148	210	0
33	CI	1032	0	1088	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DI	1032	0	1088	180	0
34	CJ	1129	0	1162	57	0
34	DJ	1129	0	1162	96	0
35	CK	939	0	1012	75	0
35	DK	939	0	1012	79	0
36	CL	1045	0	1117	130	0
36	DL	1045	0	1117	168	0
37	CM	1074	0	1157	96	0
37	DM	1074	0	1157	127	0
38	CN	961	0	1000	94	0
38	DN	961	0	1000	124	0
39	CO	892	0	923	84	0
39	DO	892	0	923	141	0
40	CP	917	0	965	93	0
40	DP	917	0	965	107	0
41	CQ	947	0	1022	63	0
41	DQ	947	0	1022	83	0
42	CR	816	0	839	84	0
42	DR	816	0	839	99	0
43	CS	857	0	922	42	0
43	DS	857	0	922	82	0
44	CT	739	0	807	71	0
44	DT	739	0	807	114	0
45	CU	780	0	834	66	0
45	DU	780	0	834	111	0
46	CV	753	0	780	59	0
46	DV	753	0	780	71	0
47	CW	575	0	589	27	0
48	CX	625	0	655	41	0
48	DX	625	0	655	58	0
49	CY	509	0	543	88	0
49	DY	509	0	543	109	0
50	CZ	449	0	491	26	0
50	DZ	449	0	491	47	0
51	C0	444	0	461	35	0
51	D0	444	0	461	41	0
52	C1	410	0	440	37	0
52	D1	410	0	440	45	0
53	C2	377	0	418	26	0
53	D2	377	0	418	18	0
54	C3	504	0	574	40	0
54	D3	504	0	574	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	C4	302	0	340	23	0
55	D4	302	0	340	34	0
56	DB	2529	0	1281	163	0
57	DW	564	0	576	36	0
58	AA	72	0	0	0	0
58	BA	56	0	0	0	0
58	CA	194	0	0	0	0
58	CB	4	0	0	0	0
58	CQ	1	0	0	0	0
58	DA	166	0	0	0	0
58	DB	3	0	0	0	0
58	DL	1	0	0	0	0
58	DQ	1	0	0	0	0
59	C4	1	0	0	0	0
59	D4	1	0	0	0	0
60	AA	197	0	0	11	0
60	AN	4	0	0	0	0
60	AT	1	0	0	0	0
60	AU	1	0	0	0	0
60	BA	190	0	0	12	0
60	BL	1	0	0	0	0
60	BN	5	0	0	1	0
60	BT	1	0	0	0	0
60	BU	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	625	0	0	62	0
60	CB	13	0	0	0	0
60	CC	8	0	0	0	0
60	CD	2	0	0	0	0
60	CE	2	0	0	0	0
60	CF	1	0	0	0	0
60	CJ	1	0	0	0	0
60	CL	6	0	0	2	0
60	CN	4	0	0	0	0
60	CS	1	0	0	0	0
60	CV	1	0	0	0	0
60	D2	1	0	0	0	0
60	D3	2	0	0	0	0
60	D4	1	0	0	0	0
60	DA	622	0	0	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DB	14	0	0	0	0
60	DC	4	0	0	0	0
60	DD	5	0	0	2	0
60	DE	2	0	0	0	0
60	DJ	1	0	0	0	0
60	DL	4	0	0	1	0
60	DN	1	0	0	0	0
60	DR	1	0	0	0	0
All	All	292354	0	195461	20868	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 43.

The worst 5 of 20868 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)
32:DH:93:SER:OG	32:DH:121:VAL:HG12	1.46	1.15
1:BA:1053:G:H4'	1:BA:1054:C:H5'	1.29	1.11
32:DH:93:SER:OG	32:DH:121:VAL:CG1	2.03	1.06
25:DA:1153:C:OP2	60:DA:3363:HOH:O	1.78	1.01
12:BL:33:CYS:HA	12:BL:54:VAL:HA	1.44	0.99

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	109 (50%)	49 (23%)	58 (27%)	0	0
2	BB	216/218 (99%)	112 (52%)	49 (23%)	55 (26%)	0	0
3	AC	204/206 (99%)	125 (61%)	49 (24%)	30 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BC	204/206 (99%)	126 (62%)	47 (23%)	31 (15%)	0	1
4	AD	203/205 (99%)	123 (61%)	41 (20%)	39 (19%)	0	0
4	BD	203/205 (99%)	136 (67%)	36 (18%)	31 (15%)	0	1
5	AE	148/150 (99%)	87 (59%)	38 (26%)	23 (16%)	0	1
5	BE	148/150 (99%)	90 (61%)	31 (21%)	27 (18%)	0	0
6	AF	98/100 (98%)	62 (63%)	21 (21%)	15 (15%)	0	1
6	BF	98/100 (98%)	54 (55%)	23 (24%)	21 (21%)	0	0
7	AG	149/151 (99%)	86 (58%)	41 (28%)	22 (15%)	0	1
7	BG	149/151 (99%)	79 (53%)	46 (31%)	24 (16%)	0	1
8	AH	127/129 (98%)	79 (62%)	37 (29%)	11 (9%)	1	3
8	BH	127/129 (98%)	82 (65%)	32 (25%)	13 (10%)	0	2
9	AI	125/127 (98%)	76 (61%)	34 (27%)	15 (12%)	0	1
9	BI	125/127 (98%)	77 (62%)	33 (26%)	15 (12%)	0	1
10	AJ	96/98 (98%)	60 (62%)	14 (15%)	22 (23%)	0	0
10	BJ	96/98 (98%)	64 (67%)	14 (15%)	18 (19%)	0	0
11	AK	115/117 (98%)	84 (73%)	17 (15%)	14 (12%)	0	1
11	BK	115/117 (98%)	81 (70%)	19 (16%)	15 (13%)	0	1
12	AL	121/123 (98%)	85 (70%)	29 (24%)	7 (6%)	1	10
12	BL	121/123 (98%)	91 (75%)	16 (13%)	14 (12%)	0	1
13	AM	112/114 (98%)	78 (70%)	22 (20%)	12 (11%)	0	2
13	BM	112/114 (98%)	65 (58%)	24 (21%)	23 (20%)	0	0
14	AN	92/100 (92%)	47 (51%)	27 (29%)	18 (20%)	0	0
14	BN	92/100 (92%)	39 (42%)	30 (33%)	23 (25%)	0	0
15	AO	86/88 (98%)	57 (66%)	22 (26%)	7 (8%)	1	4
15	BO	86/88 (98%)	52 (60%)	17 (20%)	17 (20%)	0	0
16	AP	80/82 (98%)	48 (60%)	11 (14%)	21 (26%)	0	0
16	BP	80/82 (98%)	47 (59%)	22 (28%)	11 (14%)	0	1
17	AQ	78/80 (98%)	47 (60%)	18 (23%)	13 (17%)	0	0
17	BQ	78/80 (98%)	48 (62%)	18 (23%)	12 (15%)	0	1
18	AR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	2
18	BR	53/55 (96%)	31 (58%)	19 (36%)	3 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AS	77/79 (98%)	36 (47%)	29 (38%)	12 (16%)	0	1
19	BS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	3
20	AT	83/85 (98%)	37 (45%)	31 (37%)	15 (18%)	0	0
20	BT	83/85 (98%)	46 (55%)	23 (28%)	14 (17%)	0	0
21	AU	49/51 (96%)	20 (41%)	15 (31%)	14 (29%)	0	0
21	BU	49/51 (96%)	22 (45%)	10 (20%)	17 (35%)	0	0
24	AY	181/183 (99%)	135 (75%)	35 (19%)	11 (6%)	1	8
27	CC	269/271 (99%)	216 (80%)	32 (12%)	21 (8%)	1	4
27	DC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	0	2
28	CD	207/209 (99%)	166 (80%)	30 (14%)	11 (5%)	2	11
28	DD	207/209 (99%)	162 (78%)	35 (17%)	10 (5%)	2	13
29	CE	199/201 (99%)	158 (79%)	32 (16%)	9 (4%)	2	14
29	DE	199/201 (99%)	142 (71%)	38 (19%)	19 (10%)	0	3
30	CF	175/177 (99%)	118 (67%)	38 (22%)	19 (11%)	0	2
30	DF	175/177 (99%)	113 (65%)	34 (19%)	28 (16%)	0	1
31	CG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1	3
31	DG	174/176 (99%)	106 (61%)	43 (25%)	25 (14%)	0	1
32	CH	147/149 (99%)	95 (65%)	29 (20%)	23 (16%)	0	1
32	DH	147/149 (99%)	95 (65%)	27 (18%)	25 (17%)	0	0
33	CI	139/141 (99%)	65 (47%)	47 (34%)	27 (19%)	0	0
33	DI	139/141 (99%)	71 (51%)	46 (33%)	22 (16%)	0	1
34	CJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	15
34	DJ	140/142 (99%)	112 (80%)	24 (17%)	4 (3%)	4	24
35	CK	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	6
35	DK	120/122 (98%)	87 (72%)	21 (18%)	12 (10%)	0	2
36	CL	141/143 (99%)	99 (70%)	21 (15%)	21 (15%)	0	1
36	DL	141/143 (99%)	88 (62%)	36 (26%)	17 (12%)	0	1
37	CM	134/136 (98%)	110 (82%)	15 (11%)	9 (7%)	1	6
37	DM	134/136 (98%)	97 (72%)	23 (17%)	14 (10%)	0	2
38	CN	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	2	12
38	DN	118/120 (98%)	82 (70%)	28 (24%)	8 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CO	114/116 (98%)	83 (73%)	17 (15%)	14 (12%)	0	1
39	DO	114/116 (98%)	77 (68%)	25 (22%)	12 (10%)	0	2
40	CP	112/114 (98%)	96 (86%)	12 (11%)	4 (4%)	3	19
40	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	7
41	CQ	115/117 (98%)	100 (87%)	13 (11%)	2 (2%)	9	39
41	DQ	115/117 (98%)	95 (83%)	18 (16%)	2 (2%)	9	39
42	CR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	4
42	DR	101/103 (98%)	78 (77%)	14 (14%)	9 (9%)	1	3
43	CS	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	10
43	DS	108/110 (98%)	78 (72%)	19 (18%)	11 (10%)	0	2
44	CT	91/93 (98%)	67 (74%)	13 (14%)	11 (12%)	0	1
44	DT	91/93 (98%)	59 (65%)	20 (22%)	12 (13%)	0	1
45	CU	100/102 (98%)	74 (74%)	14 (14%)	12 (12%)	0	1
45	DU	100/102 (98%)	73 (73%)	14 (14%)	13 (13%)	0	1
46	CV	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	6	31
46	DV	92/94 (98%)	71 (77%)	15 (16%)	6 (6%)	1	7
47	CW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	5	26
48	CX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	5	26
48	DX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	4
49	CY	61/63 (97%)	34 (56%)	13 (21%)	14 (23%)	0	0
49	DY	61/63 (97%)	28 (46%)	16 (26%)	17 (28%)	0	0
50	CZ	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
50	DZ	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	3	19
51	C0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	3	19
51	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	3
52	C1	48/50 (96%)	32 (67%)	12 (25%)	4 (8%)	1	4
52	D1	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	3	16
53	C2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	6	30
53	D2	44/46 (96%)	31 (70%)	8 (18%)	5 (11%)	0	2
54	C3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
54	D3	62/64 (97%)	49 (79%)	11 (18%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	C4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	25
55	D4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	25
57	DW	73/75 (97%)	57 (78%)	12 (16%)	4 (6%)	2	10
All	All	11416/11626 (98%)	7804 (68%)	2248 (20%)	1364 (12%)	0	1

5 of 1364 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	21	TYR
2	AB	33	ALA
2	AB	63	LYS
2	AB	67	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	114 (63%)	66 (37%)	0	1
2	BB	180/180 (100%)	131 (73%)	49 (27%)	0	2
3	AC	170/170 (100%)	127 (75%)	43 (25%)	0	3
3	BC	170/170 (100%)	123 (72%)	47 (28%)	0	2
4	AD	172/172 (100%)	132 (77%)	40 (23%)	1	4
4	BD	172/172 (100%)	123 (72%)	49 (28%)	0	2
5	AE	113/113 (100%)	80 (71%)	33 (29%)	0	2
5	BE	113/113 (100%)	87 (77%)	26 (23%)	1	4
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	1
6	BF	87/87 (100%)	61 (70%)	26 (30%)	0	1
7	AG	124/124 (100%)	90 (73%)	34 (27%)	0	2
7	BG	124/124 (100%)	85 (68%)	39 (32%)	0	1
8	AH	104/104 (100%)	78 (75%)	26 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BH	104/104 (100%)	78 (75%)	26 (25%)	0	3
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	1
9	BI	105/105 (100%)	67 (64%)	38 (36%)	0	1
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	0	2
10	BJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
11	AK	90/90 (100%)	66 (73%)	24 (27%)	0	2
11	BK	90/90 (100%)	67 (74%)	23 (26%)	0	3
12	AL	103/103 (100%)	86 (84%)	17 (16%)	2	11
12	BL	103/103 (100%)	75 (73%)	28 (27%)	0	2
13	AM	92/92 (100%)	73 (79%)	19 (21%)	1	6
13	BM	92/92 (100%)	71 (77%)	21 (23%)	1	4
14	AN	79/83 (95%)	56 (71%)	23 (29%)	0	2
14	BN	79/83 (95%)	60 (76%)	19 (24%)	0	3
15	AO	76/76 (100%)	61 (80%)	15 (20%)	1	7
15	BO	76/76 (100%)	60 (79%)	16 (21%)	1	5
16	AP	65/65 (100%)	45 (69%)	20 (31%)	0	1
16	BP	65/65 (100%)	48 (74%)	17 (26%)	0	2
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	0	2
17	BQ	74/74 (100%)	47 (64%)	27 (36%)	0	1
18	AR	48/48 (100%)	40 (83%)	8 (17%)	2	11
18	BR	48/48 (100%)	40 (83%)	8 (17%)	2	11
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	7
19	BS	70/70 (100%)	53 (76%)	17 (24%)	0	3
20	AT	65/65 (100%)	45 (69%)	20 (31%)	0	1
20	BT	65/65 (100%)	47 (72%)	18 (28%)	0	2
21	AU	44/44 (100%)	23 (52%)	21 (48%)	0	0
21	BU	44/44 (100%)	26 (59%)	18 (41%)	0	0
24	AY	157/157 (100%)	139 (88%)	18 (12%)	5	24
27	CC	216/216 (100%)	182 (84%)	34 (16%)	2	13
27	DC	216/216 (100%)	173 (80%)	43 (20%)	1	7
28	CD	164/164 (100%)	143 (87%)	21 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DD	164/164 (100%)	135 (82%)	29 (18%)	2	9
29	CE	165/165 (100%)	143 (87%)	22 (13%)	4	17
29	DE	165/165 (100%)	126 (76%)	39 (24%)	1	3
30	CF	148/148 (100%)	112 (76%)	36 (24%)	0	3
30	DF	148/148 (100%)	114 (77%)	34 (23%)	1	4
31	CG	137/137 (100%)	114 (83%)	23 (17%)	2	11
31	DG	137/137 (100%)	119 (87%)	18 (13%)	4	18
32	CH	114/114 (100%)	89 (78%)	25 (22%)	1	5
32	DH	114/114 (100%)	92 (81%)	22 (19%)	1	8
33	CI	109/109 (100%)	78 (72%)	31 (28%)	0	2
33	DI	109/109 (100%)	83 (76%)	26 (24%)	0	3
34	CJ	116/116 (100%)	97 (84%)	19 (16%)	2	11
34	DJ	116/116 (100%)	95 (82%)	21 (18%)	1	9
35	CK	103/103 (100%)	85 (82%)	18 (18%)	2	10
35	DK	103/103 (100%)	85 (82%)	18 (18%)	2	10
36	CL	102/102 (100%)	81 (79%)	21 (21%)	1	6
36	DL	102/102 (100%)	81 (79%)	21 (21%)	1	6
37	CM	109/109 (100%)	87 (80%)	22 (20%)	1	6
37	DM	109/109 (100%)	87 (80%)	22 (20%)	1	6
38	CN	100/100 (100%)	83 (83%)	17 (17%)	2	10
38	DN	100/100 (100%)	80 (80%)	20 (20%)	1	7
39	CO	86/86 (100%)	68 (79%)	18 (21%)	1	5
39	DO	86/86 (100%)	66 (77%)	20 (23%)	1	4
40	CP	99/99 (100%)	78 (79%)	21 (21%)	1	5
40	DP	99/99 (100%)	76 (77%)	23 (23%)	1	4
41	CQ	89/89 (100%)	76 (85%)	13 (15%)	3	15
41	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	11
42	CR	84/84 (100%)	70 (83%)	14 (17%)	2	11
42	DR	84/84 (100%)	66 (79%)	18 (21%)	1	5
43	CS	93/93 (100%)	83 (89%)	10 (11%)	6	26
43	DS	93/93 (100%)	71 (76%)	22 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	CT	80/80 (100%)	69 (86%)	11 (14%)	3	17
44	DT	80/80 (100%)	57 (71%)	23 (29%)	0	2
45	CU	83/83 (100%)	64 (77%)	19 (23%)	1	4
45	DU	83/83 (100%)	63 (76%)	20 (24%)	0	3
46	CV	78/78 (100%)	63 (81%)	15 (19%)	1	8
46	DV	78/78 (100%)	63 (81%)	15 (19%)	1	8
47	CW	56/58 (97%)	50 (89%)	6 (11%)	6	26
48	CX	67/67 (100%)	56 (84%)	11 (16%)	2	11
48	DX	67/67 (100%)	56 (84%)	11 (16%)	2	11
49	CY	55/55 (100%)	46 (84%)	9 (16%)	2	11
49	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
50	CZ	48/48 (100%)	40 (83%)	8 (17%)	2	11
50	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	5
51	C0	47/47 (100%)	41 (87%)	6 (13%)	4	19
51	D0	47/47 (100%)	41 (87%)	6 (13%)	4	19
52	C1	45/45 (100%)	38 (84%)	7 (16%)	2	13
52	D1	45/45 (100%)	37 (82%)	8 (18%)	2	9
53	C2	38/38 (100%)	32 (84%)	6 (16%)	2	12
53	D2	38/38 (100%)	33 (87%)	5 (13%)	4	18
54	C3	51/51 (100%)	48 (94%)	3 (6%)	19	54
54	D3	51/51 (100%)	48 (94%)	3 (6%)	19	54
55	C4	34/34 (100%)	28 (82%)	6 (18%)	2	10
55	D4	34/34 (100%)	27 (79%)	7 (21%)	1	6
57	DW	55/57 (96%)	47 (86%)	8 (14%)	3	15
All	All	9482/9494 (100%)	7392 (78%)	2090 (22%)	1	4

5 of 2090 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	BN	25	GLU
30	CF	55	ASP
42	DR	48	LYS
15	BO	87	ARG
21	BU	4	LYS



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
27	CC	116	GLN
34	CJ	58	ASN
45	DU	26	ASN
28	CD	67	HIS
30	CF	62	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	441 (28%)	28 (1%)
1	BA	1538/1539 (99%)	445 (28%)	20 (1%)
22	AV	75/76 (98%)	29 (38%)	1 (1%)
22	BV	75/76 (98%)	15 (20%)	1 (1%)
23	AX	14/16 (87%)	5 (35%)	0
23	BX	15/16 (93%)	4 (26%)	0
25	CA	2895/2903 (99%)	747 (25%)	53 (1%)
25	DA	2893/2903 (99%)	764 (26%)	48 (1%)
26	CB	118/119 (99%)	24 (20%)	1 (0%)
56	DB	117/118 (99%)	34 (29%)	3 (2%)
All	All	9277/9305 (99%)	2508 (27%)	155 (1%)

5 of 2508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	9	G
1	AA	12	U

5 of 155 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	CA	1046	A
25	CA	1800	C
25	DA	2311	A
25	CA	1133	A
25	CA	1301	A



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1538/1539 (99%)	-0.64	7 (0%) 91 75	0, 31, 105, 170	0
1	BA	1539/1539 (100%)	-0.58	9 (0%) 89 72	0, 33, 101, 147	0
2	AB	218/218 (100%)	0.58	13 (5%) 21 7	12, 52, 84, 115	0
2	BB	218/218 (100%)	0.41	12 (5%) 25 9	19, 59, 88, 113	0
3	AC	206/206 (100%)	-0.32	0 100 100	0, 35, 69, 93	0
3	BC	206/206 (100%)	0.23	3 (1%) 73 46	9, 46, 75, 92	0
4	AD	205/205 (100%)	0.09	4 (1%) 65 36	14, 42, 73, 98	0
4	BD	205/205 (100%)	-0.26	1 (0%) 91 75	0, 24, 64, 82	0
5	AE	150/150 (100%)	-0.15	2 (1%) 77 51	0, 32, 68, 105	0
5	BE	150/150 (100%)	-0.38	0 100 100	0, 31, 68, 98	0
6	AF	100/100 (100%)	-0.37	0 100 100	0, 33, 68, 86	0
6	BF	100/100 (100%)	-0.01	0 100 100	17, 54, 80, 93	0
7	AG	151/151 (100%)	0.50	14 (9%) 8 3	12, 56, 86, 111	0
7	BG	151/151 (100%)	0.01	5 (3%) 46 20	20, 54, 81, 94	0
8	AH	129/129 (100%)	-0.48	0 100 100	0, 32, 60, 71	0
8	BH	129/129 (100%)	-0.25	1 (0%) 86 65	4, 34, 58, 82	0
9	AI	127/127 (100%)	0.18	4 (3%) 49 21	6, 54, 79, 108	0
9	BI	127/127 (100%)	0.36	8 (6%) 20 6	20, 55, 85, 117	0
10	AJ	98/98 (100%)	0.42	5 (5%) 28 10	8, 55, 89, 104	0
10	BJ	98/98 (100%)	0.38	6 (6%) 21 7	25, 58, 82, 113	0
11	AK	117/117 (100%)	-0.37	1 (0%) 84 63	0, 19, 50, 87	0
11	BK	117/117 (100%)	-0.24	0 100 100	0, 32, 66, 79	0
12	AL	123/123 (100%)	-0.32	2 (1%) 72 44	0, 22, 67, 93	0
12	BL	123/123 (100%)	-0.27	3 (2%) 59 30	0, 17, 58, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	0.08	5 (4%) 34 13	9, 53, 87, 100	0
13	BM	114/114 (100%)	0.73	7 (6%) 21 7	26, 63, 87, 97	0
14	AN	96/100 (96%)	-0.03	1 (1%) 82 59	12, 45, 84, 107	0
14	BN	96/100 (96%)	0.26	4 (4%) 36 14	10, 56, 84, 98	0
15	AO	88/88 (100%)	-0.40	1 (1%) 80 56	0, 28, 55, 93	0
15	BO	88/88 (100%)	-0.08	1 (1%) 80 56	1, 33, 66, 89	0
16	AP	82/82 (100%)	0.13	3 (3%) 41 17	5, 30, 73, 86	0
16	BP	82/82 (100%)	-0.12	4 (4%) 29 11	0, 24, 67, 91	0
17	AQ	80/80 (100%)	0.03	1 (1%) 77 51	8, 42, 75, 96	0
17	BQ	80/80 (100%)	-0.10	1 (1%) 77 51	7, 44, 79, 94	0
18	AR	55/55 (100%)	-0.37	1 (1%) 68 40	0, 25, 59, 93	0
18	BR	55/55 (100%)	-0.10	2 (3%) 42 17	5, 38, 80, 101	0
19	AS	79/79 (100%)	0.51	4 (5%) 28 10	21, 52, 83, 98	0
19	BS	79/79 (100%)	0.78	9 (11%) 5 1	37, 65, 83, 95	0
20	AT	85/85 (100%)	0.19	3 (3%) 44 18	7, 37, 67, 80	0
20	BT	85/85 (100%)	0.20	2 (2%) 59 30	8, 38, 69, 96	0
21	AU	51/51 (100%)	0.20	5 (9%) 7 2	7, 39, 74, 77	0
21	BU	51/51 (100%)	0.27	3 (5%) 22 7	8, 47, 74, 80	0
22	AV	76/76 (100%)	-0.23	1 (1%) 77 51	0, 70, 127, 154	0
22	BV	76/76 (100%)	-0.33	0 100 100	22, 43, 72, 119	0
23	AX	15/16 (93%)	0.40	1 (6%) 17 5	6, 76, 115, 133	0
23	BX	16/16 (100%)	0.19	1 (6%) 20 6	16, 77, 102, 124	0
24	AY	183/183 (100%)	0.71	38 (20%) 1 0	0, 50, 96, 117	0
25	CA	2897/2903 (99%)	-0.52	33 (1%) 80 56	0, 0, 103, 162	0
25	DA	2896/2903 (99%)	-0.60	25 (0%) 84 63	0, 15, 109, 162	0
26	CB	119/119 (100%)	-0.84	0 100 100	0, 7, 32, 85	0
27	CC	271/271 (100%)	-0.62	0 100 100	0, 1, 29, 56	0
27	DC	271/271 (100%)	-0.53	0 100 100	0, 19, 47, 77	0
28	CD	209/209 (100%)	-0.63	0 100 100	0, 0, 19, 61	0
28	DD	209/209 (100%)	-0.55	1 (0%) 91 75	0, 10, 52, 66	0
29	CE	201/201 (100%)	-0.53	0 100 100	0, 0, 39, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	DE	201/201 (100%)	-0.39	0 100 100	0, 21, 60, 89	0
30	CF	177/177 (100%)	0.06	3 (1%) 70 41	0, 35, 82, 91	0
30	DF	177/177 (100%)	0.41	8 (4%) 33 12	12, 58, 84, 95	0
31	CG	176/176 (100%)	-0.37	0 100 100	0, 15, 48, 88	0
31	DG	176/176 (100%)	0.19	2 (1%) 80 56	15, 48, 73, 93	0
32	CH	149/149 (100%)	0.10	7 (4%) 31 11	0, 52, 87, 100	0
32	DH	149/149 (100%)	0.60	7 (4%) 31 11	8, 58, 92, 107	0
33	CI	141/141 (100%)	2.32	73 (51%) 0 0	44, 79, 102, 124	0
33	DI	141/141 (100%)	2.45	71 (50%) 0 0	54, 82, 104, 118	0
34	CJ	142/142 (100%)	-0.61	0 100 100	0, 0, 21, 56	0
34	DJ	142/142 (100%)	-0.44	0 100 100	0, 8, 37, 65	0
35	CK	122/122 (100%)	-0.64	0 100 100	0, 0, 27, 73	0
35	DK	122/122 (100%)	-0.45	0 100 100	0, 15, 50, 71	0
36	CL	143/143 (100%)	-0.54	0 100 100	0, 0, 27, 68	0
36	DL	143/143 (100%)	-0.30	3 (2%) 63 34	0, 18, 56, 82	0
37	CM	136/136 (100%)	-0.61	0 100 100	0, 0, 21, 83	0
37	DM	136/136 (100%)	-0.17	1 (0%) 87 69	0, 21, 55, 88	0
38	CN	120/120 (100%)	-0.57	0 100 100	0, 0, 14, 68	0
38	DN	120/120 (100%)	-0.50	0 100 100	0, 12, 44, 78	0
39	CO	116/116 (100%)	-0.55	0 100 100	0, 11, 39, 49	0
39	DO	116/116 (100%)	0.33	8 (6%) 16 5	5, 49, 78, 98	0
40	CP	114/114 (100%)	-0.61	0 100 100	0, 0, 47, 70	0
40	DP	114/114 (100%)	-0.46	0 100 100	0, 21, 51, 81	0
41	CQ	117/117 (100%)	-0.60	0 100 100	0, 0, 7, 63	0
41	DQ	117/117 (100%)	-0.70	0 100 100	0, 2, 27, 45	0
42	CR	103/103 (100%)	-0.57	0 100 100	0, 0, 35, 57	0
42	DR	103/103 (100%)	-0.61	1 (0%) 82 59	0, 10, 46, 78	0
43	CS	110/110 (100%)	-0.46	1 (0%) 84 63	0, 0, 22, 98	0
43	DS	110/110 (100%)	-0.63	0 100 100	0, 8, 40, 77	0
44	CT	93/93 (100%)	-0.27	2 (2%) 62 33	0, 6, 68, 78	0
44	DT	93/93 (100%)	0.13	1 (1%) 80 56	0, 35, 71, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	CU	102/102 (100%)	-0.49	2 (1%) 65 36	0, 5, 42, 79	0
45	DU	102/102 (100%)	0.36	10 (9%) 7 2	0, 34, 74, 100	0
46	CV	94/94 (100%)	-0.55	0 100 100	0, 6, 42, 62	0
46	DV	94/94 (100%)	-0.10	1 (1%) 80 56	11, 43, 68, 82	0
47	CW	76/76 (100%)	-0.54	0 100 100	0, 1, 31, 69	0
48	CX	77/77 (100%)	-0.47	0 100 100	0, 1, 47, 74	0
48	DX	77/77 (100%)	-0.42	0 100 100	0, 23, 55, 67	0
49	CY	63/63 (100%)	-0.32	2 (3%) 47 20	0, 14, 56, 97	0
49	DY	63/63 (100%)	-0.18	0 100 100	8, 43, 70, 111	0
50	CZ	58/58 (100%)	-0.53	0 100 100	0, 0, 13, 50	0
50	DZ	58/58 (100%)	-0.39	1 (1%) 70 41	0, 20, 52, 72	0
51	C0	56/56 (100%)	-0.60	0 100 100	0, 0, 25, 69	0
51	D0	56/56 (100%)	-0.54	0 100 100	0, 10, 53, 94	0
52	C1	50/50 (100%)	-0.03	1 (2%) 65 36	0, 8, 51, 93	0
52	D1	50/50 (100%)	0.47	3 (6%) 21 7	21, 38, 70, 88	0
53	C2	46/46 (100%)	-0.50	1 (2%) 62 33	0, 0, 15, 101	0
53	D2	46/46 (100%)	-0.64	0 100 100	0, 10, 26, 94	0
54	C3	64/64 (100%)	-0.61	0 100 100	0, 0, 11, 38	0
54	D3	64/64 (100%)	-0.42	0 100 100	0, 15, 35, 52	0
55	C4	38/38 (100%)	-0.38	0 100 100	0, 1, 32, 72	0
55	D4	38/38 (100%)	-0.12	0 100 100	3, 26, 59, 65	0
56	DB	118/118 (100%)	-0.71	0 100 100	6, 58, 86, 106	0
57	DW	75/75 (100%)	-0.16	0 100 100	0, 27, 54, 94	0
All	All	20908/20931 (99%)	-0.31	466 (2%) 62 33	0, 23, 86, 170	0

The worst 5 of 466 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	CI	52	LEU	10.6
33	DI	2	LYS	9.5
33	DI	59	THR	9.0
33	DI	4	VAL	8.9
33	CI	48	ILE	8.7



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3115	1/1	0.60	0.18	27,27,27,27	0
58	MG	DA	3083	1/1	0.64	0.22	31,31,31,31	0
58	MG	DA	3098	1/1	0.65	0.54	49,49,49,49	0
58	MG	DA	3055	1/1	0.71	0.13	28,28,28,28	0
58	MG	DA	3091	1/1	0.71	0.26	50,50,50,50	0
58	MG	DA	3088	1/1	0.74	0.11	12,12,12,12	0
58	MG	AA	1640	1/1	0.74	0.18	34,34,34,34	0
58	MG	BA	1631	1/1	0.78	0.13	35,35,35,35	0
58	MG	CA	3084	1/1	0.78	0.11	22,22,22,22	0
58	MG	CA	3015	1/1	0.79	0.25	36,36,36,36	0
58	MG	BA	1630	1/1	0.80	0.07	41,41,41,41	0
58	MG	CA	3062	1/1	0.80	0.46	46,46,46,46	0
58	MG	DA	3061	1/1	0.81	0.19	24,24,24,24	0
58	MG	BA	1602	1/1	0.82	0.08	21,21,21,21	0
58	MG	AA	1631	1/1	0.82	0.17	35,35,35,35	0
58	MG	AA	1601	1/1	0.82	0.10	44,44,44,44	0
58	MG	DA	3078	1/1	0.82	0.09	15,15,15,15	0
58	MG	AA	1620	1/1	0.83	0.07	10,10,10,10	0
58	MG	AA	1644	1/1	0.83	0.19	5,5,5,5	0
58	MG	DA	3116	1/1	0.84	0.14	13,13,13,13	0
58	MG	CA	3106	1/1	0.84	0.18	0,0,0,0	0
58	MG	CA	3105	1/1	0.84	0.16	0,0,0,0	0
58	MG	DA	3080	1/1	0.85	0.09	1,1,1,1	0
58	MG	DA	3136	1/1	0.85	0.11	28,28,28,28	0
58	MG	AA	1626	1/1	0.85	0.10	0,0,0,0	0
58	MG	AA	1603	1/1	0.85	0.08	28,28,28,28	0
58	MG	AA	1611	1/1	0.85	0.09	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3090	1/1	0.86	0.08	15,15,15,15	0
58	MG	CA	3082	1/1	0.86	0.12	0,0,0,0	0
58	MG	BA	1636	1/1	0.86	0.10	42,42,42,42	0
58	MG	AA	1639	1/1	0.86	0.10	22,22,22,22	0
58	MG	DA	3005	1/1	0.87	0.11	25,25,25,25	0
58	MG	DA	3165	1/1	0.87	0.23	0,0,0,0	0
58	MG	DA	3101	1/1	0.87	0.12	0,0,0,0	0
58	MG	BA	1618	1/1	0.87	0.19	4,4,4,4	0
58	MG	AA	1623	1/1	0.87	0.07	24,24,24,24	0
58	MG	DA	3084	1/1	0.87	0.12	32,32,32,32	0
58	MG	AA	1658	1/1	0.87	0.19	16,16,16,16	0
58	MG	AA	1662	1/1	0.87	0.10	8,8,8,8	0
58	MG	DA	3015	1/1	0.87	0.18	23,23,23,23	0
58	MG	DB	203	1/1	0.88	0.06	16,16,16,16	0
58	MG	CA	3099	1/1	0.88	0.85	53,53,53,53	0
58	MG	DA	3064	1/1	0.88	0.10	0,0,0,0	0
58	MG	CA	3014	1/1	0.88	0.14	12,12,12,12	0
58	MG	BA	1641	1/1	0.88	0.09	20,20,20,20	0
58	MG	AA	1617	1/1	0.88	0.05	21,21,21,21	0
58	MG	DA	3025	1/1	0.88	0.20	16,16,16,16	0
58	MG	CA	3134	1/1	0.89	0.32	14,14,14,14	0
58	MG	DA	3050	1/1	0.89	0.06	0,0,0,0	0
58	MG	BA	1624	1/1	0.89	0.07	1,1,1,1	0
58	MG	DA	3057	1/1	0.89	0.14	14,14,14,14	0
58	MG	CA	3019	1/1	0.89	0.09	0,0,0,0	0
58	MG	AA	1645	1/1	0.89	0.24	8,8,8,8	0
58	MG	CA	3117	1/1	0.89	0.14	5,5,5,5	0
58	MG	AA	1634	1/1	0.90	0.05	2,2,2,2	0
58	MG	BA	1614	1/1	0.90	0.07	19,19,19,19	0
58	MG	DA	3036	1/1	0.90	0.08	21,21,21,21	0
58	MG	BA	1609	1/1	0.90	0.09	26,26,26,26	0
58	MG	DA	3131	1/1	0.90	0.59	55,55,55,55	0
58	MG	DA	3103	1/1	0.90	0.08	0,0,0,0	0
58	MG	BA	1627	1/1	0.90	0.12	35,35,35,35	0
58	MG	AA	1669	1/1	0.90	0.14	10,10,10,10	0
58	MG	DA	3087	1/1	0.90	0.05	20,20,20,20	0
58	MG	CA	3092	1/1	0.90	0.09	16,16,16,16	0
58	MG	CA	3089	1/1	0.90	0.08	19,19,19,19	0
58	MG	DA	3102	1/1	0.90	0.09	12,12,12,12	0
58	MG	AA	1666	1/1	0.90	0.16	13,13,13,13	0
58	MG	CA	3114	1/1	0.91	0.10	0,0,0,0	0
58	MG	AA	1637	1/1	0.91	0.09	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1604	1/1	0.91	0.18	22,22,22,22	0
58	MG	CA	3026	1/1	0.91	0.33	30,30,30,30	0
58	MG	DA	3047	1/1	0.91	0.05	28,28,28,28	0
58	MG	AA	1660	1/1	0.91	0.12	15,15,15,15	0
58	MG	DA	3133	1/1	0.91	0.17	16,16,16,16	0
58	MG	AA	1635	1/1	0.91	0.09	18,18,18,18	0
58	MG	BA	1653	1/1	0.91	0.08	7,7,7,7	0
58	MG	AA	1606	1/1	0.91	0.06	6,6,6,6	0
58	MG	DA	3160	1/1	0.91	0.12	0,0,0,0	0
58	MG	BA	1655	1/1	0.91	0.11	9,9,9,9	0
58	MG	DA	3071	1/1	0.92	0.08	0,0,0,0	0
58	MG	BA	1629	1/1	0.92	0.06	17,17,17,17	0
58	MG	DA	3092	1/1	0.92	0.25	34,34,34,34	0
58	MG	CA	3102	1/1	0.92	0.15	0,0,0,0	0
58	MG	AA	1659	1/1	0.92	0.08	12,12,12,12	0
58	MG	DA	3095	1/1	0.92	0.11	10,10,10,10	0
58	MG	CA	3091	1/1	0.92	0.08	3,3,3,3	0
58	MG	AA	1655	1/1	0.92	0.15	0,0,0,0	0
58	MG	AA	1636	1/1	0.92	0.08	0,0,0,0	0
58	MG	AA	1613	1/1	0.92	0.06	2,2,2,2	0
58	MG	BA	1611	1/1	0.92	0.11	13,13,13,13	0
58	MG	BA	1605	1/1	0.92	0.06	21,21,21,21	0
58	MG	AA	1630	1/1	0.92	0.09	16,16,16,16	0
58	MG	CA	3164	1/1	0.92	0.24	0,0,0,0	0
58	MG	AA	1632	1/1	0.92	0.07	15,15,15,15	0
58	MG	DA	3030	1/1	0.92	0.12	0,0,0,0	0
58	MG	DA	3152	1/1	0.92	0.17	6,6,6,6	0
58	MG	CA	3138	1/1	0.92	0.43	0,0,0,0	0
58	MG	BA	1608	1/1	0.92	0.15	18,18,18,18	0
58	MG	DA	3070	1/1	0.92	0.08	0,0,0,0	0
58	MG	DA	3019	1/1	0.92	0.11	0,0,0,0	0
58	MG	BA	1635	1/1	0.92	0.08	21,21,21,21	0
58	MG	BA	1649	1/1	0.92	0.15	11,11,11,11	0
58	MG	DA	3079	1/1	0.92	0.08	27,27,27,27	0
58	MG	DA	3006	1/1	0.92	0.05	10,10,10,10	0
58	MG	AA	1667	1/1	0.92	0.26	13,13,13,13	0
58	MG	CA	3028	1/1	0.92	0.14	21,21,21,21	0
58	MG	DA	3138	1/1	0.92	0.45	0,0,0,0	0
58	MG	CA	3048	1/1	0.92	0.09	13,13,13,13	0
58	MG	AA	1670	1/1	0.92	0.27	11,11,11,11	0
58	MG	DA	3063	1/1	0.92	0.15	0,0,0,0	0
58	MG	CA	3154	1/1	0.93	0.29	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3025	1/1	0.93	0.17	0,0,0,0	0
58	MG	DL	201	1/1	0.93	0.05	10,10,10,10	0
58	MG	CA	3112	1/1	0.93	0.10	4,4,4,4	0
58	MG	DA	3065	1/1	0.93	0.08	0,0,0,0	0
58	MG	AA	1641	1/1	0.93	0.09	0,0,0,0	0
58	MG	CA	3076	1/1	0.93	0.15	0,0,0,0	0
58	MG	CA	3129	1/1	0.93	0.12	0,0,0,0	0
58	MG	DA	3062	1/1	0.93	0.09	0,0,0,0	0
58	MG	CA	3080	1/1	0.93	0.07	1,1,1,1	0
58	MG	CA	3132	1/1	0.93	0.40	24,24,24,24	0
58	MG	BA	1634	1/1	0.93	0.05	10,10,10,10	0
58	MG	CA	3002	1/1	0.93	0.07	0,0,0,0	0
58	MG	DA	3038	1/1	0.93	0.12	0,0,0,0	0
58	MG	DA	3016	1/1	0.93	0.08	1,1,1,1	0
58	MG	CA	3024	1/1	0.93	0.11	0,0,0,0	0
58	MG	AA	1654	1/1	0.93	0.16	5,5,5,5	0
58	MG	CA	3116	1/1	0.93	0.22	10,10,10,10	0
58	MG	CA	3185	1/1	0.93	0.28	0,0,0,0	0
58	MG	BA	1625	1/1	0.93	0.06	0,0,0,0	0
58	MG	AA	1627	1/1	0.93	0.14	19,19,19,19	0
58	MG	DA	3075	1/1	0.93	0.12	8,8,8,8	0
58	MG	DA	3161	1/1	0.93	0.09	15,15,15,15	0
58	MG	CA	3187	1/1	0.93	0.16	0,0,0,0	0
58	MG	BA	1645	1/1	0.93	0.08	8,8,8,8	0
58	MG	DA	3014	1/1	0.93	0.11	12,12,12,12	0
58	MG	DA	3034	1/1	0.94	0.06	11,11,11,11	0
58	MG	BA	1615	1/1	0.94	0.18	9,9,9,9	0
58	MG	DA	3004	1/1	0.94	0.10	30,30,30,30	0
58	MG	CA	3160	1/1	0.94	0.32	0,0,0,0	0
58	MG	DA	3135	1/1	0.94	0.08	11,11,11,11	0
58	MG	CA	3191	1/1	0.94	0.20	0,0,0,0	0
58	MG	CA	3040	1/1	0.94	0.16	0,0,0,0	0
58	MG	DA	3009	1/1	0.94	0.09	4,4,4,4	0
58	MG	DA	3112	1/1	0.94	0.09	5,5,5,5	0
58	MG	DA	3124	1/1	0.94	0.05	0,0,0,0	0
58	MG	DA	3109	1/1	0.94	0.13	2,2,2,2	0
58	MG	DA	3126	1/1	0.94	0.14	0,0,0,0	0
58	MG	CA	3100	1/1	0.94	0.10	0,0,0,0	0
58	MG	CA	3178	1/1	0.94	0.13	0,0,0,0	0
58	MG	DA	3120	1/1	0.94	0.11	8,8,8,8	0
58	MG	BA	1617	1/1	0.94	0.06	13,13,13,13	0
58	MG	DA	3119	1/1	0.94	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3162	1/1	0.94	0.20	4,4,4,4	0
58	MG	BA	1633	1/1	0.94	0.12	11,11,11,11	0
58	MG	AA	1625	1/1	0.94	0.07	6,6,6,6	0
58	MG	CB	201	1/1	0.94	0.05	0,0,0,0	0
58	MG	AA	1671	1/1	0.94	0.17	6,6,6,6	0
58	MG	AA	1607	1/1	0.94	0.08	10,10,10,10	0
58	MG	BA	1622	1/1	0.94	0.05	4,4,4,4	0
58	MG	DA	3059	1/1	0.94	0.11	6,6,6,6	0
58	MG	DA	3077	1/1	0.94	0.05	12,12,12,12	0
58	MG	AA	1616	1/1	0.94	0.09	11,11,11,11	0
58	MG	CA	3135	1/1	0.94	0.12	0,0,0,0	0
58	MG	CA	3030	1/1	0.94	0.11	0,0,0,0	0
58	MG	CA	3035	1/1	0.94	0.07	1,1,1,1	0
58	MG	AA	1619	1/1	0.94	0.16	32,32,32,32	0
58	MG	BA	1612	1/1	0.94	0.05	18,18,18,18	0
58	MG	DA	3156	1/1	0.94	0.23	3,3,3,3	0
58	MG	DA	3003	1/1	0.94	0.07	8,8,8,8	0
58	MG	BA	1626	1/1	0.94	0.06	14,14,14,14	0
58	MG	DA	3085	1/1	0.94	0.20	0,0,0,0	0
58	MG	DA	3033	1/1	0.94	0.12	0,0,0,0	0
58	MG	DA	3010	1/1	0.94	0.09	7,7,7,7	0
58	MG	DA	3026	1/1	0.94	0.09	0,0,0,0	0
58	MG	CA	3006	1/1	0.94	0.07	1,1,1,1	0
58	MG	DA	3044	1/1	0.94	0.05	11,11,11,11	0
58	MG	DA	3114	1/1	0.94	0.08	14,14,14,14	0
58	MG	DA	3110	1/1	0.94	0.05	18,18,18,18	0
58	MG	BA	1632	1/1	0.94	0.04	18,18,18,18	0
58	MG	CA	3194	1/1	0.94	0.19	0,0,0,0	0
58	MG	CA	3056	1/1	0.94	0.08	10,10,10,10	0
58	MG	BA	1603	1/1	0.94	0.09	13,13,13,13	0
58	MG	CA	3120	1/1	0.94	0.12	2,2,2,2	0
58	MG	BA	1613	1/1	0.95	0.13	0,0,0,0	0
58	MG	CA	3061	1/1	0.95	0.12	9,9,9,9	0
58	MG	CA	3041	1/1	0.95	0.16	0,0,0,0	0
58	MG	CA	3121	1/1	0.95	0.19	0,0,0,0	0
58	MG	DA	3096	1/1	0.95	0.06	13,13,13,13	0
58	MG	DA	3111	1/1	0.95	0.08	1,1,1,1	0
58	MG	CA	3180	1/1	0.95	0.19	6,6,6,6	0
58	MG	DA	3076	1/1	0.95	0.09	5,5,5,5	0
58	MG	AA	1653	1/1	0.95	0.15	1,1,1,1	0
58	MG	BA	1637	1/1	0.95	0.16	19,19,19,19	0
58	MG	CA	3169	1/1	0.95	0.22	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3046	1/1	0.95	0.06	0,0,0,0	0
58	MG	DA	3045	1/1	0.95	0.09	0,0,0,0	0
58	MG	DA	3099	1/1	0.95	0.07	0,0,0,0	0
58	MG	AA	1665	1/1	0.95	0.08	0,0,0,0	0
58	MG	DA	3149	1/1	0.95	0.18	0,0,0,0	0
58	MG	DA	3021	1/1	0.95	0.08	3,3,3,3	0
58	MG	CA	3171	1/1	0.95	0.14	0,0,0,0	0
58	MG	DA	3027	1/1	0.95	0.10	14,14,14,14	0
58	MG	AA	1663	1/1	0.95	0.10	6,6,6,6	0
58	MG	CA	3051	1/1	0.95	0.09	3,3,3,3	0
58	MG	CA	3168	1/1	0.95	0.20	0,0,0,0	0
58	MG	CA	3027	1/1	0.95	0.14	0,0,0,0	0
58	MG	CA	3059	1/1	0.95	0.07	4,4,4,4	0
58	MG	CA	3173	1/1	0.95	0.25	0,0,0,0	0
58	MG	DA	3028	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3085	1/1	0.95	0.21	12,12,12,12	0
58	MG	CA	3058	1/1	0.95	0.10	10,10,10,10	0
58	MG	CA	3032	1/1	0.95	0.07	0,0,0,0	0
58	MG	DA	3117	1/1	0.95	0.05	5,5,5,5	0
58	MG	CA	3044	1/1	0.95	0.06	0,0,0,0	0
58	MG	DA	3082	1/1	0.95	0.05	7,7,7,7	0
58	MG	CA	3081	1/1	0.95	0.07	0,0,0,0	0
58	MG	DA	3060	1/1	0.95	0.13	5,5,5,5	0
58	MG	CA	3175	1/1	0.95	0.17	0,0,0,0	0
58	MG	BA	1639	1/1	0.95	0.06	0,0,0,0	0
58	MG	CA	3045	1/1	0.95	0.10	0,0,0,0	0
58	MG	DA	3113	1/1	0.95	0.12	0,0,0,0	0
58	MG	BA	1616	1/1	0.95	0.11	0,0,0,0	0
58	MG	AA	1602	1/1	0.95	0.11	17,17,17,17	0
58	MG	CA	3001	1/1	0.95	0.10	0,0,0,0	0
58	MG	DA	3118	1/1	0.95	0.10	7,7,7,7	0
58	MG	CA	3063	1/1	0.95	0.12	0,0,0,0	0
58	MG	DA	3145	1/1	0.95	0.11	0,0,0,0	0
58	MG	DA	3037	1/1	0.95	0.18	0,0,0,0	0
58	MG	CA	3126	1/1	0.95	0.13	0,0,0,0	0
58	MG	AA	1608	1/1	0.95	0.20	0,0,0,0	0
58	MG	CA	3101	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3109	1/1	0.95	0.15	0,0,0,0	0
58	MG	BA	1652	1/1	0.95	0.10	1,1,1,1	0
58	MG	DB	201	1/1	0.95	0.05	24,24,24,24	0
58	MG	BA	1646	1/1	0.95	0.14	10,10,10,10	0
58	MG	CA	3034	1/1	0.95	0.20	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3122	1/1	0.95	0.15	0,0,0,0	0
58	MG	CA	3009	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3098	1/1	0.95	0.14	0,0,0,0	0
58	MG	DA	3066	1/1	0.95	0.05	0,0,0,0	0
58	MG	CA	3127	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3153	1/1	0.95	0.29	0,0,0,0	0
58	MG	CA	3124	1/1	0.96	0.09	0,0,0,0	0
58	MG	BA	1654	1/1	0.96	0.10	22,22,22,22	0
58	MG	AA	1649	1/1	0.96	0.23	0,0,0,0	0
58	MG	CA	3007	1/1	0.96	0.04	0,0,0,0	0
58	MG	CA	3071	1/1	0.96	0.07	0,0,0,0	0
58	MG	AA	1657	1/1	0.96	0.18	2,2,2,2	0
58	MG	DA	3139	1/1	0.96	0.28	0,0,0,0	0
58	MG	CA	3070	1/1	0.96	0.12	25,25,25,25	0
58	MG	CA	3137	1/1	0.96	0.09	4,4,4,4	0
58	MG	AA	1618	1/1	0.96	0.07	21,21,21,21	0
58	MG	CA	3150	1/1	0.96	0.10	0,0,0,0	0
58	MG	CA	3188	1/1	0.96	0.15	2,2,2,2	0
58	MG	CA	3179	1/1	0.96	0.15	0,0,0,0	0
58	MG	CA	3021	1/1	0.96	0.10	0,0,0,0	0
58	MG	CA	3125	1/1	0.96	0.08	0,0,0,0	0
58	MG	CA	3086	1/1	0.96	0.16	0,0,0,0	0
58	MG	DA	3073	1/1	0.96	0.11	6,6,6,6	0
58	MG	CA	3067	1/1	0.96	0.13	0,0,0,0	0
58	MG	DA	3154	1/1	0.96	0.17	0,0,0,0	0
58	MG	CA	3181	1/1	0.96	0.15	0,0,0,0	0
58	MG	BA	1620	1/1	0.96	0.07	19,19,19,19	0
58	MG	BA	1643	1/1	0.96	0.14	3,3,3,3	0
58	MG	DA	3150	1/1	0.96	0.15	0,0,0,0	0
58	MG	AA	1646	1/1	0.96	0.17	0,0,0,0	0
58	MG	DA	3001	1/1	0.96	0.05	0,0,0,0	0
58	MG	AA	1672	1/1	0.96	0.21	3,3,3,3	0
58	MG	BA	1642	1/1	0.96	0.23	6,6,6,6	0
58	MG	DA	3040	1/1	0.96	0.14	5,5,5,5	0
58	MG	CA	3193	1/1	0.96	0.25	0,0,0,0	0
58	MG	DA	3166	1/1	0.96	0.20	9,9,9,9	0
58	MG	CA	3075	1/1	0.96	0.07	0,0,0,0	0
58	MG	CA	3140	1/1	0.96	0.52	0,0,0,0	0
58	MG	DB	202	1/1	0.96	0.04	9,9,9,9	0
58	MG	DA	3105	1/1	0.96	0.11	0,0,0,0	0
58	MG	CA	3003	1/1	0.96	0.06	0,0,0,0	0
58	MG	CA	3172	1/1	0.96	0.17	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1633	1/1	0.96	0.04	3,3,3,3	0
58	MG	BA	1656	1/1	0.96	0.19	9,9,9,9	0
58	MG	AA	1647	1/1	0.96	0.23	1,1,1,1	0
58	MG	AA	1612	1/1	0.96	0.05	0,0,0,0	0
58	MG	CA	3111	1/1	0.96	0.04	6,6,6,6	0
58	MG	CA	3177	1/1	0.96	0.13	0,0,0,0	0
58	MG	CA	3094	1/1	0.96	0.06	3,3,3,3	0
58	MG	CA	3165	1/1	0.96	0.20	0,0,0,0	0
58	MG	CA	3166	1/1	0.96	0.14	0,0,0,0	0
58	MG	DA	3094	1/1	0.96	0.08	43,43,43,43	0
58	MG	DA	3121	1/1	0.96	0.07	7,7,7,7	0
58	MG	DA	3132	1/1	0.96	0.05	6,6,6,6	0
58	MG	CA	3090	1/1	0.96	0.08	1,1,1,1	0
58	MG	AA	1656	1/1	0.96	0.13	14,14,14,14	0
58	MG	AA	1643	1/1	0.96	0.27	0,0,0,0	0
58	MG	DA	3013	1/1	0.96	0.14	0,0,0,0	0
58	MG	BA	1638	1/1	0.96	0.09	27,27,27,27	0
58	MG	AA	1622	1/1	0.96	0.17	0,0,0,0	0
58	MG	CA	3155	1/1	0.96	0.37	0,0,0,0	0
58	MG	DA	3093	1/1	0.96	0.08	2,2,2,2	0
58	MG	DA	3046	1/1	0.96	0.07	1,1,1,1	0
58	MG	CB	202	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3100	1/1	0.96	0.06	4,4,4,4	0
58	MG	AA	1648	1/1	0.96	0.12	4,4,4,4	0
58	MG	AA	1614	1/1	0.96	0.05	12,12,12,12	0
58	MG	DA	3012	1/1	0.96	0.11	0,0,0,0	0
58	MG	DA	3002	1/1	0.96	0.06	1,1,1,1	0
58	MG	BA	1648	1/1	0.96	0.17	0,0,0,0	0
58	MG	DA	3042	1/1	0.96	0.06	5,5,5,5	0
58	MG	CA	3093	1/1	0.96	0.12	11,11,11,11	0
58	MG	DA	3018	1/1	0.96	0.07	6,6,6,6	0
58	MG	CA	3136	1/1	0.96	0.09	0,0,0,0	0
58	MG	AA	1651	1/1	0.96	0.24	0,0,0,0	0
58	MG	CA	3146	1/1	0.96	0.33	0,0,0,0	0
58	MG	CA	3049	1/1	0.97	0.07	0,0,0,0	0
58	MG	BA	1623	1/1	0.97	0.08	3,3,3,3	0
58	MG	DA	3056	1/1	0.97	0.05	5,5,5,5	0
58	MG	CA	3011	1/1	0.97	0.20	0,0,0,0	0
58	MG	BA	1610	1/1	0.97	0.03	0,0,0,0	0
58	MG	CQ	201	1/1	0.97	0.31	0,0,0,0	0
58	MG	DA	3023	1/1	0.97	0.06	0,0,0,0	0
58	MG	DA	3072	1/1	0.97	0.09	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	CA	3104	1/1	0.97	0.06	0,0,0,0	0
58	MG	CA	3060	1/1	0.97	0.04	4,4,4,4	0
58	MG	CA	3184	1/1	0.97	0.22	0,0,0,0	0
58	MG	DA	3123	1/1	0.97	0.05	6,6,6,6	0
58	MG	CA	3170	1/1	0.97	0.07	0,0,0,0	0
58	MG	CA	3145	1/1	0.97	0.13	0,0,0,0	0
58	MG	CA	3108	1/1	0.97	0.10	0,0,0,0	0
58	MG	CA	3053	1/1	0.97	0.08	0,0,0,0	0
58	MG	CA	3037	1/1	0.97	0.06	11,11,11,11	0
58	MG	AA	1610	1/1	0.97	0.07	32,32,32,32	0
58	MG	CA	3052	1/1	0.97	0.12	0,0,0,0	0
58	MG	CA	3158	1/1	0.97	0.33	0,0,0,0	0
58	MG	CA	3103	1/1	0.97	0.09	0,0,0,0	0
58	MG	DQ	801	1/1	0.97	0.26	0,0,0,0	0
58	MG	AA	1621	1/1	0.97	0.03	10,10,10,10	0
58	MG	DA	3147	1/1	0.97	0.19	0,0,0,0	0
58	MG	CA	3079	1/1	0.97	0.05	3,3,3,3	0
58	MG	CA	3183	1/1	0.97	0.18	0,0,0,0	0
58	MG	DA	3164	1/1	0.97	0.15	0,0,0,0	0
58	MG	CA	3013	1/1	0.97	0.15	0,0,0,0	0
58	MG	DA	3128	1/1	0.97	0.11	0,0,0,0	0
58	MG	CA	3113	1/1	0.97	0.12	0,0,0,0	0
58	MG	CA	3023	1/1	0.97	0.13	0,0,0,0	0
58	MG	CA	3074	1/1	0.97	0.15	0,0,0,0	0
58	MG	DA	3146	1/1	0.97	0.18	0,0,0,0	0
58	MG	AA	1668	1/1	0.97	0.09	0,0,0,0	0
58	MG	CA	3004	1/1	0.97	0.05	11,11,11,11	0
58	MG	DA	3067	1/1	0.97	0.07	0,0,0,0	0
58	MG	CA	3031	1/1	0.97	0.22	0,0,0,0	0
58	MG	CA	3157	1/1	0.97	0.21	0,0,0,0	0
58	MG	CA	3008	1/1	0.97	0.09	0,0,0,0	0
58	MG	DA	3043	1/1	0.97	0.05	6,6,6,6	0
58	MG	AA	1650	1/1	0.97	0.11	0,0,0,0	0
58	MG	CA	3163	1/1	0.97	0.20	0,0,0,0	0
58	MG	CA	3167	1/1	0.97	0.30	0,0,0,0	0
58	MG	DA	3031	1/1	0.97	0.11	0,0,0,0	0
58	MG	DA	3144	1/1	0.97	0.07	0,0,0,0	0
58	MG	CA	3065	1/1	0.97	0.09	0,0,0,0	0
58	MG	CA	3115	1/1	0.97	0.06	0,0,0,0	0
58	MG	DA	3137	1/1	0.97	0.47	0,0,0,0	0
58	MG	CA	3110	1/1	0.97	0.17	0,0,0,0	0
58	MG	DA	3140	1/1	0.97	0.28	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3104	1/1	0.97	0.09	0,0,0,0	0
58	MG	DA	3068	1/1	0.97	0.06	6,6,6,6	0
58	MG	AA	1624	1/1	0.97	0.06	10,10,10,10	0
58	MG	BA	1607	1/1	0.97	0.06	1,1,1,1	0
58	MG	DA	3069	1/1	0.97	0.09	41,41,41,41	0
58	MG	DA	3081	1/1	0.97	0.06	0,0,0,0	0
58	MG	DA	3157	1/1	0.97	0.22	0,0,0,0	0
58	MG	CA	3176	1/1	0.97	0.14	10,10,10,10	0
58	MG	AA	1661	1/1	0.97	0.15	15,15,15,15	0
58	MG	DA	3051	1/1	0.97	0.07	0,0,0,0	0
58	MG	CA	3042	1/1	0.97	0.10	0,0,0,0	0
58	MG	DA	3097	1/1	0.97	0.08	13,13,13,13	0
58	MG	AA	1615	1/1	0.97	0.08	9,9,9,9	0
58	MG	BA	1644	1/1	0.97	0.09	0,0,0,0	0
58	MG	BA	1604	1/1	0.97	0.07	13,13,13,13	0
58	MG	BA	1651	1/1	0.97	0.14	7,7,7,7	0
58	MG	BA	1606	1/1	0.97	0.12	24,24,24,24	0
58	MG	CA	3186	1/1	0.98	0.27	0,0,0,0	0
58	MG	DA	3159	1/1	0.98	0.26	3,3,3,3	0
58	MG	CA	3012	1/1	0.98	0.18	0,0,0,0	0
58	MG	CA	3152	1/1	0.98	0.17	0,0,0,0	0
58	MG	DA	3011	1/1	0.98	0.08	0,0,0,0	0
58	MG	DA	3032	1/1	0.98	0.08	0,0,0,0	0
58	MG	CA	3148	1/1	0.98	0.47	0,0,0,0	0
58	MG	CA	3118	1/1	0.98	0.08	0,0,0,0	0
58	MG	CA	3097	1/1	0.98	0.12	0,0,0,0	0
58	MG	DA	3048	1/1	0.98	0.06	0,0,0,0	0
58	MG	CA	3047	1/1	0.98	0.09	0,0,0,0	0
58	MG	CA	3162	1/1	0.98	0.28	0,0,0,0	0
58	MG	CA	3156	1/1	0.98	0.30	0,0,0,0	0
58	MG	CA	3073	1/1	0.98	0.12	0,0,0,0	0
58	MG	DA	3035	1/1	0.98	0.10	0,0,0,0	0
58	MG	CA	3020	1/1	0.98	0.12	0,0,0,0	0
58	MG	DA	3049	1/1	0.98	0.05	0,0,0,0	0
58	MG	DA	3041	1/1	0.98	0.04	6,6,6,6	0
58	MG	AA	1609	1/1	0.98	0.05	0,0,0,0	0
58	MG	CA	3131	1/1	0.98	0.15	0,0,0,0	0
58	MG	AA	1628	1/1	0.98	0.04	1,1,1,1	0
58	MG	CA	3149	1/1	0.98	0.32	0,0,0,0	0
58	MG	BA	1647	1/1	0.98	0.06	0,0,0,0	0
58	MG	DA	3125	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3072	1/1	0.98	0.07	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	BA	1640	1/1	0.98	0.14	0,0,0,0	0
58	MG	CB	204	1/1	0.98	0.39	0,0,0,0	0
58	MG	CA	3057	1/1	0.98	0.04	0,0,0,0	0
58	MG	CA	3043	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3189	1/1	0.98	0.14	0,0,0,0	0
58	MG	CB	203	1/1	0.98	0.04	5,5,5,5	0
58	MG	CA	3141	1/1	0.98	0.27	0,0,0,0	0
58	MG	BA	1601	1/1	0.98	0.08	2,2,2,2	0
58	MG	CA	3095	1/1	0.98	0.16	17,17,17,17	0
58	MG	AA	1664	1/1	0.98	0.11	4,4,4,4	0
58	MG	DA	3127	1/1	0.98	0.05	0,0,0,0	0
58	MG	CA	3078	1/1	0.98	0.07	0,0,0,0	0
58	MG	DA	3039	1/1	0.98	0.09	3,3,3,3	0
58	MG	BA	1619	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3107	1/1	0.98	0.17	0,0,0,0	0
58	MG	CA	3066	1/1	0.98	0.21	0,0,0,0	0
58	MG	DA	3142	1/1	0.98	0.16	0,0,0,0	0
58	MG	DA	3163	1/1	0.98	0.09	0,0,0,0	0
58	MG	CA	3161	1/1	0.98	0.19	0,0,0,0	0
58	MG	DA	3058	1/1	0.98	0.07	6,6,6,6	0
58	MG	DA	3020	1/1	0.98	0.06	0,0,0,0	0
58	MG	CA	3039	1/1	0.98	0.11	0,0,0,0	0
58	MG	CA	3192	1/1	0.98	0.11	0,0,0,0	0
58	MG	CA	3077	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3174	1/1	0.98	0.31	0,0,0,0	0
58	MG	BA	1650	1/1	0.98	0.21	5,5,5,5	0
58	MG	DA	3106	1/1	0.98	0.17	0,0,0,0	0
58	MG	DA	3054	1/1	0.98	0.09	0,0,0,0	0
58	MG	DA	3086	1/1	0.98	0.15	0,0,0,0	0
58	MG	CA	3123	1/1	0.98	0.20	0,0,0,0	0
58	MG	CA	3036	1/1	0.98	0.16	0,0,0,0	0
58	MG	CA	3054	1/1	0.98	0.14	0,0,0,0	0
58	MG	CA	3128	1/1	0.98	0.14	0,0,0,0	0
58	MG	DA	3017	1/1	0.98	0.13	0,0,0,0	0
58	MG	CA	3088	1/1	0.98	0.10	0,0,0,0	0
58	MG	CA	3064	1/1	0.98	0.18	0,0,0,0	0
58	MG	CA	3029	1/1	0.98	0.13	0,0,0,0	0
58	MG	DA	3089	1/1	0.98	0.08	24,24,24,24	0
58	MG	DA	3143	1/1	0.98	0.21	0,0,0,0	0
58	MG	CA	3147	1/1	0.98	0.27	0,0,0,0	0
58	MG	CA	3159	1/1	0.98	0.26	0,0,0,0	0
58	MG	DA	3008	1/1	0.98	0.11	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	AA	1642	1/1	0.98	0.06	1,1,1,1	0
58	MG	CA	3069	1/1	0.98	0.14	0,0,0,0	0
58	MG	AA	1652	1/1	0.98	0.12	13,13,13,13	0
58	MG	AA	1638	1/1	0.98	0.06	12,12,12,12	0
58	MG	CA	3033	1/1	0.98	0.14	0,0,0,0	0
58	MG	DA	3052	1/1	0.98	0.05	0,0,0,0	0
58	MG	DA	3022	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3010	1/1	0.98	0.11	0,0,0,0	0
58	MG	CA	3083	1/1	0.98	0.04	10,10,10,10	0
58	MG	BA	1621	1/1	0.98	0.05	12,12,12,12	0
58	MG	DA	3107	1/1	0.98	0.09	9,9,9,9	0
58	MG	DA	3024	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3017	1/1	0.98	0.16	0,0,0,0	0
58	MG	DA	3155	1/1	0.98	0.18	1,1,1,1	0
58	MG	CA	3096	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3144	1/1	0.98	0.33	0,0,0,0	0
58	MG	CA	3055	1/1	0.98	0.10	6,6,6,6	0
58	MG	CA	3130	1/1	0.98	0.18	0,0,0,0	0
58	MG	DA	3153	1/1	0.99	0.10	11,11,11,11	0
58	MG	CA	3005	1/1	0.99	0.05	14,14,14,14	0
58	MG	DA	3158	1/1	0.99	0.14	0,0,0,0	0
58	MG	DA	3148	1/1	0.99	0.27	0,0,0,0	0
58	MG	BA	1628	1/1	0.99	0.08	25,25,25,25	0
58	MG	DA	3130	1/1	0.99	0.11	0,0,0,0	0
58	MG	CA	3068	1/1	0.99	0.12	0,0,0,0	0
58	MG	CA	3016	1/1	0.99	0.12	0,0,0,0	0
58	MG	DA	3074	1/1	0.99	0.13	0,0,0,0	0
58	MG	CA	3182	1/1	0.99	0.30	0,0,0,0	0
58	MG	DA	3007	1/1	0.99	0.19	26,26,26,26	0
58	MG	CA	3119	1/1	0.99	0.02	8,8,8,8	0
58	MG	CA	3190	1/1	0.99	0.23	0,0,0,0	0
59	ZN	C4	101	1/1	0.99	0.07	0,0,0,0	0
58	MG	DA	3108	1/1	0.99	0.17	0,0,0,0	0
58	MG	CA	3139	1/1	0.99	0.42	0,0,0,0	0
58	MG	CA	3151	1/1	0.99	0.32	0,0,0,0	0
58	MG	CA	3143	1/1	0.99	0.29	0,0,0,0	0
58	MG	CA	3022	1/1	0.99	0.14	0,0,0,0	0
58	MG	DA	3134	1/1	0.99	0.07	0,0,0,0	0
58	MG	DA	3029	1/1	0.99	0.05	0,0,0,0	0
59	ZN	D4	101	1/1	0.99	0.06	41,41,41,41	0
58	MG	CA	3018	1/1	0.99	0.18	0,0,0,0	0
58	MG	CA	3142	1/1	0.99	0.41	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	DA	3129	1/1	0.99	0.08	0,0,0,0	0
58	MG	DA	3151	1/1	0.99	0.15	11,11,11,11	0
58	MG	CA	3133	1/1	0.99	0.05	0,0,0,0	0
58	MG	DA	3141	1/1	0.99	0.23	0,0,0,0	0
58	MG	AA	1629	1/1	0.99	0.07	0,0,0,0	0
58	MG	CA	3038	1/1	0.99	0.20	0,0,0,0	0
58	MG	DA	3053	1/1	0.99	0.06	0,0,0,0	0
58	MG	AA	1605	1/1	0.99	0.07	0,0,0,0	0
58	MG	CA	3087	1/1	0.99	0.13	0,0,0,0	0
58	MG	CA	3050	1/1	1.00	0.15	0,0,0,0	0
58	MG	CA	3122	1/1	1.00	0.11	0,0,0,0	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.