



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 05:54 PM BST

PDB ID : 4V4A  
Title : Crystal Structure of the Wild Type Ribosome from E. Coli 70S Ribosome.  
Authors : Vila-Sanjurjo, A.; Ridgeway, W.K.; Seymaner, V.; Zhang, W.; Santoso, S.;  
Yu, K.; Cate, J.H.D.  
Deposited on : 2003-06-13  
Resolution : 9.50 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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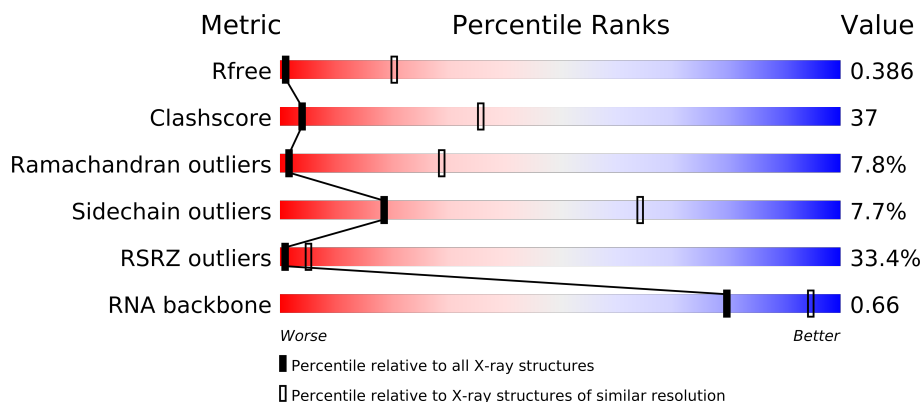
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 9.50 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))
$R_{free}$	66092	1106 (11.50-3.50)
Clashscore	79885	1010 (15.00-3.54)
Ramachandran outliers	78287	1304 (15.00-3.50)
Sidechain outliers	78261	1278 (15.00-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)
RNA backbone	1838	1055 (11.50-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1537	
2	AB	234	
3	AC	206	
4	AD	208	
5	AE	150	
6	AF	101	
7	AG	155	
8	AH	138	
9	AI	127	
10	AJ	98	
11	AK	119	
12	AL	124	

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Mol	Chain	Length	Quality of chain
13	AM	125	
14	AN	60	
15	AO	88	
16	AP	83	
17	AQ	104	
18	AR	73	
19	AS	80	
20	AT	99	
21	B0	2887	
22	B9	118	
23	BA	270	
24	BB	205	
25	BC	197	
26	BD	178	
27	BE	177	
28	BF	52	
29	BG	143	
30	BH	143	
31	BI	132	
32	BJ	141	
33	BK	124	
34	BL	114	
35	BM	111	
36	BN	125	
37	BO	117	
38	BP	100	
39	BQ	130	
40	BR	93	
41	BS	113	
42	BT	173	
43	BU	86	
44	BV	16	
45	BW	65	
46	BX	55	
47	BY	73	
48	BZ	58	
49	B1	53	
50	B2	46	
51	B3	63	
52	B4	35	
53	B5	217	

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 118711 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0	0
			32939	14664	6099	10643	1533			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- 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
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- 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
			1146	724	217	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- 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
			1010	639	198	173				

- 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
			794	499	156	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	0
			996	617	207	170	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- 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
			733	459	147	125	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	104	Total	C	N	O	S	0	0	0
			856	547	161	146	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	73	Total	C	N	O	0	0	0
			596	380	118	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	B0	2825	Total	C	N	O	P	0	0	0
			60636	27047	11191	19573	2825			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B9	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
23	BA	270	Total	C	0	0	270
			270	270			

- Molecule 24 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
24	BB	205	Total	C	0	0	205
			205	205			

- Molecule 25 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	BC	197	Total	C	0	0	197
			197	197			

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
26	BD	178	Total	C	0	0	178
			178	178			

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
27	BE	177	Total	C	0	0	177
			177	177			

- Molecule 28 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
28	BF	52	Total	C	0	0	52
			52	52			

- Molecule 29 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
29	BG	143	Total	C	0	0	143
			143	143			

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
30	BH	143	Total	C	0	0	143
			143	143			

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
31	BI	132	Total	C	0	0	132
			132	132			

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
32	BJ	141	Total	C	0	0	141
			141	141			

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
33	BK	124	Total	C	0	0	124
			124	124			

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
34	BL	114	Total	C	0	0	114
			114	114			

- Molecule 35 is a protein called 50S ribosomal protein L18.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	BM	111	Total C 111 111	0	0	111

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BN	125	Total C 125 125	0	0	125

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BO	117	Total C 117 117	0	0	117

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BP	100	Total C 100 100	0	0	100

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	BQ	130	Total C 130 130	0	0	130

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	BR	93	Total C 93 93	0	0	93

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	BS	113	Total C 113 113	0	0	113

- Molecule 42 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	BT	173	Total C 173 173	0	0	173

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	BU	86	Total C 86 86	0	0	86

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	BV	16	Total C 16 16	0	0	16

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	BW	65	Total C 65 65	0	0	65

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	BX	55	Total C 55 55	0	0	55

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	BY	73	Total C 73 73	0	0	73

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	BZ	58	Total C 58 58	0	0	58

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
49	B1	53	Total	C	0	0	53
			53	53			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
50	B2	46	Total	C	0	0	46
			46	46			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
51	B3	63	Total	C	0	0	63
			63	63			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
52	B4	35	Total	C	0	0	35
			35	35			

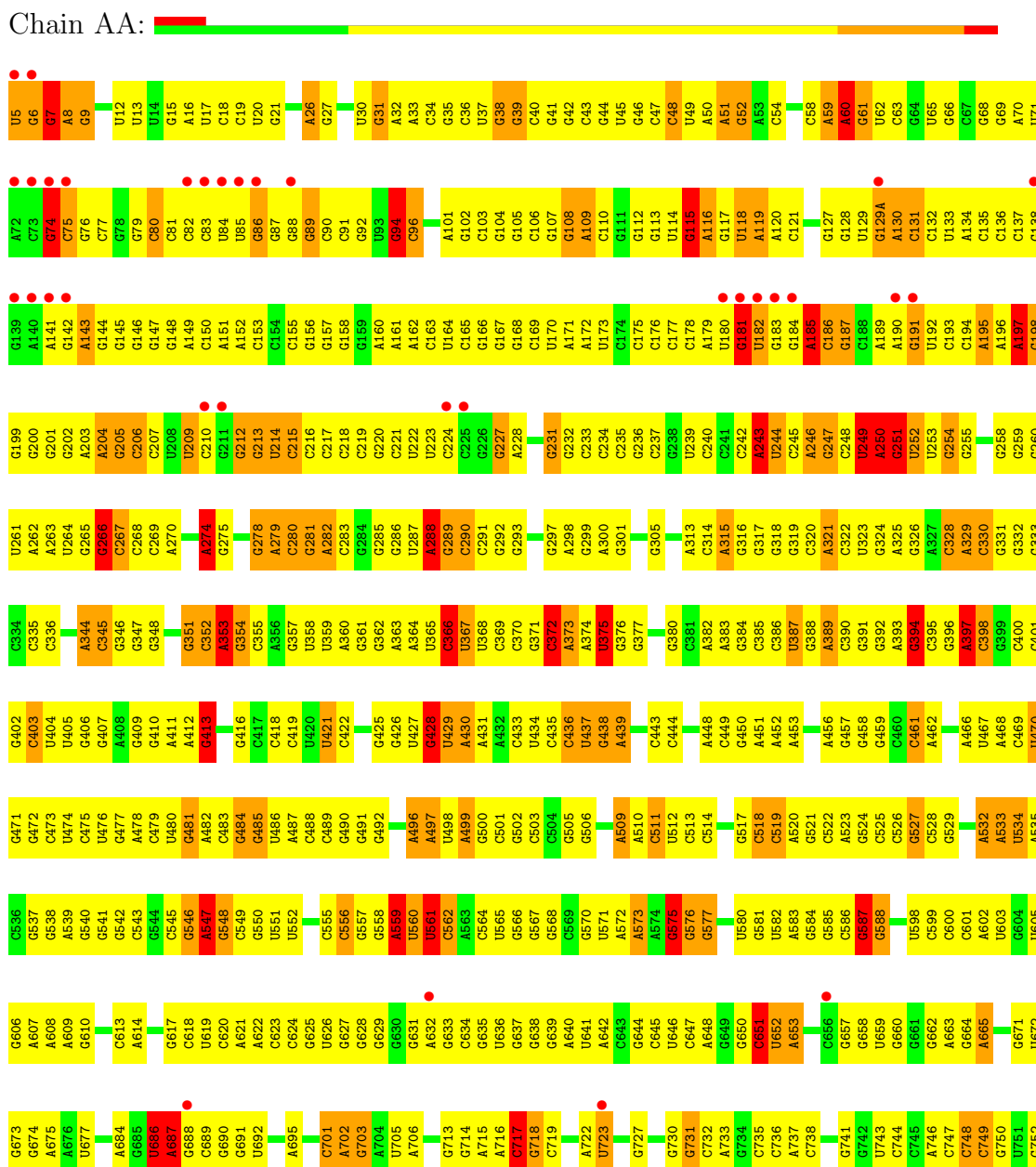
- Molecule 53 is a protein called 50S ribosomal protein L1P.

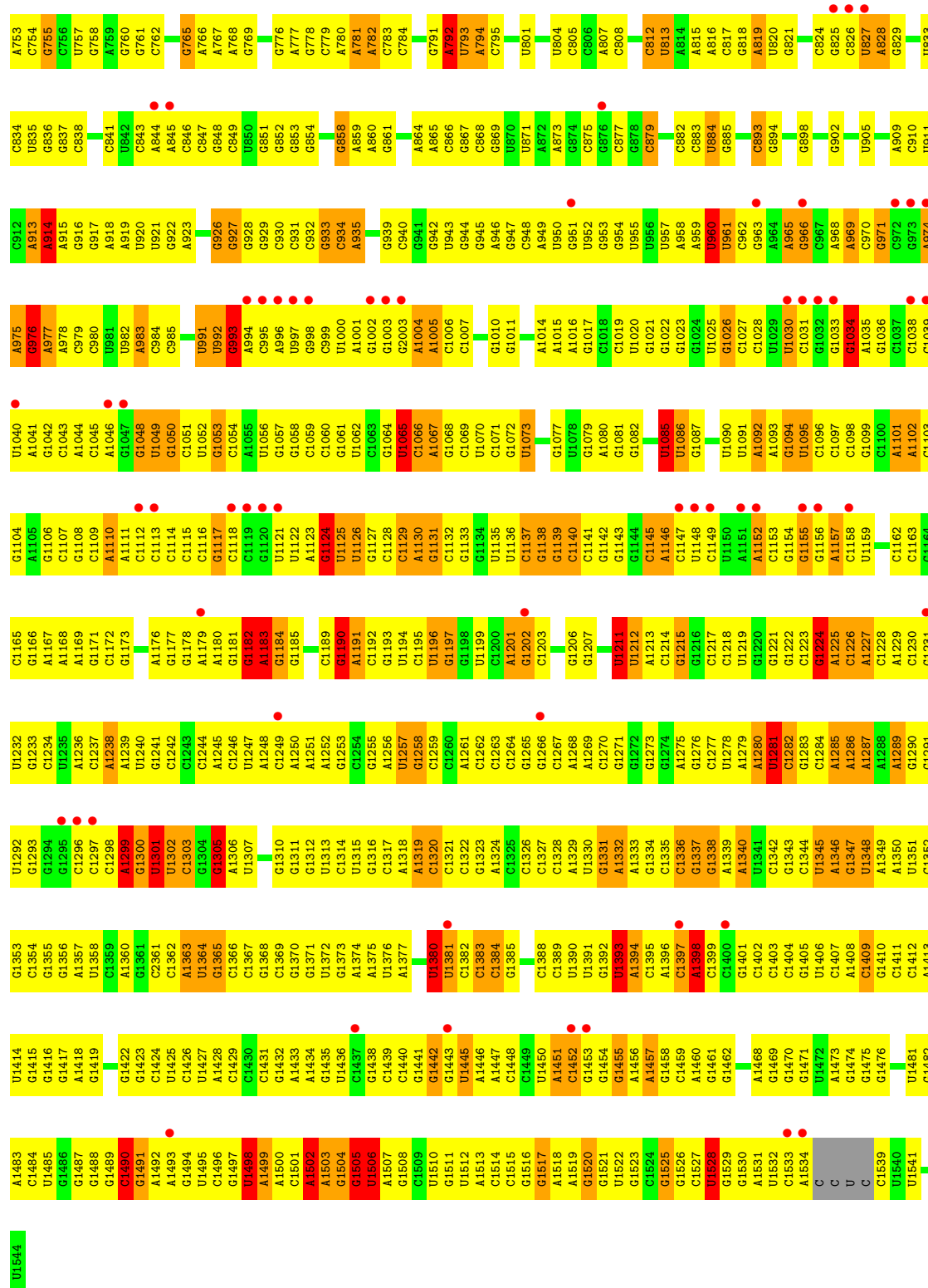
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
53	B5	217	Total	C	0	0	217
			217	217			

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

#### • Molecule 1: 16S RIBOSOMAL RNA

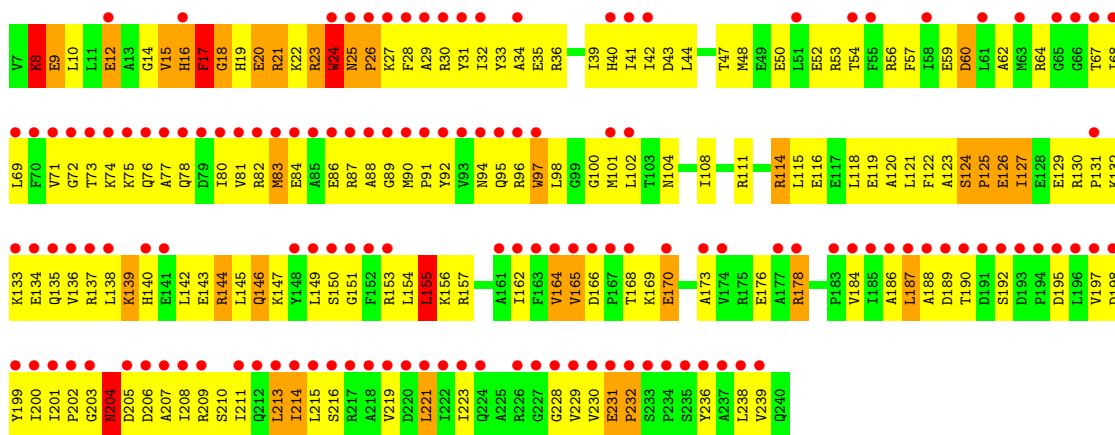




• Molecule 2: 30S ribosomal protein S2

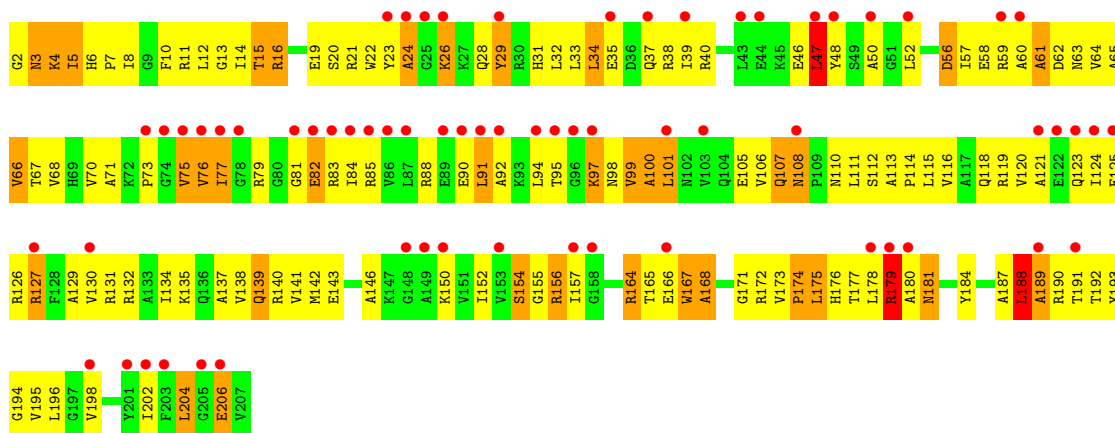
Chain AB:





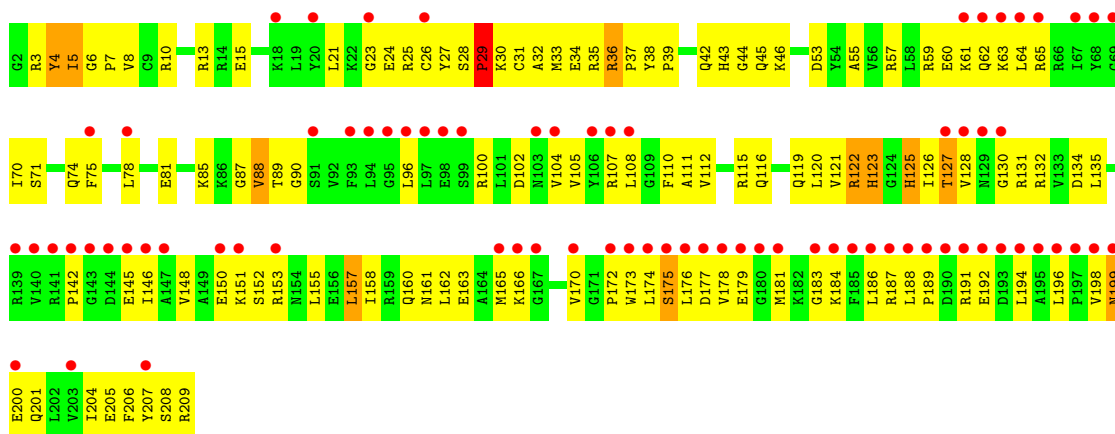
• Molecule 3: 30S ribosomal protein S3

Chain AC:



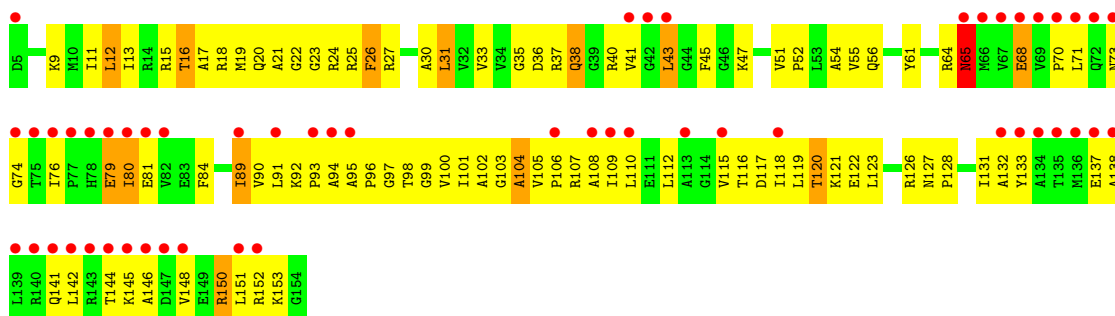
• Molecule 4: 30S ribosomal protein S4

Chain AD:



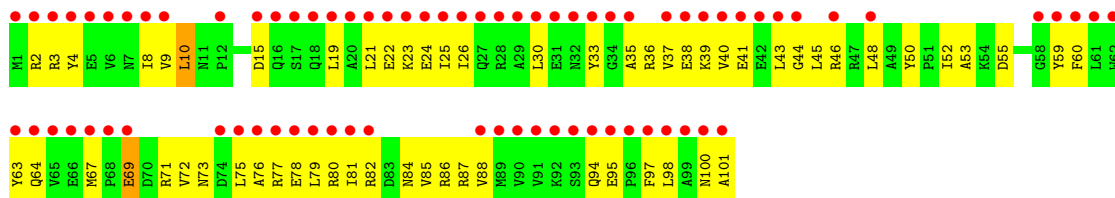
• Molecule 5: 30S ribosomal protein S5

Chain AE:



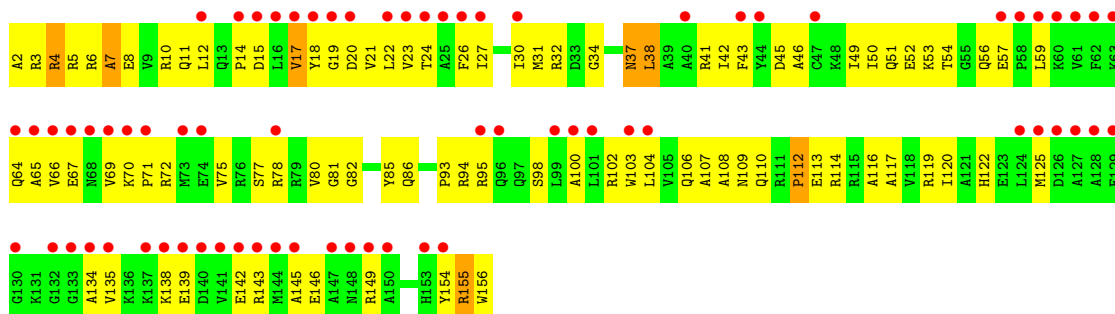
- Molecule 6: 30S ribosomal protein S6

Chain AF:



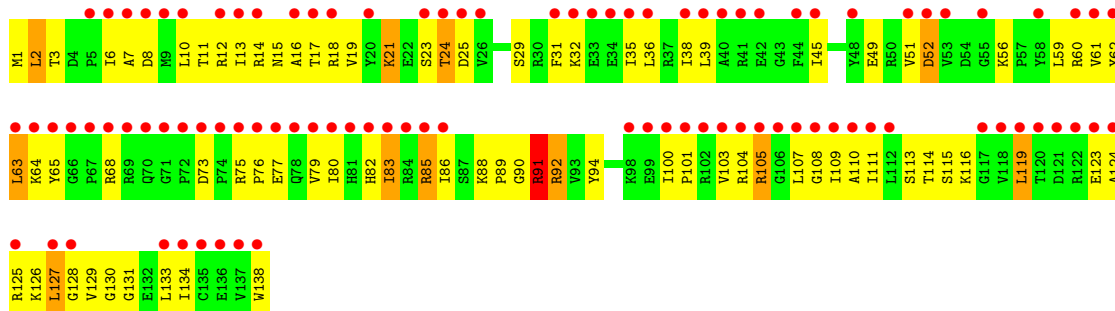
- Molecule 7: 30S ribosomal protein S7

Chain AG:



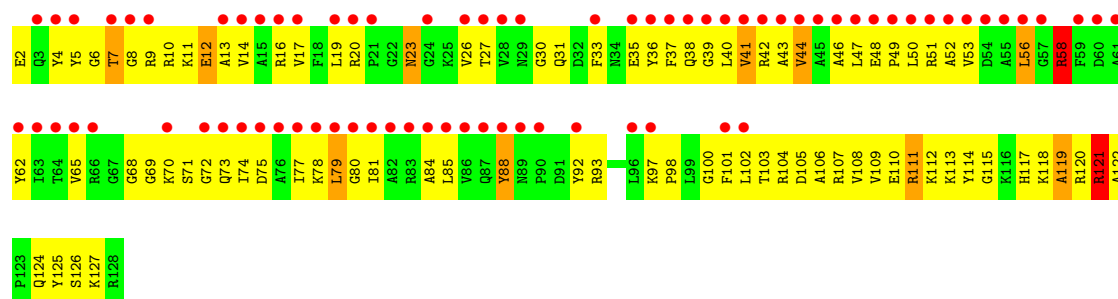
- Molecule 8: 30S ribosomal protein S8

Chain AH:



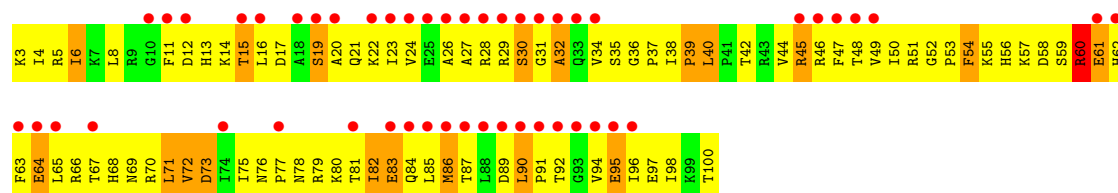
- Molecule 9: 30S ribosomal protein S9

Chain AI:



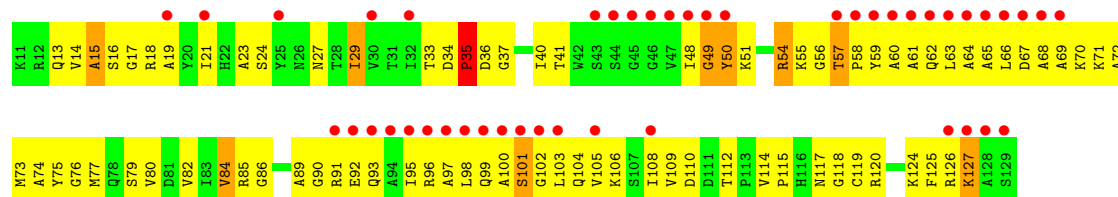
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



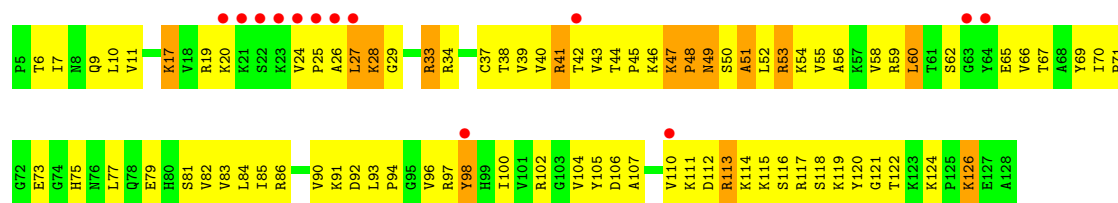
• Molecule 11: 30S ribosomal protein S11

Chain AK:



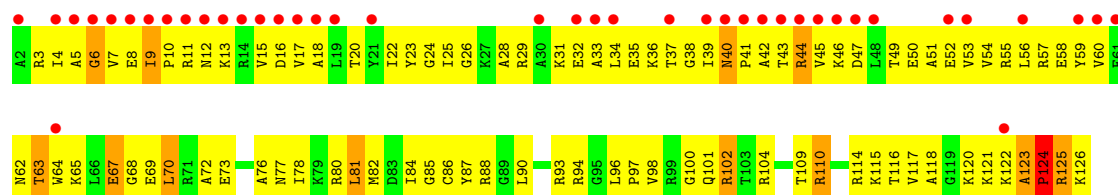
• Molecule 12: 30S ribosomal protein S12

Chain AL:



• Molecule 13: 30S ribosomal protein S13

Chain AM:



• Molecule 14: 30S ribosomal protein S14

Chain AN:





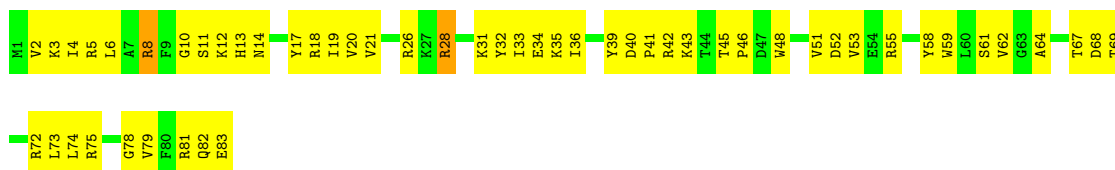
• Molecule 15: 30S ribosomal protein S15

Chain AO:



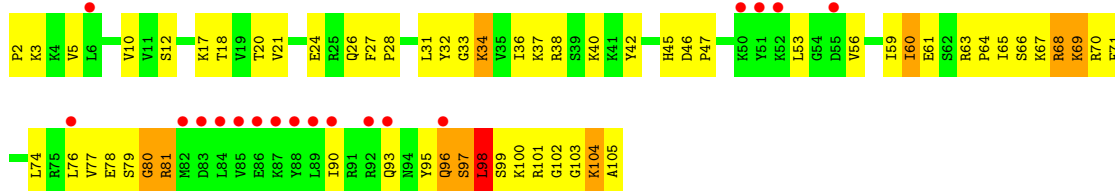
• Molecule 16: 30S ribosomal protein S16

Chain AP:



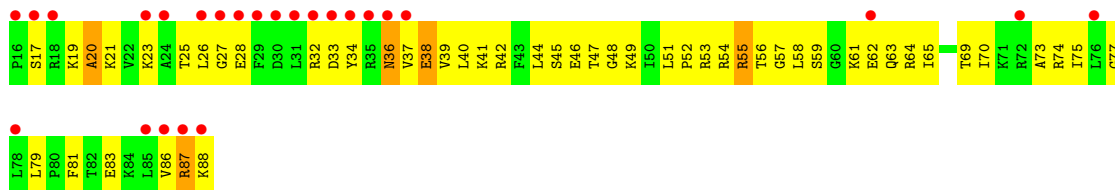
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



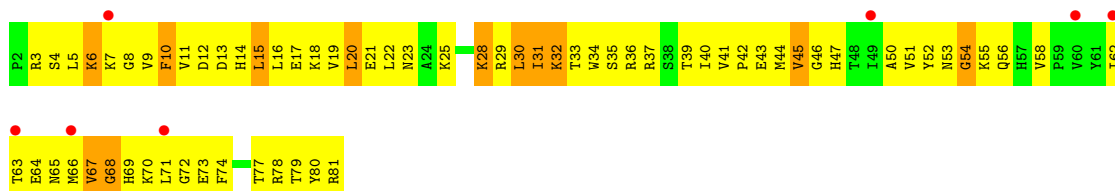
• Molecule 18: 30S ribosomal protein S18

Chain AR:



• Molecule 19: 30S ribosomal protein S19

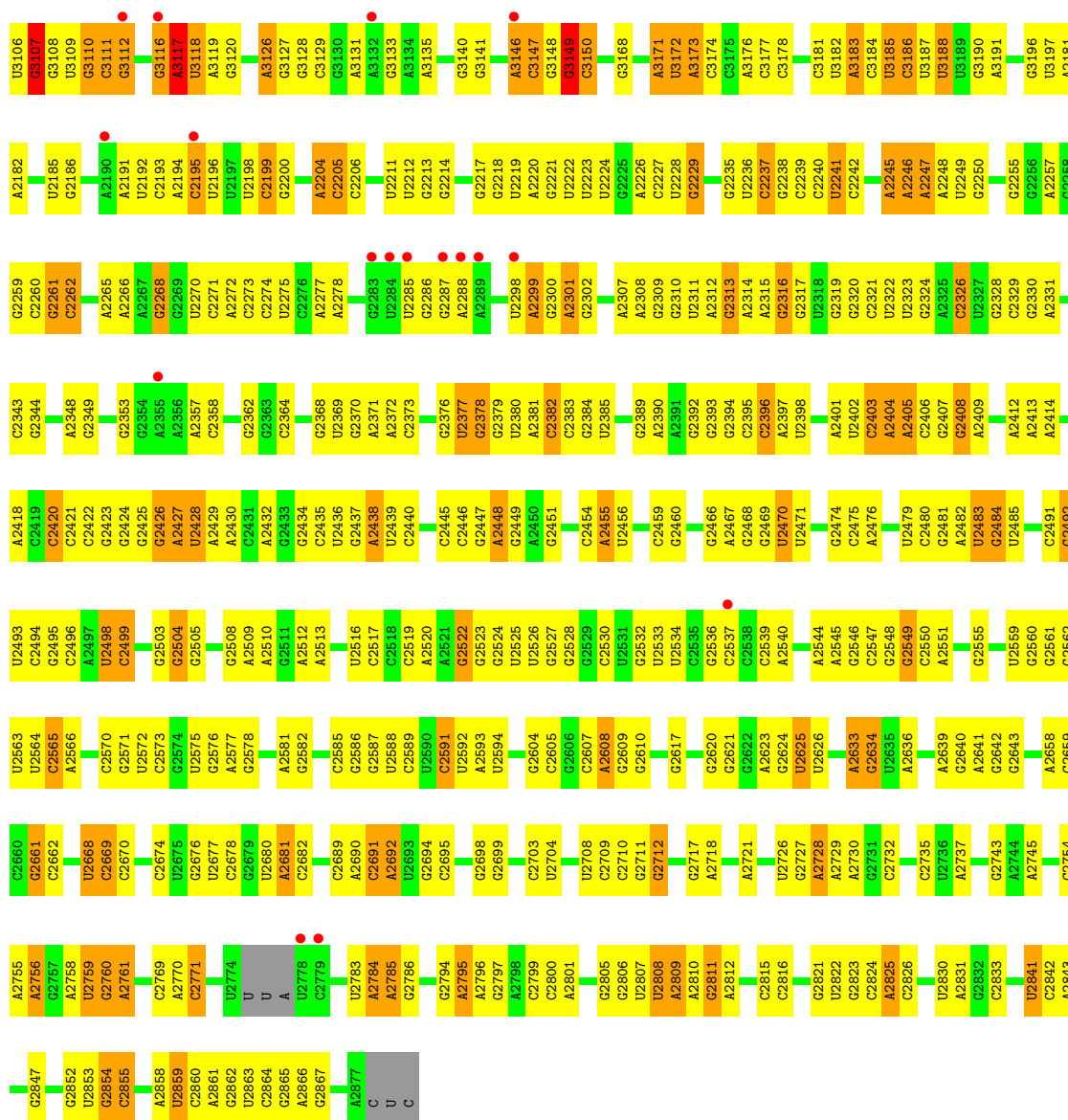
Chain AS:



- Chain AT:

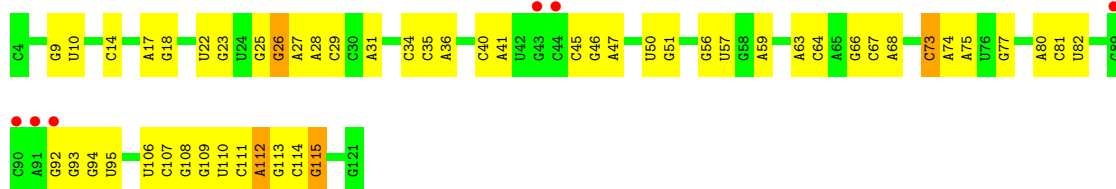






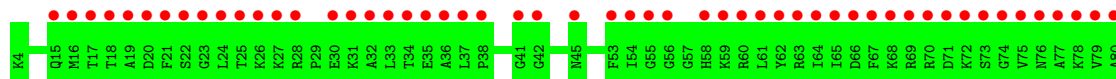
• Molecule 22: 5S RIBOSOMAL RNA

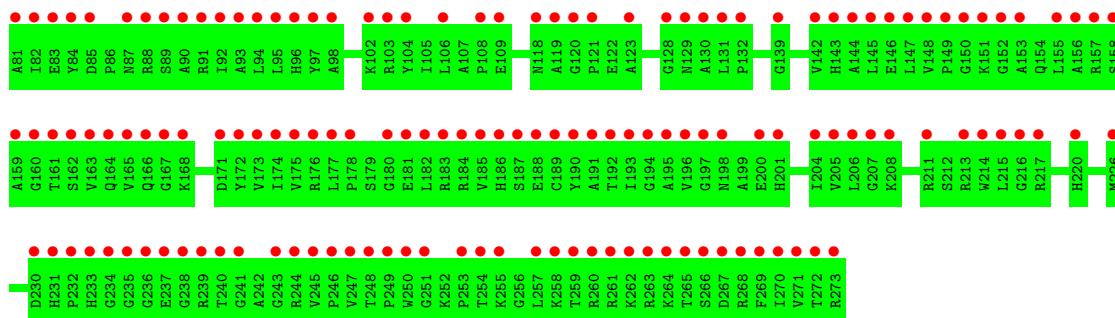
Chain B9:



• Molecule 23: 50S ribosomal protein L2

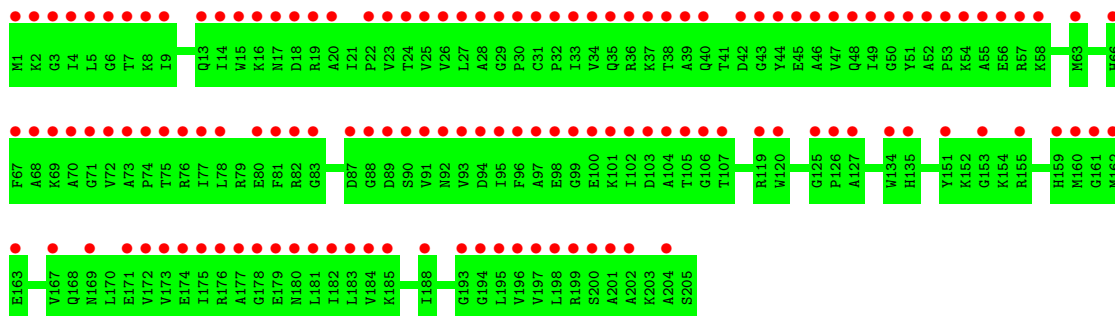
Chain BA:





• Molecule 24: 50S ribosomal protein L3

Chain BB:



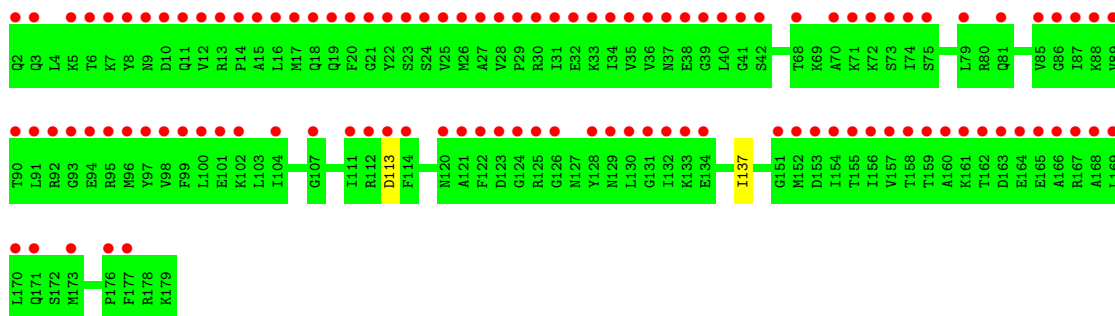
• Molecule 25: 50S ribosomal protein L4

Chain BC:



• Molecule 26: 50S ribosomal protein L5

Chain BD:



• Molecule 27: 50S ribosomal protein L6

The diagram illustrates a sequence of 100 numbered nodes, labeled G159 through G181, arranged in three rows. The nodes are connected by lines, forming a complex network structure. The top row contains nodes G159 to G173. The middle row contains nodes E28 to G181. The bottom row contains nodes G5 to G45. The nodes are connected in a way that suggests a hierarchical or sequential relationship, with some nodes having multiple connections.

- |    |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| H1 | Q2 | V3 | L4 | L5 | L6 | E7 | P8 | S9 | R10 | L11 | G12 | K13 | T14 | G15 | E16 | V17 | V18 | S19 | V20 | K21 | D22 | C23 | Y24 | A25 | R26 | T27 | N28 | L29 | L30 | F31 | Q32 | Q33 | G34 | L35 | A36 | S37 | S38 | A39 | T39 | R40 | R41 | N42 | M43 | K44 | T45 | L46 | E47 | E48 | R51 | R52 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- 
- | Item Type | Count |
|-----------|-------|
| E121      | 1     |
| E122      | 1     |
| A123      | 1     |
| A124      | 1     |
| N125      | 1     |
| T126      | 1     |
| V127      | 1     |
| A128      | 1     |
| G129      | 1     |
| T130      | 1     |
| A131      | 1     |
| E132      | 1     |
| S133      | 1     |
| M134      | 1     |
| G135      | 1     |
| P142      | 1     |
| N143      | 1     |
| W1        | 2     |
| L10       | 2     |
| V23       | 2     |
| G24       | 2     |
| P25       | 2     |
| A26       | 2     |
| L27       | 2     |
| G28       | 2     |
| A32       | 2     |
| N33       | 2     |
| L34       | 2     |
| M35       | 2     |
| E36       | 2     |
| F37       | 2     |
| T38       | 2     |
| K39       | 2     |
| A40       | 2     |
| F41       | 2     |
| N42       | 2     |
| A43       | 2     |
| Q44       | 2     |
| T45       | 2     |
| A46       | 2     |
| E52       | 2     |
| E53       | 2     |
| P54       | 2     |
| E55       | 2     |
| E56       | 2     |
| E59       | 2     |
| V60       | 2     |
| A61       | 2     |
| D62       | 2     |
| S63       | 2     |
| S64       | 2     |
| F65       | 2     |
| T66       | 2     |
| P67       | 2     |
| E68       | 2     |
| E69       | 2     |
| P72       | 2     |
| G87       | 2     |
| L105      | 2     |
| A108      | 2     |
| X111      | 2     |
| M112      | 2     |
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| G118      | 2     |
| S119      | 2     |
| V120      | 2     |

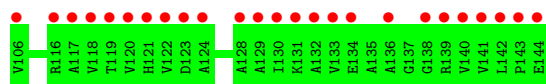
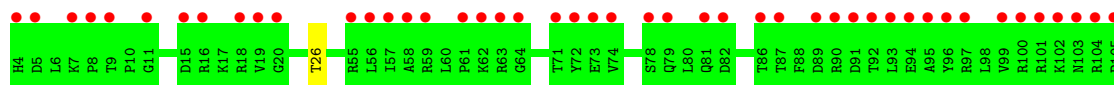
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| Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 | V131 | F132 | Q140 | G141 | R142 | A143 | M144 | H145 | T146 | R147 | L148 | K149 | V150 | L151 | A152 | G153 | E154 | F155 | H156 | P157 | H158 | S159 | A160 | Q161 | K162 | P163 | Q164 | V165 | L166 | L167 | T168 | Q169 | P170 | L171 | D97 | X98 | V99 | T100 | L101 | R102 | G105 | Y106 | E113 | T114 | A115 | R116 | E117 | A118 | L119 | S120 | K121 | H122 | P123 | E124 | R125 | V126 | L127 | E128 | H129 | A130 |
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- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| V69 | V70 | K71 | A72 | V73 | V74 | V75 | R76 | T77 | H79 | A80 | I81 | K82 | R83 | A84 | D85 | G86 | S87 | T88 | I89 | R90 | F91 | D92 | R93 | N94 | A95 | A96 | V97 | I98 | I99 | N100 | N101 | Q102 | G103 | E104 | P105 | R106 | G107 | T108 | R109 | V110 | F111 | G112 | P113 | V114 | A115 | R116 | E117 | L118 | R119 | D120 | R121 | R122 | F123 | M124 | K125 | I126 | V127 | F128 |
| I2  | M3  | P4  | Q5  | S6  | R7  | L8  | D9  | V10 | A11 | D12 | M13 | S14 | G15 | A16 | R17 | E18 | I19 | M20 | C21 | I22 | R23 | V24 | L25 | N26 | S27 | G28 | I29 | G30 | G33 | L34  | T35  | R43  | Y44  | A45  | R46  | V47  | G48  | D49  | I50  | I51  | V52  | A53  | S54  | V55  | K56  | D57  | A58  | P60  | R61  | G62  | A63  | V64  | A65  | G66  | G67  | R68  |      |      |



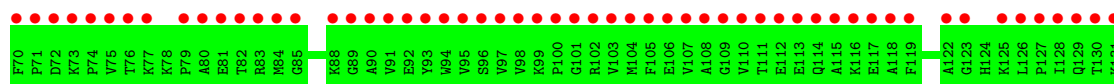
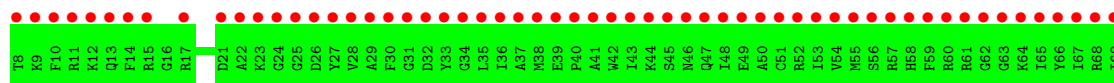
- Molecule 32: 50S ribosomal protein L15

Chain BJ:



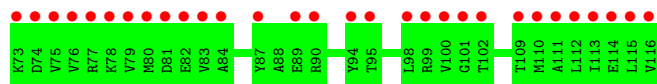
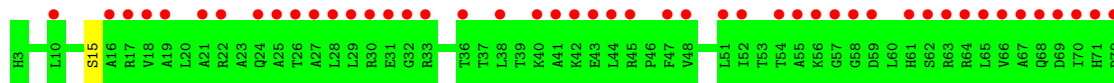
- Molecule 33: 50S ribosomal protein L16

Chain BK:



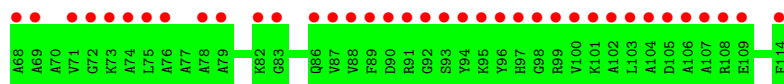
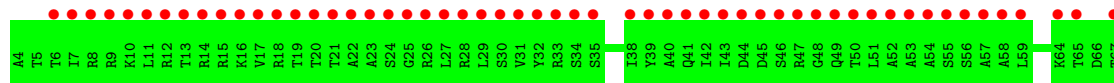
- Molecule 34: 50S ribosomal protein L17

Chain BL:



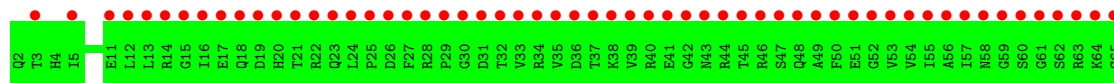
- Molecule 35: 50S ribosomal protein L18

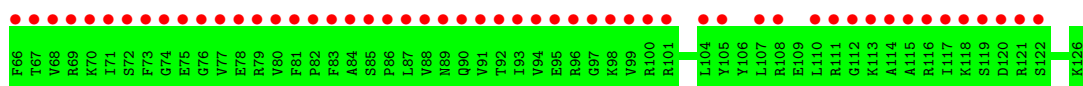
Chain BM:



- Molecule 36: 50S ribosomal protein L19

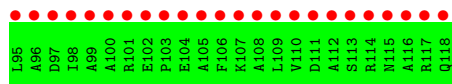
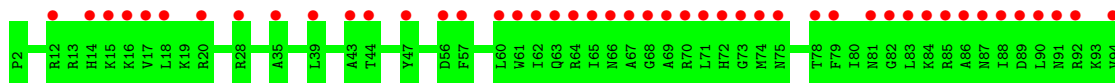
Chain BN:





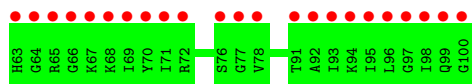
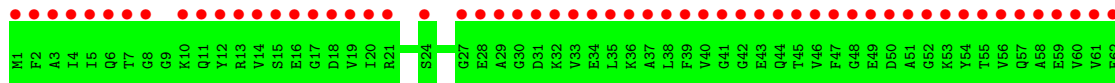
- Molecule 37: 50S ribosomal protein L20

Chain BO:



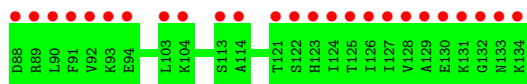
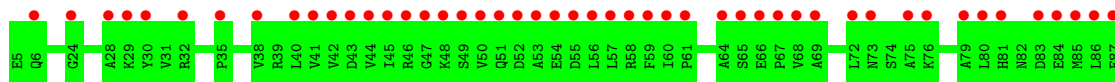
- Molecule 38: 50S ribosomal protein L21

Chain BP:



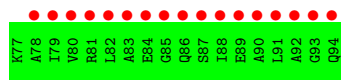
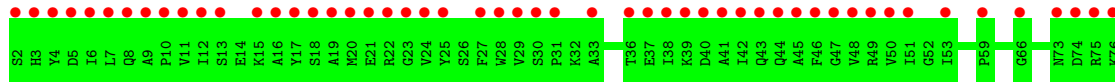
- Molecule 39: 50S ribosomal protein L22

Chain BQ:



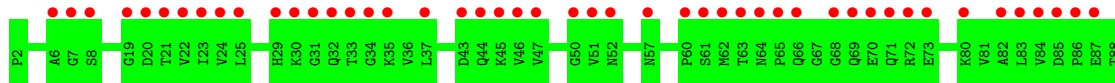
- Molecule 40: 50S ribosomal protein L23

Chain BR:

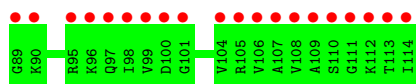


- Molecule 41: 50S ribosomal protein L24

Chain BS:

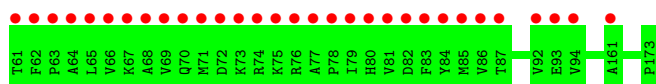
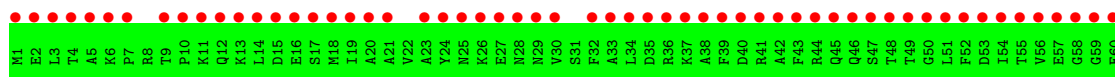






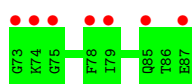
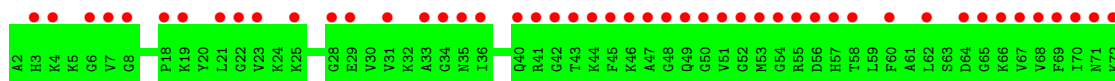
- Molecule 42: general stress protein Ctc

Chain BT:



- Molecule 43: 50S ribosomal protein L27

Chain BU:



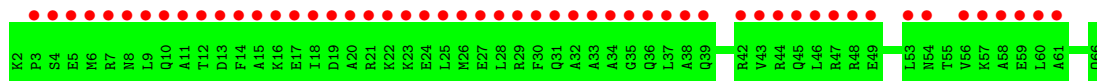
- Molecule 44: 50S RIBOSOMAL PROTEIN L28

Chain BV:

There are no outlier residues recorded for this chain.

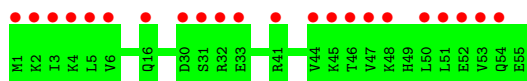
- Molecule 45: 50S ribosomal protein L29

Chain BW:



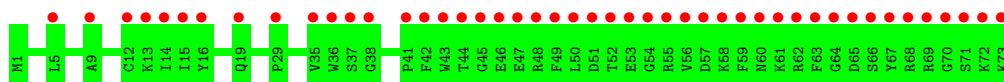
- Molecule 46: 50S ribosomal protein L30

Chain BX:



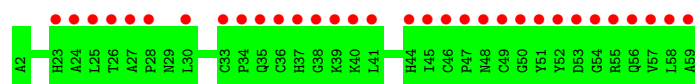
- Molecule 47: 50S ribosomal protein L31

Chain BY:



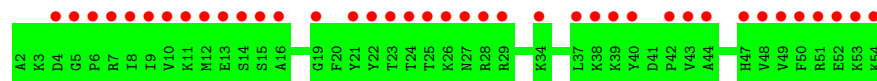
- Molecule 48: 50S ribosomal protein L32

Chain BZ:



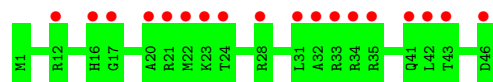
- Molecule 49: 50S ribosomal protein L33

Chain B1:



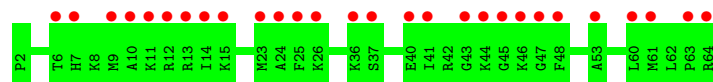
- Molecule 50: 50S ribosomal protein L34

Chain B2:



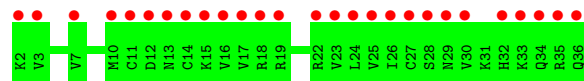
- Molecule 51: 50S ribosomal protein L35

Chain B3:



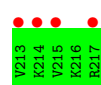
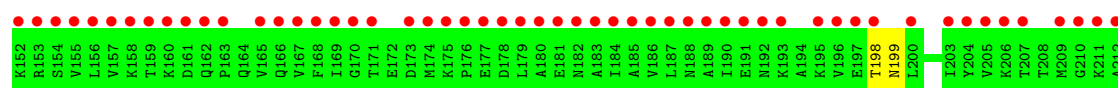
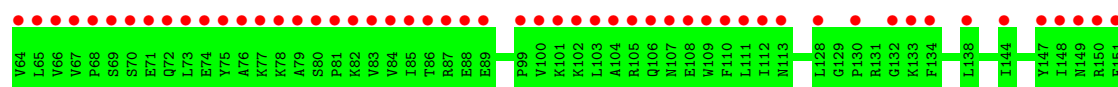
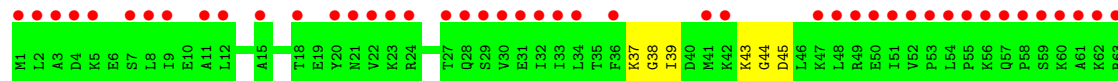
- Molecule 52: 50S ribosomal protein L36

Chain B4:



- Molecule 53: 50S ribosomal protein L1P

Chain B5:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	683.89Å 683.89Å 386.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 9.50 241.79 – 9.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (70.00-9.50) 87.2 (241.79-9.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.49 (at 9.99Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.389 , 0.407 0.369 , 0.386	Depositor DCC
$R_{free}$ test set	1209 reflections (4.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	437.2	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	-0.34 , 4859.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 26821 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	118711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	680.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	1.68	75/36823 (0.2%)	1.26	270/57351 (0.5%)
2	AB	0.37	0/1935	0.68	1/2609 (0.0%)
3	AC	0.38	0/1636	0.66	0/2205
4	AD	0.37	0/1732	0.63	0/2318
5	AE	0.49	0/1162	0.79	0/1564
6	AF	0.33	0/855	0.62	0/1154
7	AG	0.34	0/1275	0.62	0/1709
8	AH	0.44	0/1135	0.74	0/1527
9	AI	0.36	0/1028	0.62	0/1378
10	AJ	0.36	0/807	0.71	0/1085
11	AK	0.39	0/899	0.70	0/1213
12	AL	0.43	0/985	0.73	0/1317
13	AM	0.36	0/1006	0.67	0/1344
14	AN	0.40	0/500	0.78	0/664
15	AO	0.36	0/744	0.63	1/992 (0.1%)
16	AP	0.43	0/716	0.76	0/963
17	AQ	0.44	0/869	0.75	0/1159
18	AR	0.36	0/602	0.63	0/799
19	AS	0.35	0/661	0.72	1/890 (0.1%)
20	AT	0.39	0/764	0.73	0/1006
21	B0	0.50	17/67885 (0.0%)	0.75	48/105852 (0.0%)
22	B9	0.68	1/2815 (0.0%)	0.76	3/4384 (0.1%)
All	All	0.99	93/126834 (0.1%)	0.93	324/193483 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	2	40
21	B0	0	5
All	All	2	45

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	59	A	O3'-P	-120.85	0.16	1.61
1	AA	1398	A	O3'-P	-86.38	0.57	1.61
1	AA	214	U	O3'-P	-73.42	0.73	1.61
1	AA	394	G	O3'-P	-71.42	0.75	1.61
1	AA	1505	G	O3'-P	-71.04	0.76	1.61

The worst 5 of 324 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	59	A	P-O3'-C3'	-58.31	49.73	119.70
21	B0	1856	U	O3'-P-O5'	-48.57	11.72	104.00
21	B0	3098	U	P-O3'-C3'	42.71	170.95	119.70
1	AA	1490	C	P-O3'-C3'	40.44	168.23	119.70
1	AA	651	C	P-O3'-C3'	-39.22	72.64	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	181	G	C3'
1	AA	1528	U	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	187	G	Sidechain
1	AA	191	G	Sidechain
1	AA	197	A	Sidechain
1	AA	231	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32939	0	16652	3455	1
2	AB	1900	0	1951	209	0
3	AC	1612	0	1675	286	0
4	AD	1702	0	1767	217	2
5	AE	1146	0	1207	255	0
6	AF	842	0	855	75	2
7	AG	1256	0	1296	138	2
8	AH	1115	0	1177	126	0
9	AI	1010	0	1043	183	0
10	AJ	794	0	839	206	2
11	AK	884	0	904	81	0
12	AL	970	0	1056	151	0
13	AM	996	0	1068	184	0
14	AN	491	0	529	153	0
15	AO	733	0	770	57	0
16	AP	700	0	720	78	0
17	AQ	856	0	925	239	0
18	AR	596	0	668	77	0
19	AS	647	0	673	156	0
20	AT	762	0	853	286	0
21	B0	60636	0	30557	1717	1
22	B9	2519	0	1287	43	0
23	BA	270	0	0	0	0
24	BB	205	0	0	0	0
25	BC	197	0	0	0	0
26	BD	178	0	0	4	0
27	BE	177	0	0	0	0
28	BF	52	0	0	0	0
29	BG	143	0	0	1	0
30	BH	143	0	0	0	0
31	BI	132	0	0	2	0
32	BJ	141	0	0	1	0
33	BK	124	0	0	0	0
34	BL	114	0	0	1	0
35	BM	111	0	0	0	0
36	BN	125	0	0	0	0
37	BO	117	0	0	0	0
38	BP	100	0	0	0	0
39	BQ	130	0	0	0	0
40	BR	93	0	0	0	0
41	BS	113	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BT	173	0	0	0	0
43	BU	86	0	0	0	0
44	BV	16	0	0	0	0
45	BW	65	0	0	0	0
46	BX	55	0	0	0	0
47	BY	73	0	0	0	0
48	BZ	58	0	0	0	0
49	B1	53	0	0	0	0
50	B2	46	0	0	0	0
51	B3	63	0	0	0	0
52	B4	35	0	0	0	0
53	B5	217	0	0	22	0
All	All	118711	0	68472	6990	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 6990 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:1278:U:H5''	1:AA:1279:A:P	1.31	1.68
1:AA:1458:G:C8	1:AA:1459:C:H2'	1.27	1.63
1:AA:191:G:C6	1:AA:192:U:C2	1.90	1.60
1:AA:1475:G:H5''	21:B0:1706:A:C4'	1.13	1.60
1:AA:1475:G:C5'	21:B0:1706:A:H4'	1.32	1.59

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:AD:172:PRO:O	6:AF:15:ASP:CB[3.555]	1.83	0.37
1:AA:416:G:OP1	21:B0:3140:G:O2'[3.555]	1.99	0.21
7:AG:51:GLN:NE2	10:AJ:87:THR:OG1[4.555]	2.08	0.12
4:AD:186:LEU:CD1	6:AF:15:ASP:OD2[3.555]	2.14	0.06
7:AG:57:GLU:OE2	10:AJ:89:ASP:OD1[4.555]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	174 (75%)	34 (15%)	24 (10%)	1	19
3	AC	204/206 (99%)	135 (66%)	40 (20%)	29 (14%)	0	11
4	AD	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	4	47
5	AE	148/150 (99%)	130 (88%)	13 (9%)	5 (3%)	6	55
6	AF	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	22	80
7	AG	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	2	35
8	AH	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	7	58
9	AI	125/127 (98%)	88 (70%)	27 (22%)	10 (8%)	1	28
10	AJ	96/98 (98%)	59 (62%)	20 (21%)	17 (18%)	0	6
11	AK	117/119 (98%)	88 (75%)	20 (17%)	9 (8%)	1	29
12	AL	120/124 (97%)	96 (80%)	15 (12%)	9 (8%)	2	30
13	AM	121/125 (97%)	87 (72%)	26 (22%)	8 (7%)	2	35
14	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	1	14
15	AO	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	3	38
16	AP	81/83 (98%)	65 (80%)	15 (18%)	1 (1%)	19	77
17	AQ	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	29
18	AR	71/73 (97%)	62 (87%)	7 (10%)	2 (3%)	8	59
19	AS	78/80 (98%)	48 (62%)	19 (24%)	11 (14%)	0	11
20	AT	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	1	14
All	All	2330/2372 (98%)	1788 (77%)	361 (16%)	181 (8%)	1	29

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/202 (100%)	180 (89%)	22 (11%)	9	46
3	AC	160/160 (100%)	142 (89%)	18 (11%)	9	43
4	AD	180/180 (100%)	172 (96%)	8 (4%)	39	82
5	AE	115/115 (100%)	100 (87%)	15 (13%)	6	36
6	AF	90/90 (100%)	88 (98%)	2 (2%)	64	91
7	AG	126/126 (100%)	122 (97%)	4 (3%)	51	87
8	AH	119/119 (100%)	109 (92%)	10 (8%)	16	60
9	AI	98/98 (100%)	90 (92%)	8 (8%)	17	61
10	AJ	88/88 (100%)	79 (90%)	9 (10%)	11	49
11	AK	90/90 (100%)	84 (93%)	6 (7%)	23	70
12	AL	104/104 (100%)	96 (92%)	8 (8%)	18	64
13	AM	100/100 (100%)	90 (90%)	10 (10%)	11	50
14	AN	49/49 (100%)	47 (96%)	2 (4%)	41	83
15	AO	79/79 (100%)	72 (91%)	7 (9%)	14	57
16	AP	72/72 (100%)	67 (93%)	5 (7%)	22	68
17	AQ	96/96 (100%)	90 (94%)	6 (6%)	25	72
18	AR	64/64 (100%)	61 (95%)	3 (5%)	36	80
19	AS	71/71 (100%)	68 (96%)	3 (4%)	40	82
20	AT	76/76 (100%)	69 (91%)	7 (9%)	13	55
All	All	1979/1979 (100%)	1826 (92%)	153 (8%)	18	64

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	AH	2	LEU
9	AI	111	ARG
18	AR	38	GLU
8	AH	52	ASP
8	AH	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
6	AF	64	GLN
9	AI	23	ASN
18	AR	36	ASN
6	AF	94	GLN
7	AG	37	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1487/1537 (96%)	218 (14%)	89 (5%)
21	B0	2802/2887 (97%)	430 (15%)	55 (1%)
22	B9	116/118 (98%)	10 (8%)	0
All	All	4405/4542 (96%)	658 (14%)	144 (3%)

5 of 658 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1196	U
1	AA	1380	U
21	B0	3171	A
1	AA	1214	C
1	AA	1300	G

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	82
21	B0	26
22	B9	2
12	AL	1
13	AM	1

The worst 5 of 112 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1443:G	O3'	1445:U	P	9.14
1	AA	1458:G	O3'	1459:C	P	8.01
1	B0	1888:C	O3'	1889:G	P	6.96
1	AA	1459:C	O3'	1460:A	P	6.03
1	B0	3180:U	O3'	3181:C	P	5.42

## 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	1533/1537 (99%)	0.23	94 (6%) 21 26	207, 548, 819, 940	0
2	AB	234/234 (100%)	2.55	138 (58%) 0 4	754, 754, 754, 754	0
3	AC	206/206 (100%)	1.76	65 (31%) 1 5	378, 378, 378, 378	0
4	AD	208/208 (100%)	1.61	77 (37%) 1 5	709, 709, 709, 709	0
5	AE	150/150 (100%)	1.77	53 (35%) 1 5	756, 756, 756, 756	0
6	AF	101/101 (100%)	3.20	76 (75%) 0 3	748, 748, 748, 748	0
7	AG	155/155 (100%)	2.19	70 (45%) 1 4	374, 374, 374, 374	0
8	AH	138/138 (100%)	3.51	95 (68%) 0 4	856, 856, 856, 856	0
9	AI	127/127 (100%)	2.64	76 (59%) 0 4	439, 439, 439, 439	0
10	AJ	98/98 (100%)	2.37	49 (50%) 0 4	430, 430, 430, 430	0
11	AK	119/119 (100%)	2.04	45 (37%) 1 4	652, 652, 652, 652	0
12	AL	124/124 (100%)	0.74	13 (10%) 7 15	423, 541, 541, 541	0
13	AM	125/125 (100%)	1.51	41 (32%) 1 5	378, 572, 572, 572	0
14	AN	60/60 (100%)	1.33	15 (25%) 1 6	378, 378, 378, 378	0
15	AO	88/88 (100%)	0.94	4 (4%) 32 33	740, 740, 740, 740	0
16	AP	83/83 (100%)	-0.09	0 100 100	781, 781, 781, 781	0
17	AQ	104/104 (100%)	1.10	18 (17%) 2 8	857, 857, 857, 857	0
18	AR	73/73 (100%)	1.70	25 (34%) 1 5	748, 748, 748, 748	0
19	AS	80/80 (100%)	0.63	7 (8%) 10 19	633, 633, 633, 633	0
20	AT	99/99 (100%)	1.08	14 (14%) 3 10	940, 940, 940, 940	0
21	B0	2825/2887 (97%)	-0.32	100 (3%) 42 39	462, 737, 737, 940	0
22	B9	118/118 (100%)	-0.06	6 (5%) 27 30	772, 938, 938, 938	0
23	BA	270/270 (100%)	5.47	196 (72%) 0 3	737, 737, 737, 737	0
24	BB	205/205 (100%)	4.25	136 (66%) 0 4	737, 737, 737, 737	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BC	197/197 (100%)	2.55	129 (65%) 0 4	737, 737, 737, 737	0
26	BD	178/178 (100%)	5.92	111 (62%) 0 4	938, 938, 938, 938	0
27	BE	177/177 (100%)	4.68	110 (62%) 0 4	737, 737, 737, 737	0
28	BF	52/52 (100%)	5.66	43 (82%) 0 3	737, 737, 737, 737	0
29	BG	143/143 (100%)	2.50	59 (41%) 1 4	907, 907, 907, 907	0
30	BH	143/143 (100%)	4.35	113 (79%) 0 3	737, 737, 737, 737	0
31	BI	132/132 (100%)	7.07	118 (89%) 0 2	737, 737, 737, 737	0
32	BJ	141/141 (100%)	2.63	71 (50%) 0 4	737, 737, 737, 737	0
33	BK	124/124 (100%)	9.13	114 (91%) 0 2	737, 737, 737, 737	0
34	BL	114/114 (100%)	3.43	77 (67%) 0 4	737, 737, 737, 737	0
35	BM	111/111 (100%)	6.72	92 (82%) 0 3	938, 938, 938, 938	0
36	BN	125/125 (100%)	7.36	110 (88%) 0 3	737, 737, 737, 737	0
37	BO	117/117 (100%)	3.04	70 (59%) 0 4	737, 737, 737, 737	0
38	BP	100/100 (100%)	3.46	80 (80%) 0 3	737, 737, 737, 737	0
39	BQ	130/130 (100%)	2.66	73 (56%) 0 4	737, 737, 737, 737	0
40	BR	93/93 (100%)	3.98	69 (74%) 0 3	737, 737, 737, 737	0
41	BS	113/113 (100%)	2.24	67 (59%) 0 4	737, 737, 737, 737	0
42	BT	173/173 (100%)	4.75	88 (50%) 0 4	737, 772, 772, 772	0
43	BU	86/86 (100%)	4.10	55 (63%) 0 4	737, 737, 737, 737	0
44	BV	0/16	-	-	-	-
45	BW	65/65 (100%)	3.72	53 (81%) 0 3	737, 737, 737, 737	0
46	BX	55/55 (100%)	3.06	22 (40%) 1 4	737, 737, 737, 737	0
47	BY	73/73 (100%)	4.16	46 (63%) 0 4	737, 737, 737, 737	0
48	BZ	58/58 (100%)	3.10	32 (55%) 0 4	737, 737, 737, 737	0
49	B1	53/53 (100%)	5.34	39 (73%) 0 3	737, 737, 737, 737	0
50	B2	46/46 (100%)	1.87	18 (39%) 1 4	737, 737, 737, 737	0
51	B3	63/63 (100%)	2.36	28 (44%) 1 4	737, 737, 737, 737	0
52	B4	35/35 (100%)	4.74	27 (77%) 0 3	737, 737, 737, 737	0
53	B5	217/217 (100%)	6.13	156 (71%) 0 3	940, 940, 940, 940	0
All	All	10437/10519 (99%)	1.92	3483 (33%) 1 5	207, 737, 938, 940	0

The worst 5 of 3483 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	BD	17	MET	31.7
26	BD	167	ARG	28.1
26	BD	165	GLU	27.5
26	BD	13	ARG	27.3
53	B5	81	PRO	26.6

## 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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.