wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:24 PM GMT

PDB ID	:	4V4S
Title	:	Crystal structure of the whole ribosomal complex.
Authors	:	Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2005-10-12
Resolution	:	6.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

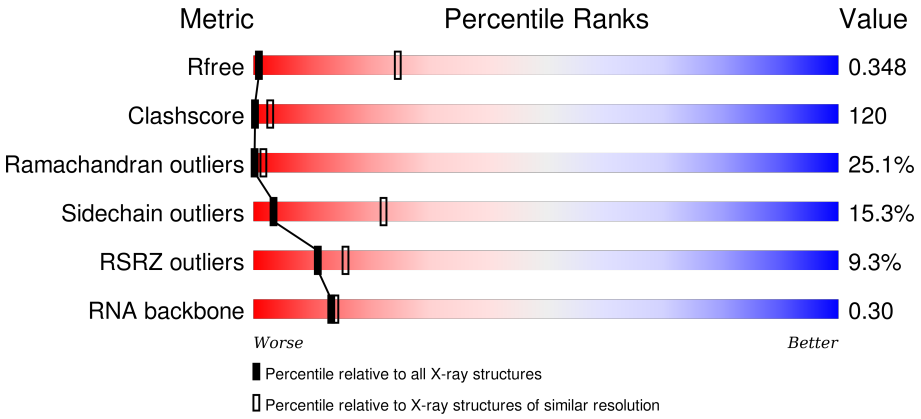
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.76 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)
RNA backbone	2183	1105 (10.00-2.80)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	1522	12% 25% 42% 24% 9%
2	AV	76	12% 16% 59% 22% .
3	AW	76	29% 30% 47% 16% 7%
4	AX	18	72% 61% 33% 6%

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Mol	Chain	Length	Quality of chain
5	AB	256	2% 44% 39% 7% 9%
6	AC	239	10% 48% 29% 8% 14%
7	AD	209	9% 36% 52% 11%
8	AE	162	9% 48% 35% 10% 7%
9	AF	101	7% 66% 29%
10	AG	156	10% 60% 35%
11	AH	138	8% 38% 47% 14%
12	AI	128	20% 50% 41% 7%
13	AJ	105	19% 42% 40% 11% 7%
14	AK	129	2% 50% 40% 8%
15	AL	135	13% 39% 45% 7% 8%
16	AM	126	16% 50% 40% 9%
17	AN	61	13% 34% 56% 8%
18	AO	89	17% 63% 29% 7%
19	AP	88	24% 44% 35% 13% 6%
20	AQ	105	7% 40% 51% 7%
21	AR	88	13% 41% 33% 9% 17%
22	AS	93	20% 39% 43% 14%
23	AT	106	11% 49% 38% 7% 7%
24	AU	27	11% 30% 52% 7% 11%
25	AY	365	21% 98%
26	BB	123	2% 28% 45% 24%
27	BA	2916	5% 11% 34% 38% 13%
28	BD	173	5% 44% 46% 9%
29	BE	338	5% 30% 20% 43%

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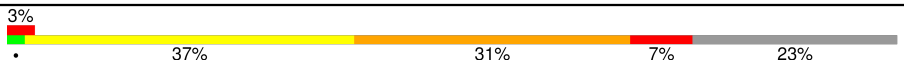
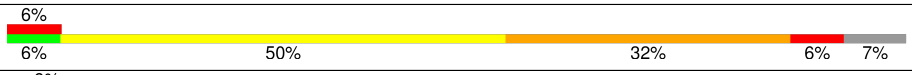
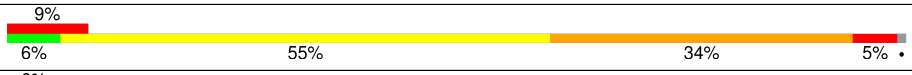
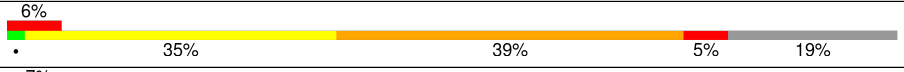
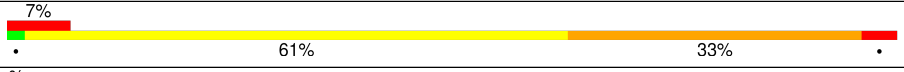
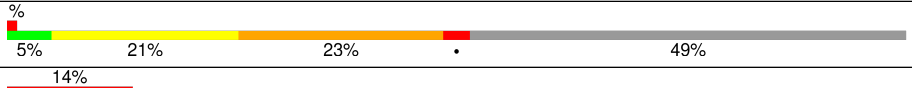
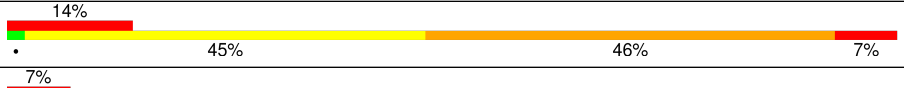
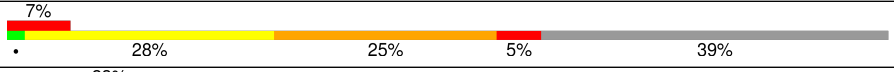
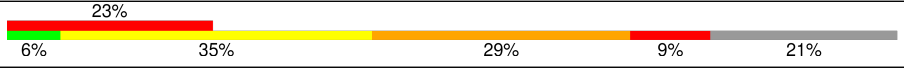
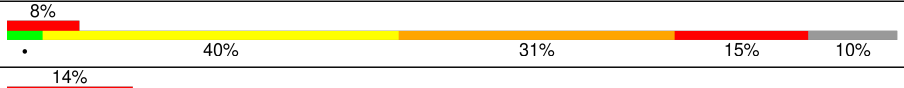
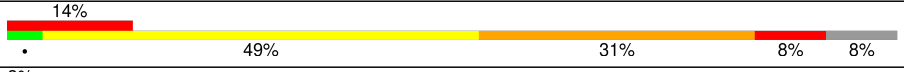
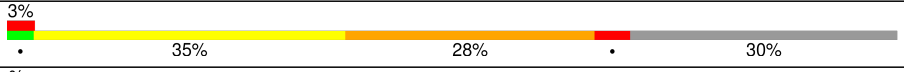
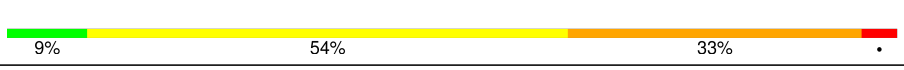
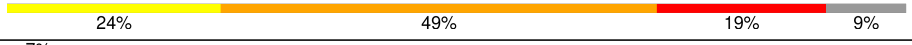
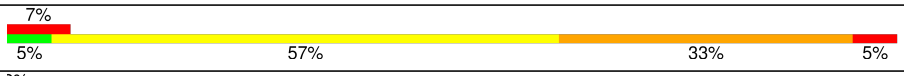
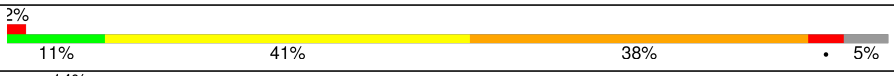
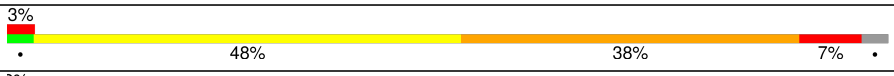
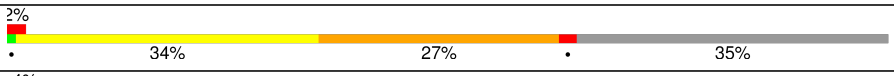
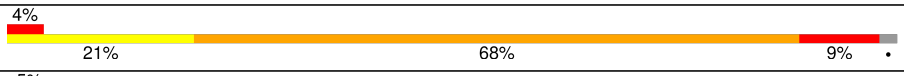
Mol	Chain	Length	Quality of chain
30	BF	246	
31	BG	176	
32	BH	177	
33	BI	149	
34	BN	145	
35	BO	122	
36	BP	164	
37	BQ	138	
38	BS	186	
39	BT	66	
40	BW	113	
41	BX	84	
42	BY	119	
43	BZ	253	
44	BR	118	
45	BU	118	
46	BV	100	
47	B2	70	
48	B3	60	
49	B0	91	
50	B4	73	
51	B5	60	
52	B6	82	
53	B7	47	
54	B8	64	

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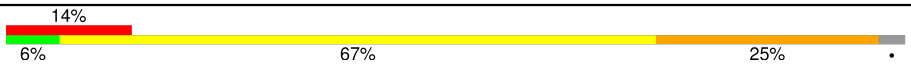
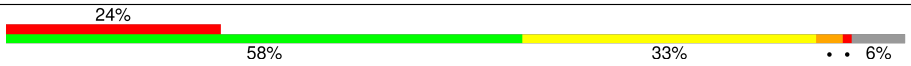
Mol	Chain	Length	Quality of chain
55	B9	36	
56	BK	141	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	YYG	AW	37	X	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1515	32551	14490	6022	10525	1514	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	416	G	-	INSERTION	GB 155076
AA	905	U	-	INSERTION	GB 155076
AA	1395	C	-	INSERTION	GB 155076

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AV	76	1622	725	293	529	75	0	0	0

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AW	76	1638	736	294	533	75	0	0	0

- Molecule 4 is a RNA chain called 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*AP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	AX	17	136	56	19	44	17	0	0	11

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AR	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 25 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	AY	365	Total	C	0	0	365
			365	365			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	123	Total	C	N	O	P	0	0	0
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2814	Total	C	N	O	P	0	0	0
			60599	26974	11331	19482	2812			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	INSERTION	GB 48268

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BP	84	Total	C	N	O	0	0	0
			639	391	109	139			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BW	108	Total	C	N	O	0	0	0
			860	542	169	149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 42 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BY	110	Total	C	N	O	0	0	0
			879	531	166	182			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 44 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BR	105	Total	C	N	O	0	0	0
			855	536	174	145			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BU	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

- Molecule 56 is a protein called 50S ribosomal protein L11.

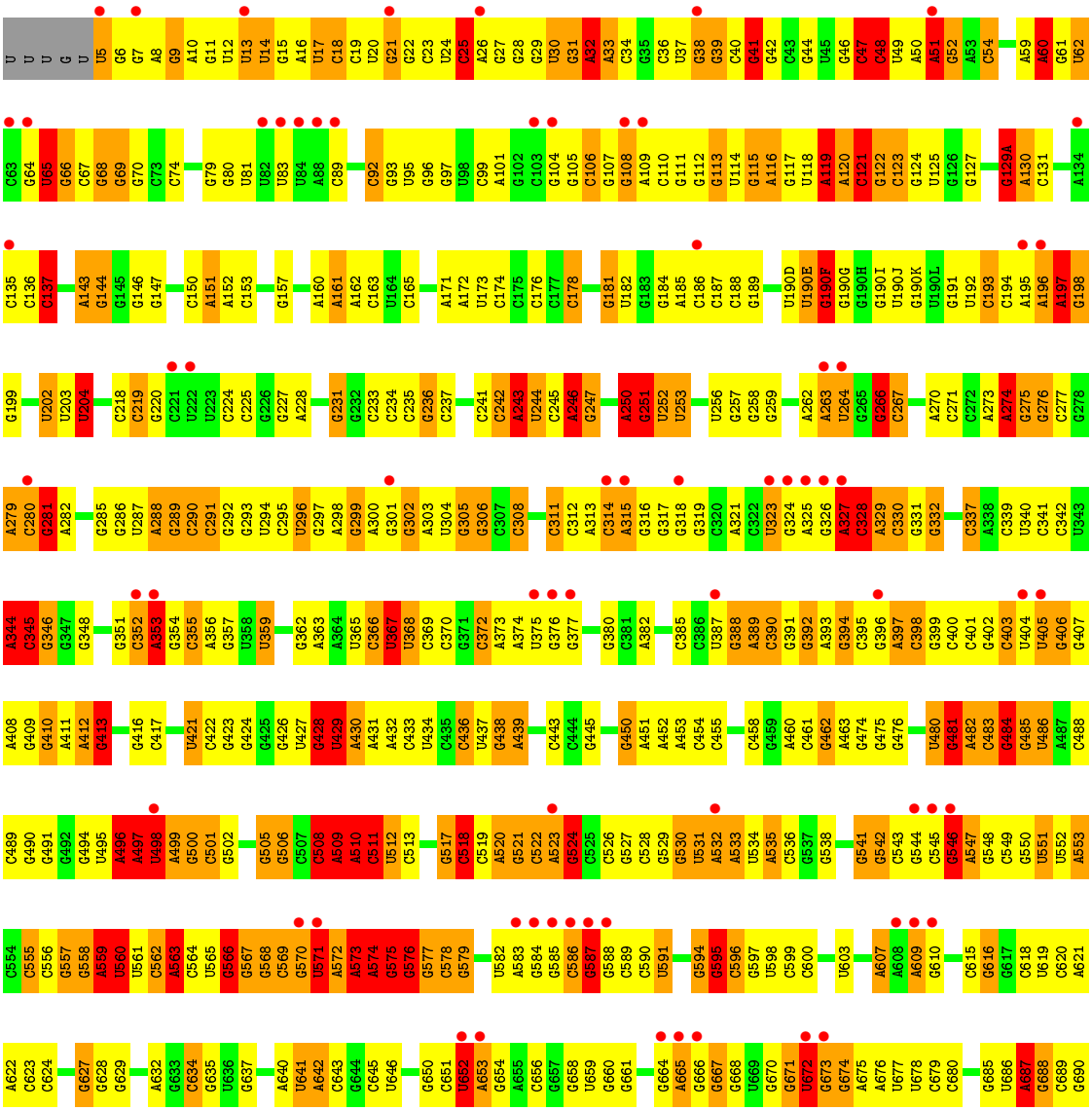
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

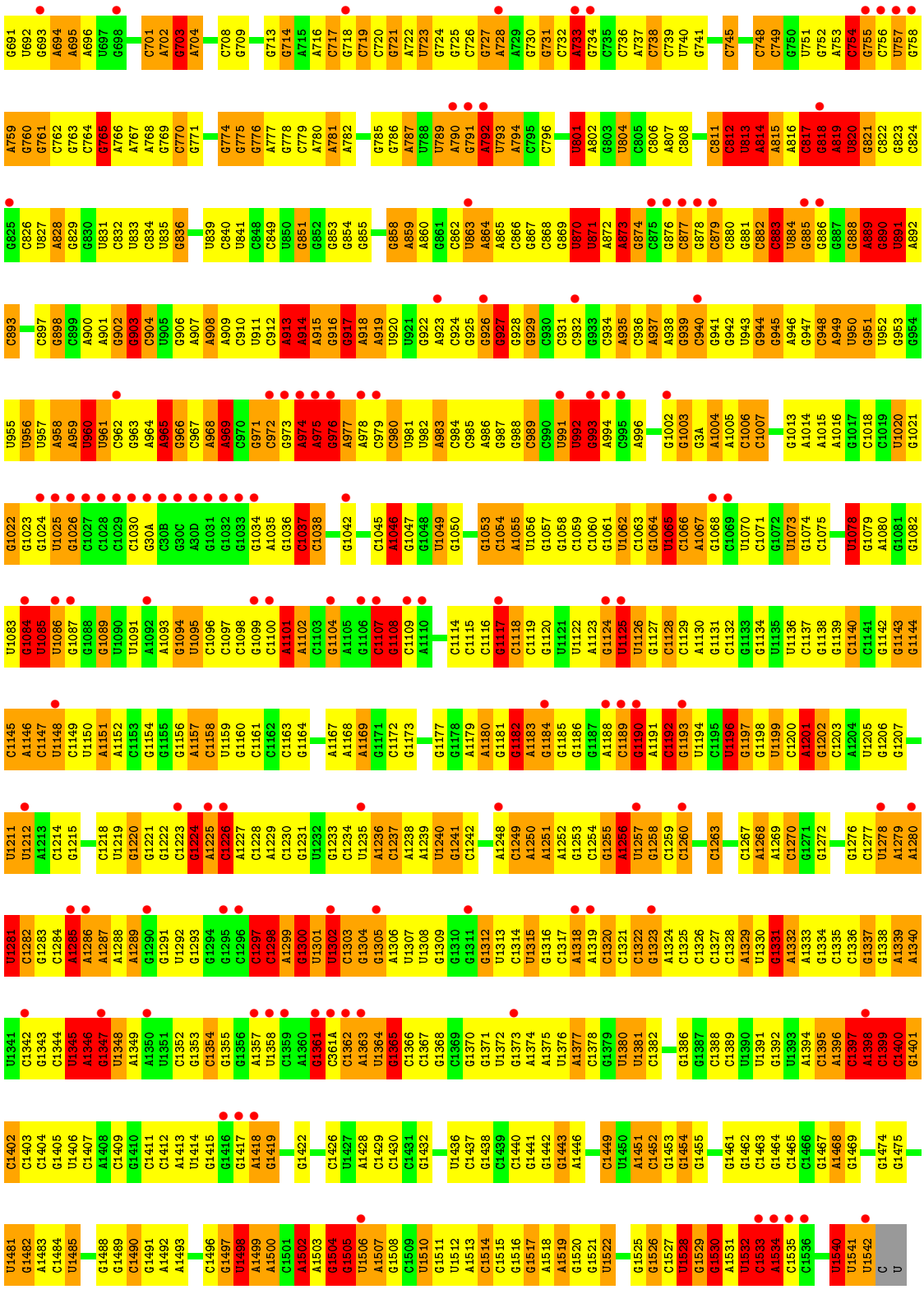
3 Residue-property plots (i)

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.

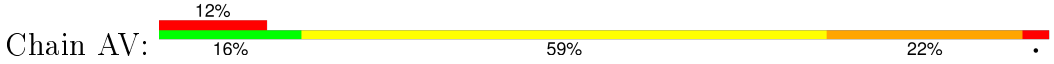
- Molecule 1: 16S ribosomal RNA

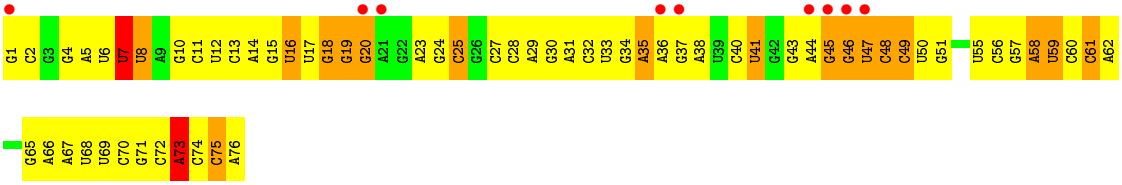
Chain AA: 12% 25% 42% 24% 9%





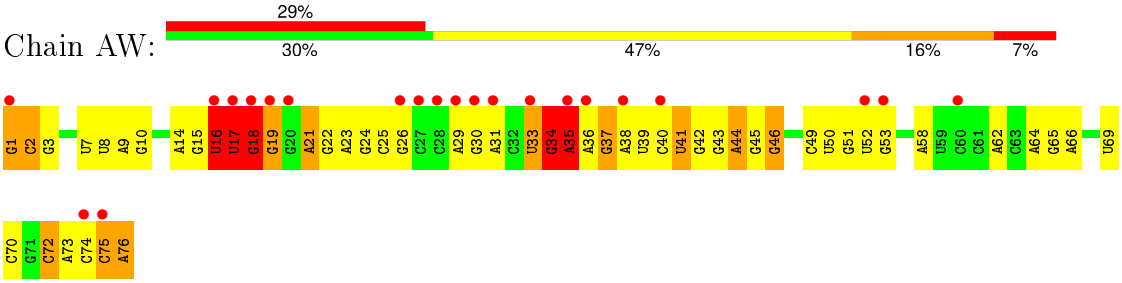
- Molecule 2: P-site tRNA (Phe)





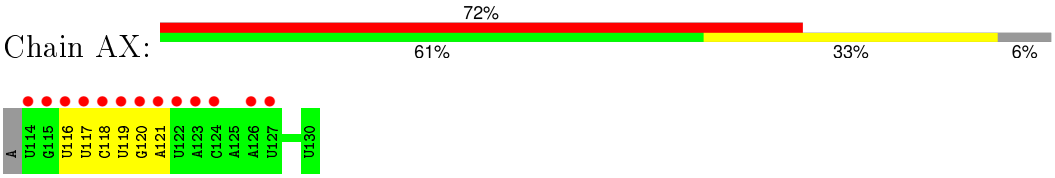
• Molecule 3: E-site tRNA (Phe)

Chain AW:



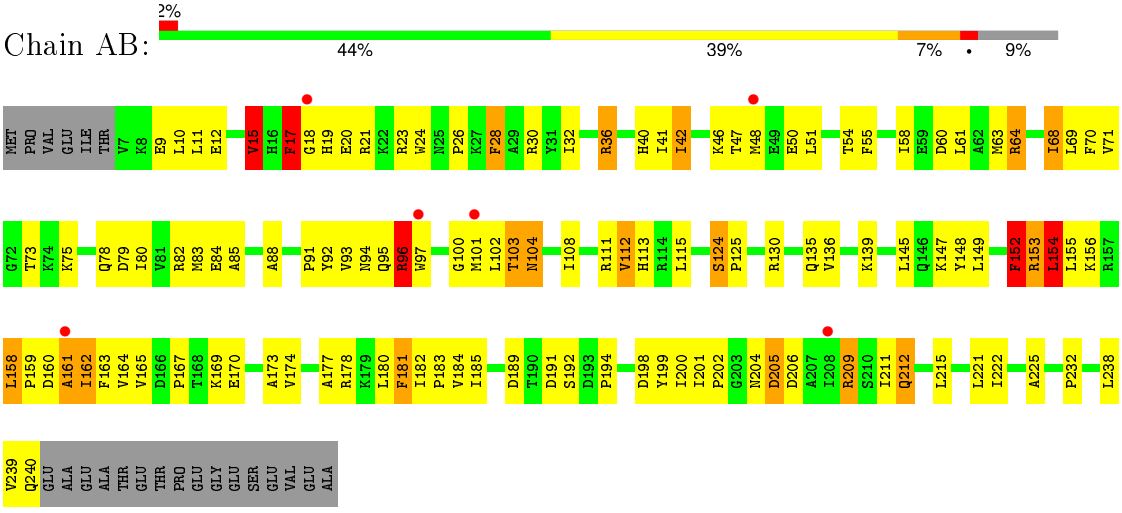
• Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*AP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

Chain AX:



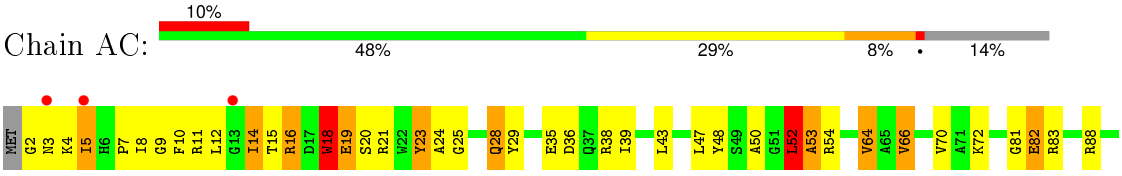
• Molecule 5: 30S ribosomal protein S2

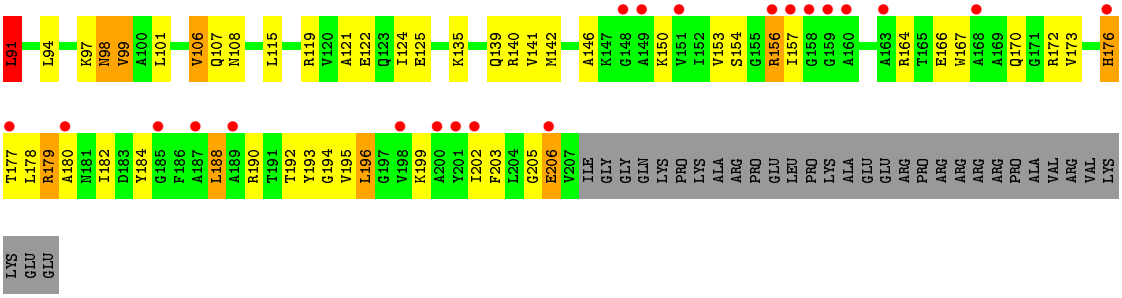
Chain AB:

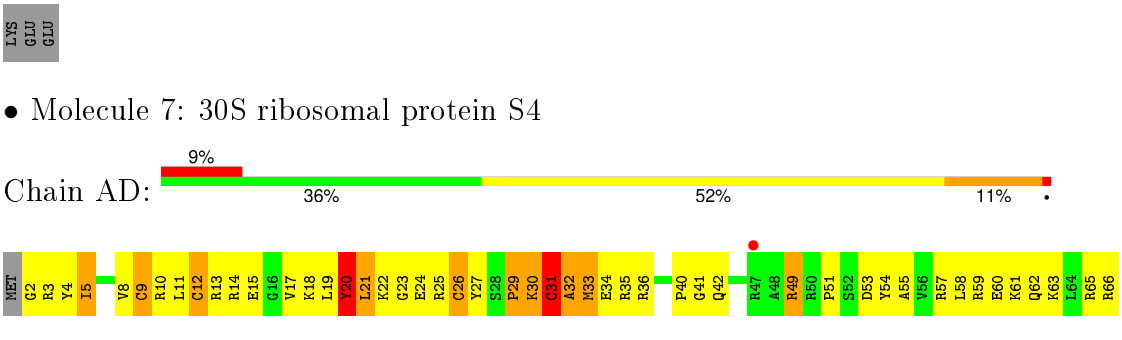


• Molecule 6: 30S ribosomal protein S3

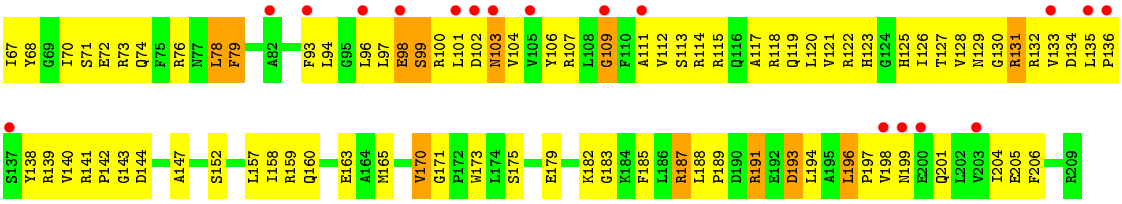
Chain AC:



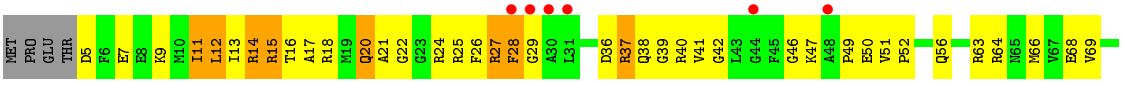


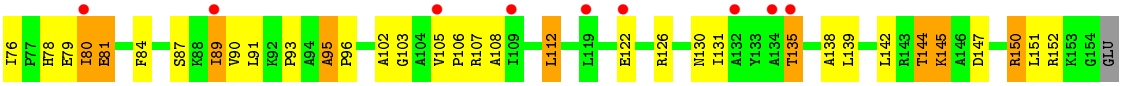


• Molecule 7: 30S ribosomal protein S4

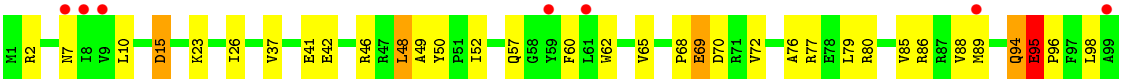


• Molecule 8: 30S ribosomal protein S5

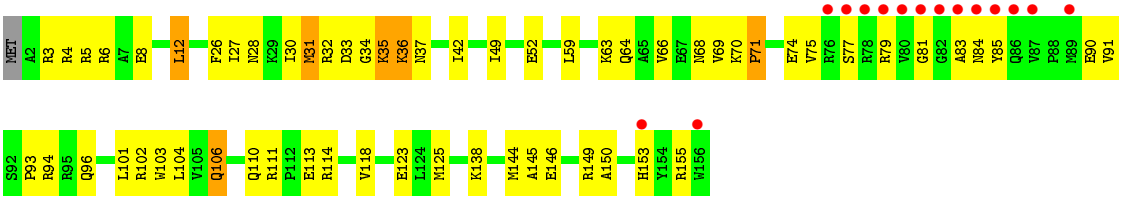




• Molecule 9: 30S ribosomal protein S6

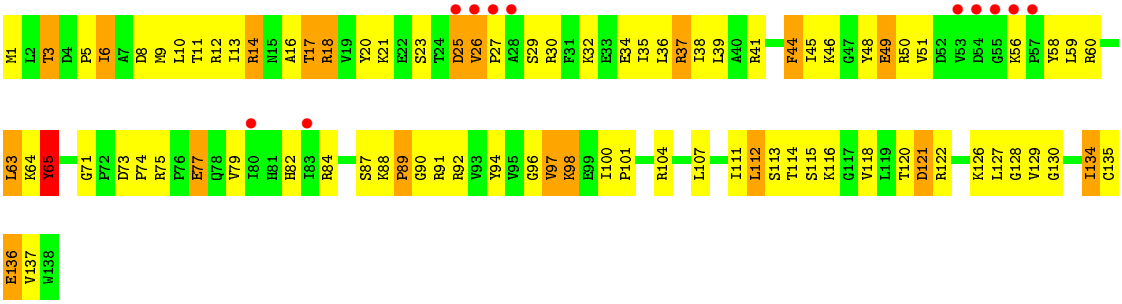


• Molecule 10: 30S ribosomal protein S7



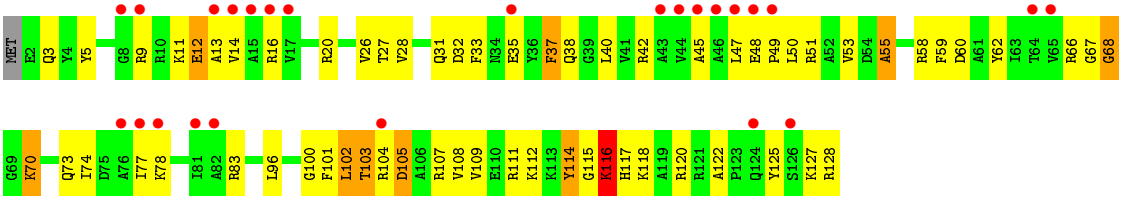
• Molecule 11: 30S ribosomal protein S8

Chain AH:



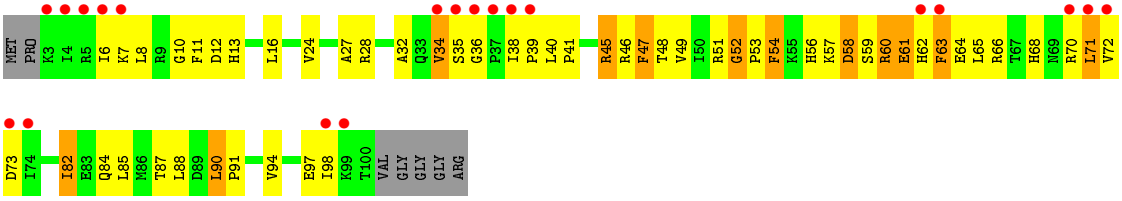
• Molecule 12: 30S ribosomal protein S9

Chain AI:



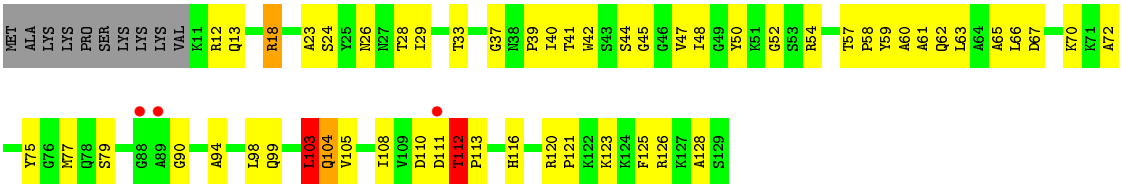
• Molecule 13: 30S ribosomal protein S10

Chain AJ:



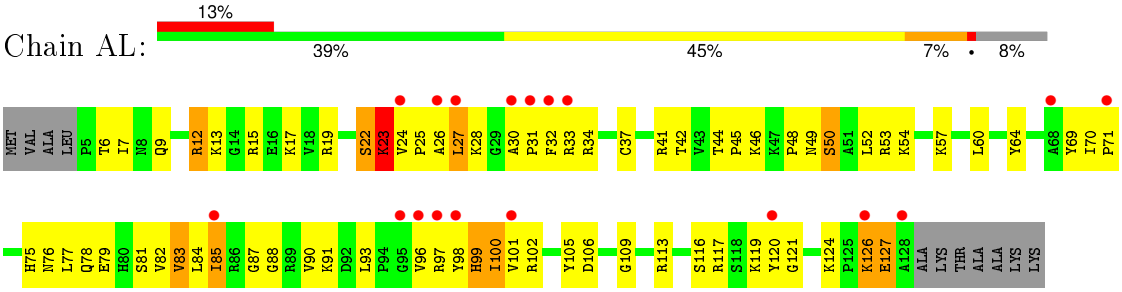
• Molecule 14: 30S ribosomal protein S11

Chain AK:



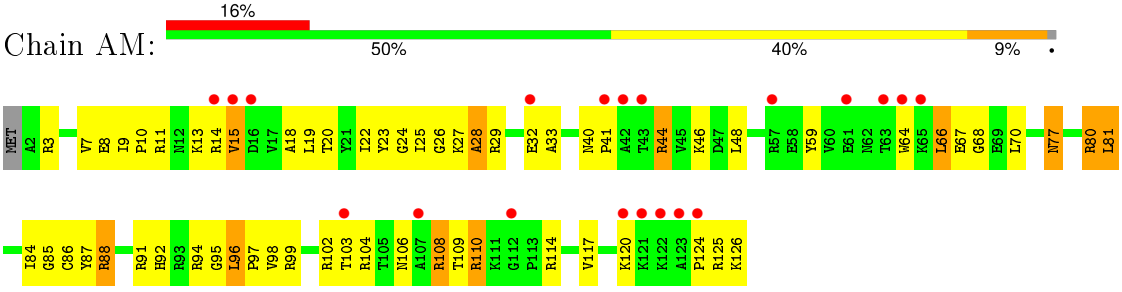
- Molecule 15: 30S ribosomal protein S12

Chain AL:



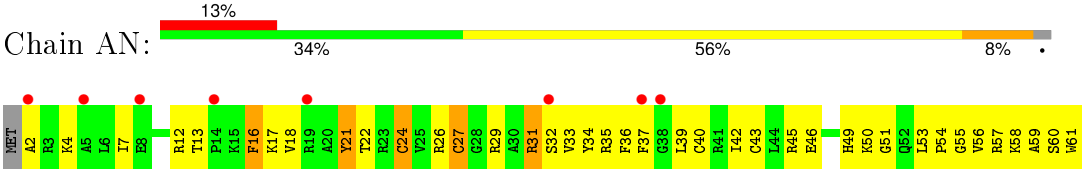
- Molecule 16: 30S ribosomal protein S13

Chain AM:



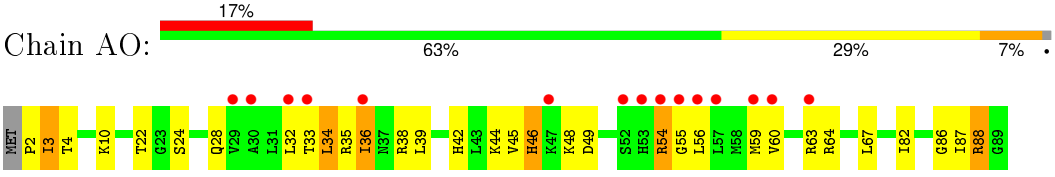
- Molecule 17: 30S ribosomal protein S14

Chain AN:



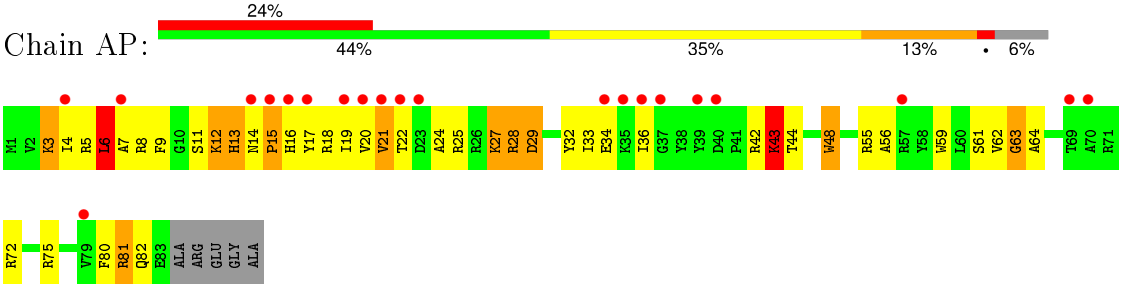
- Molecule 18: 30S ribosomal protein S15

Chain AO:



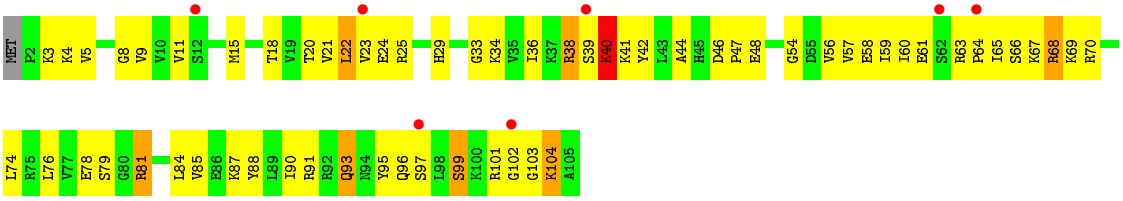
- Molecule 19: 30S ribosomal protein S16

Chain AP:



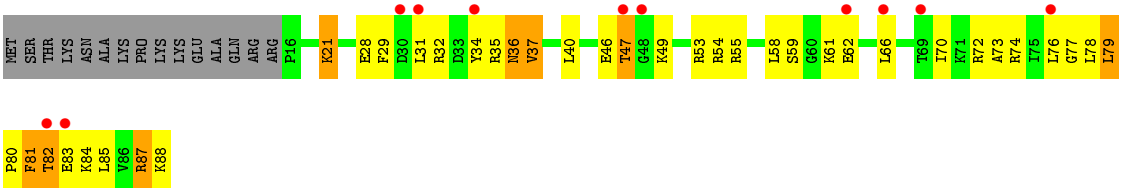
- Molecule 20: 30S ribosomal protein S17

Chain AQ:



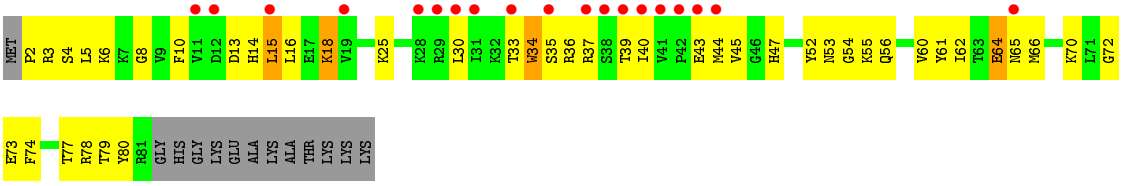
• Molecule 21: 30S ribosomal protein S18

Chain AR:



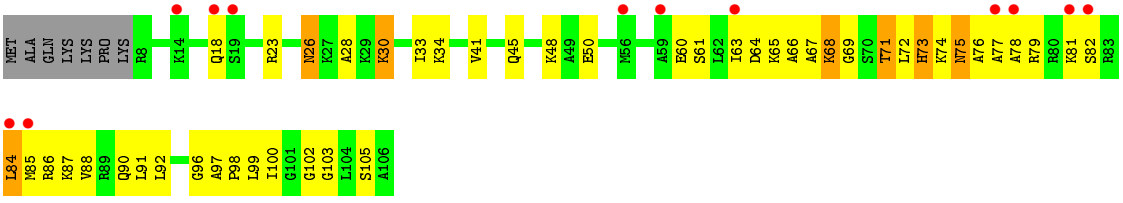
• Molecule 22: 30S ribosomal protein S19

Chain AS:



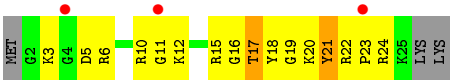
• Molecule 23: 30S ribosomal protein S20

Chain AT:



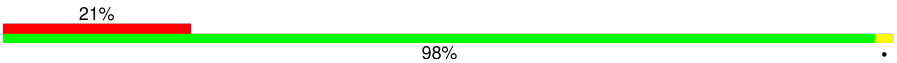
• Molecule 24: 30S ribosomal protein Thx

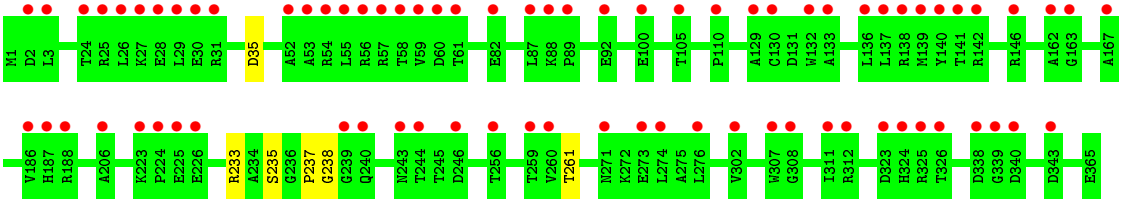
Chain AU:



• Molecule 25: Peptide chain release factor 2

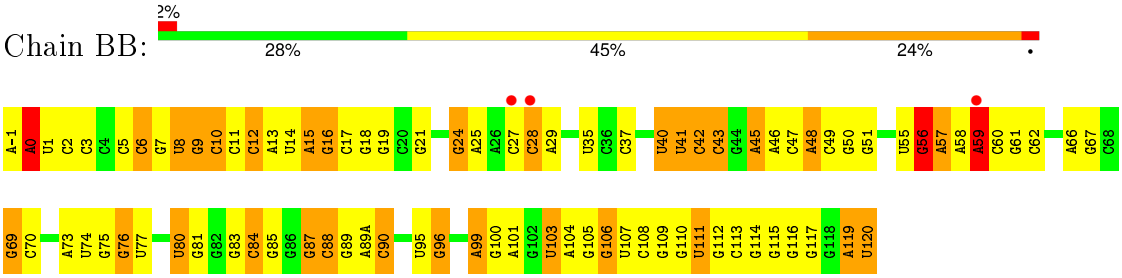
Chain AY:





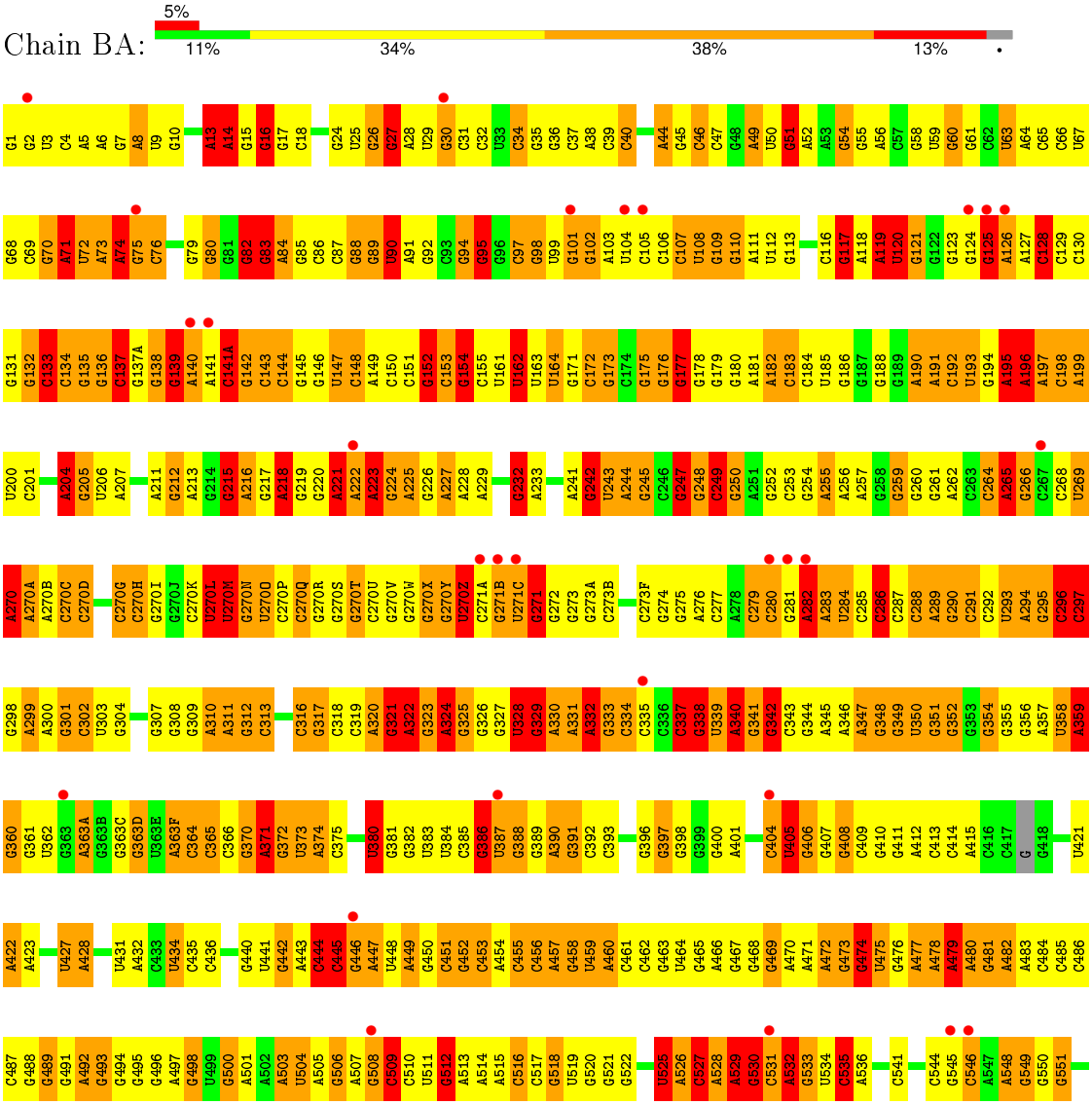
- Molecule 26: 5S ribosomal RNA

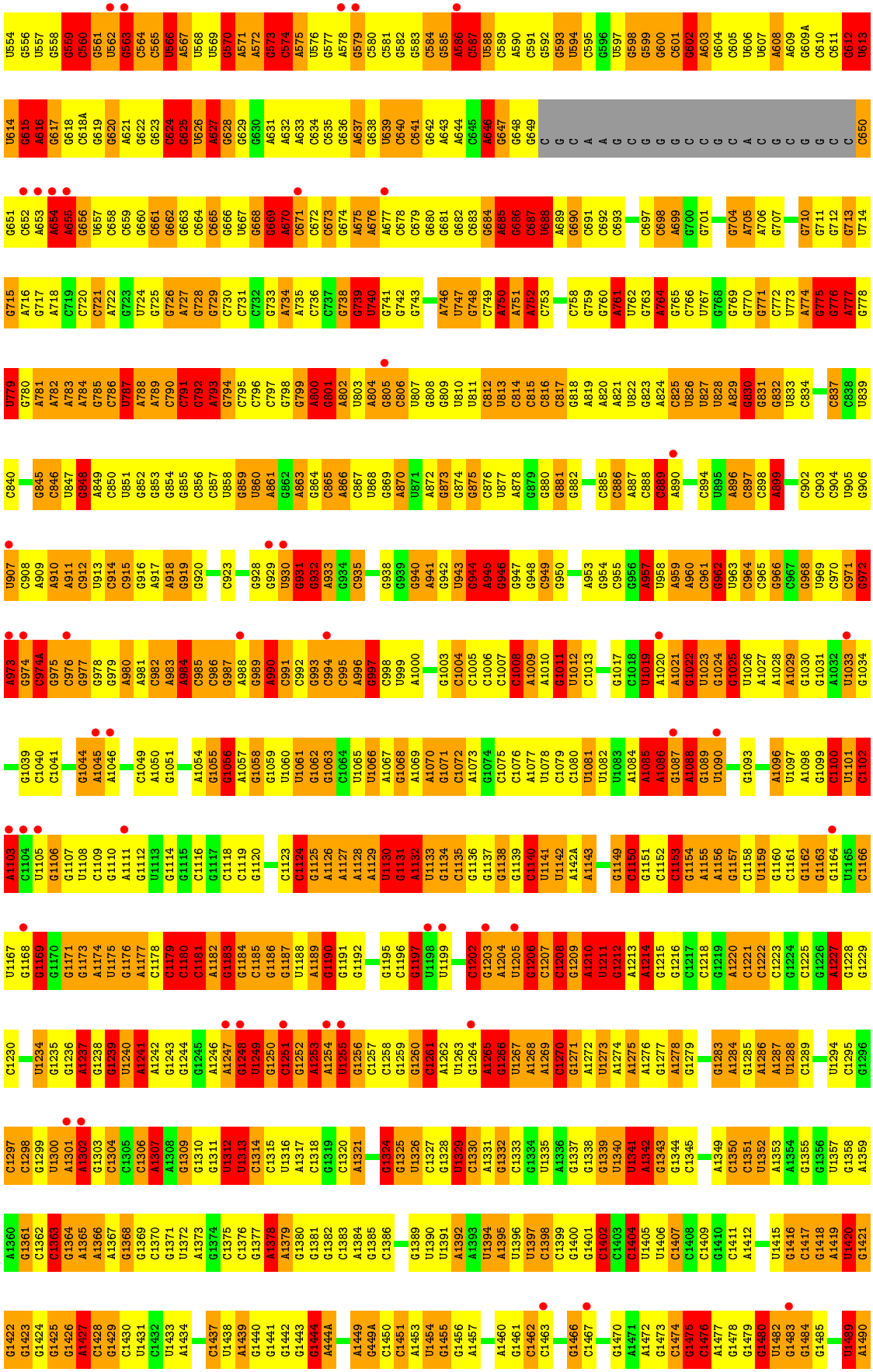
Chain BB:

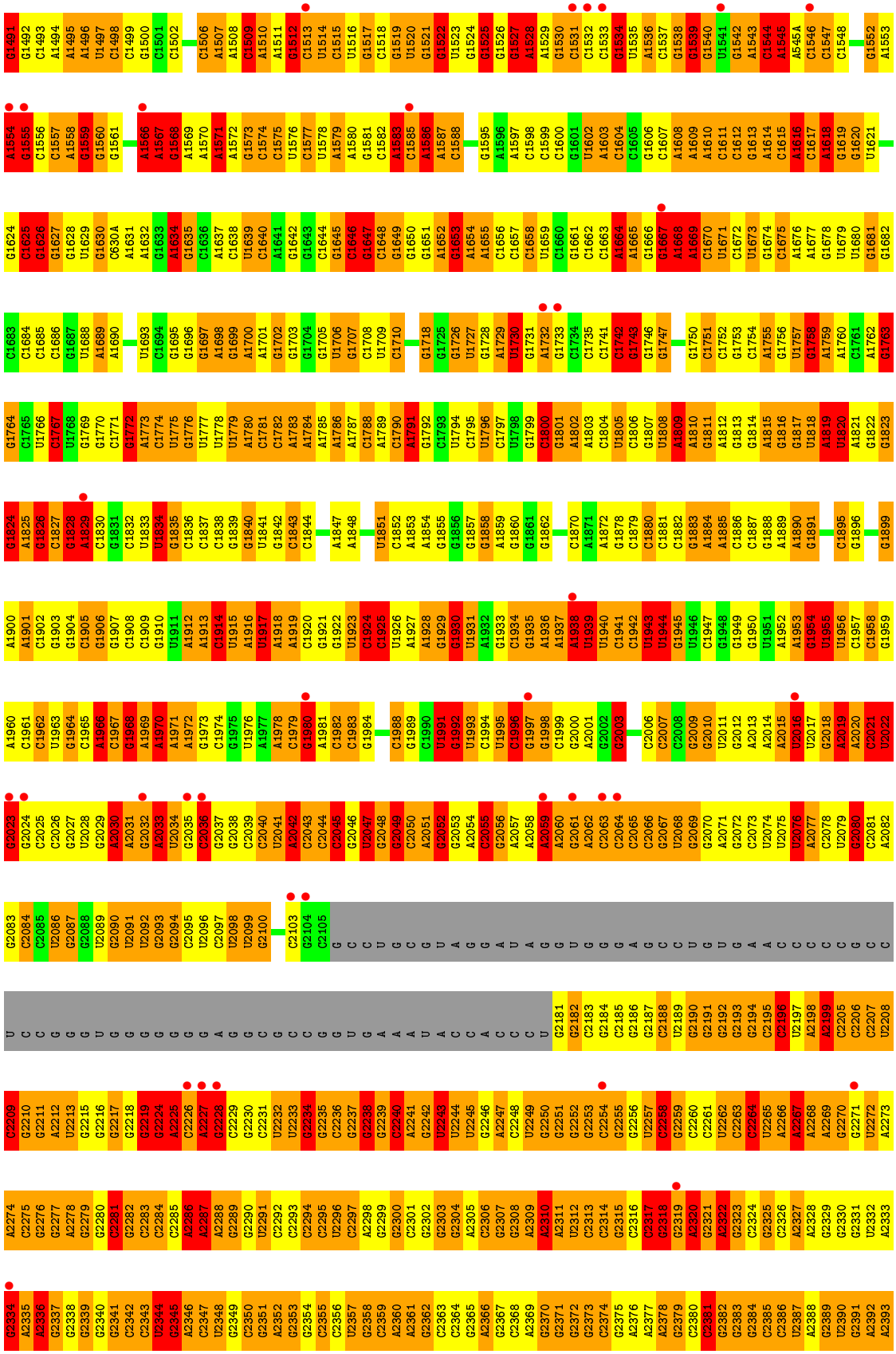


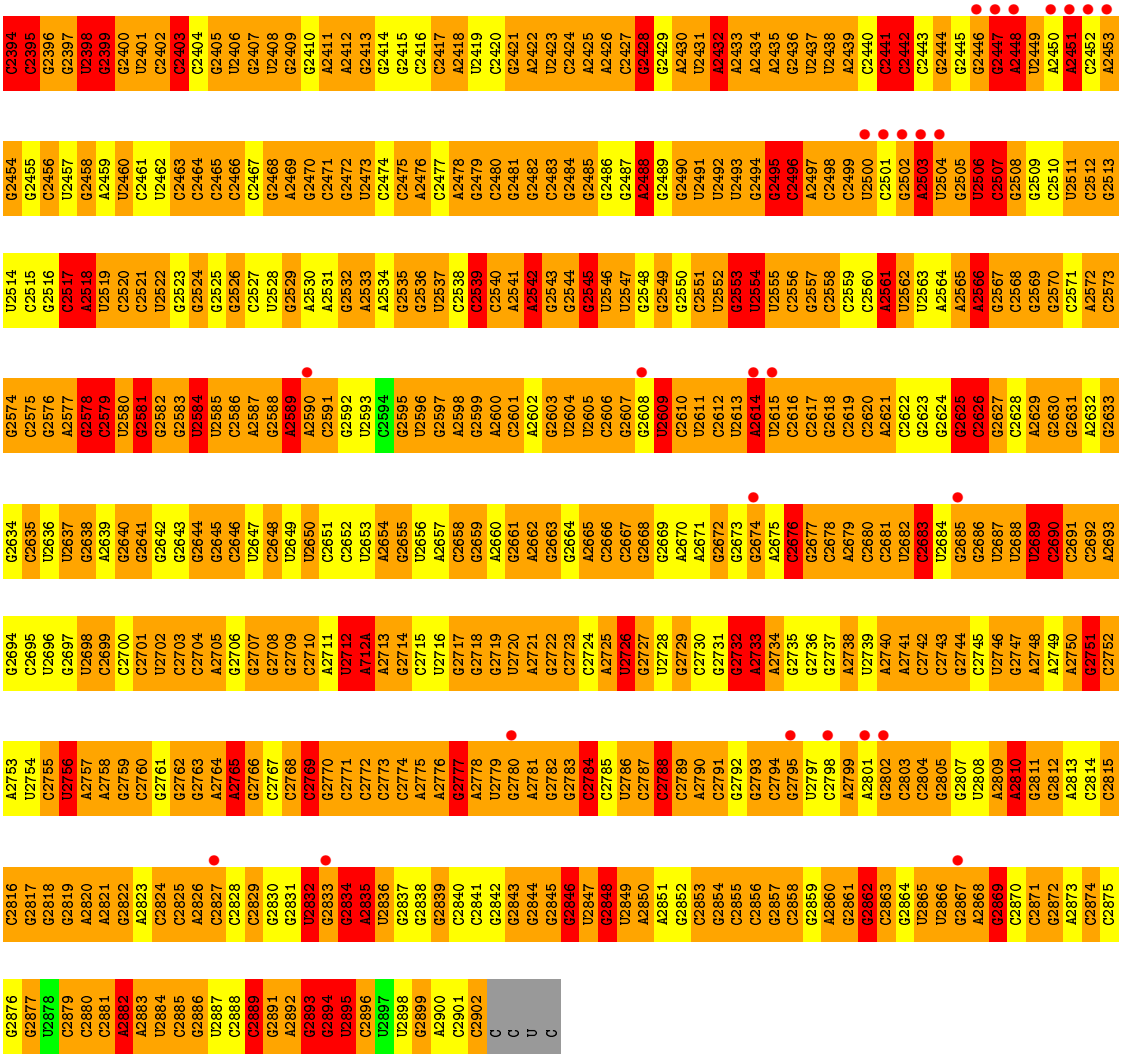
- Molecule 27: 23S ribosomal RNA

Chain BA:



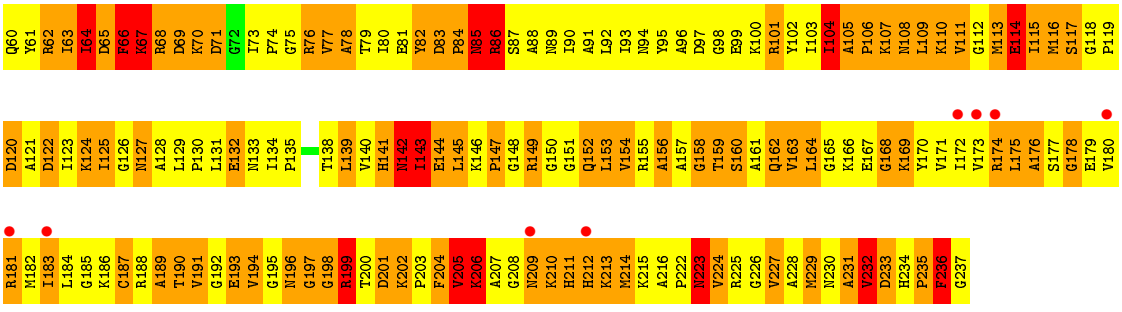






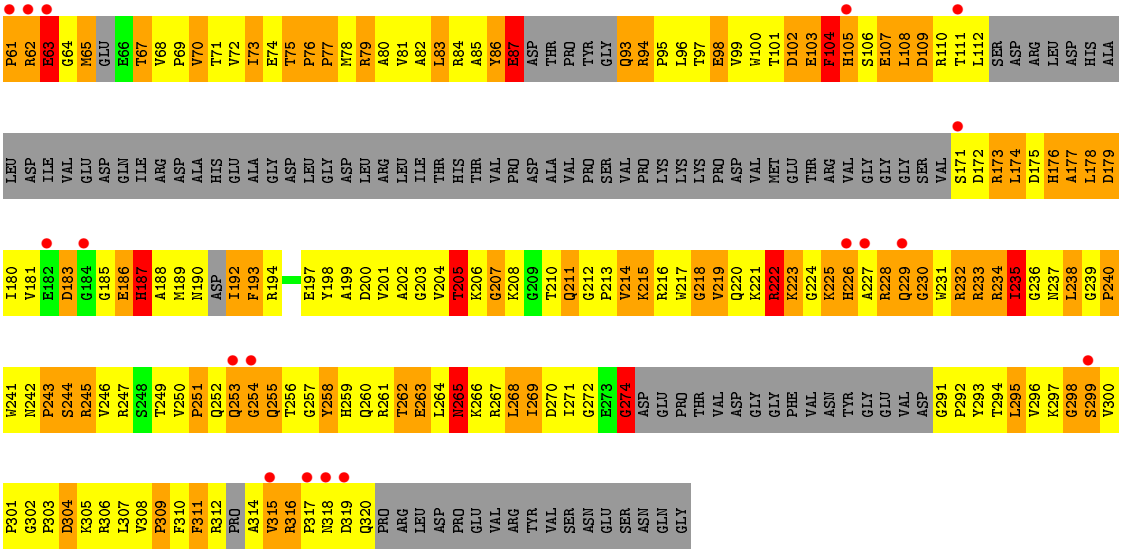
• Molecule 28: 50S ribosomal protein L2

Chain BD:



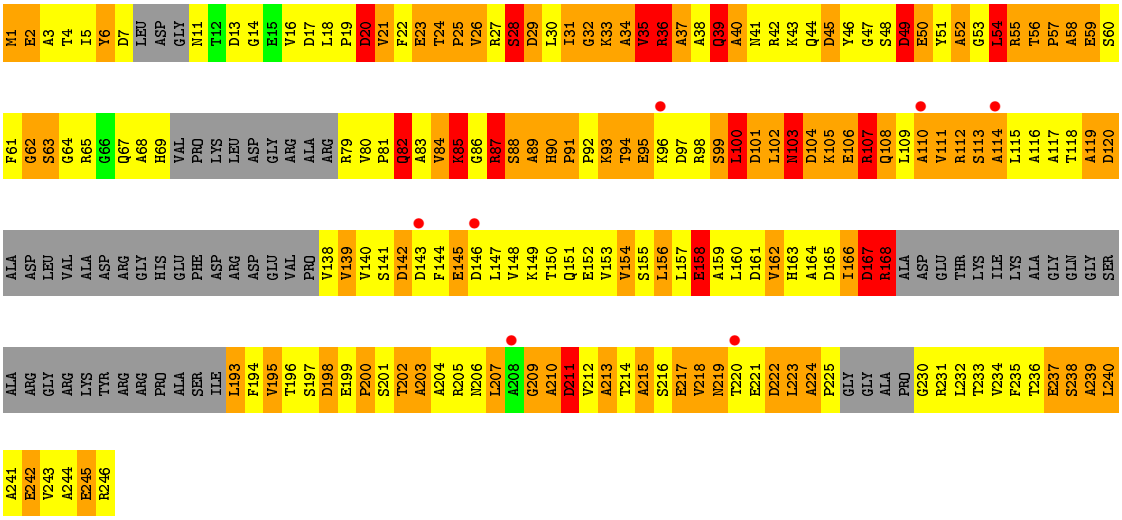
• Molecule 29: 50S ribosomal protein L3

Chain BE:



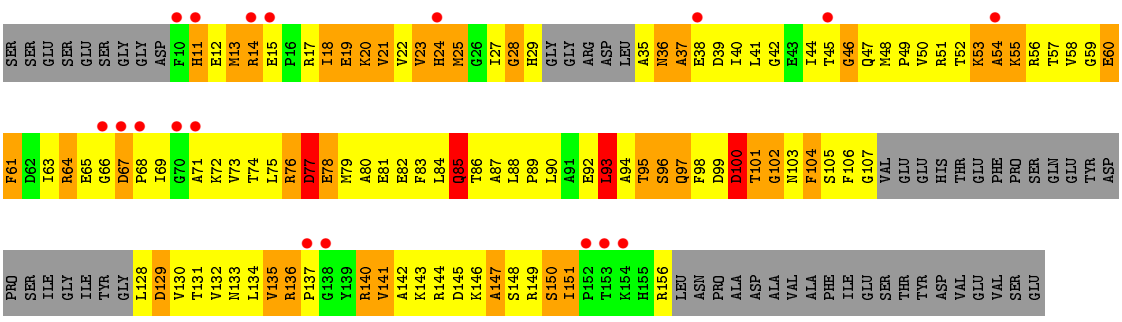
• Molecule 30: 50S ribosomal protein L4

Chain BF:

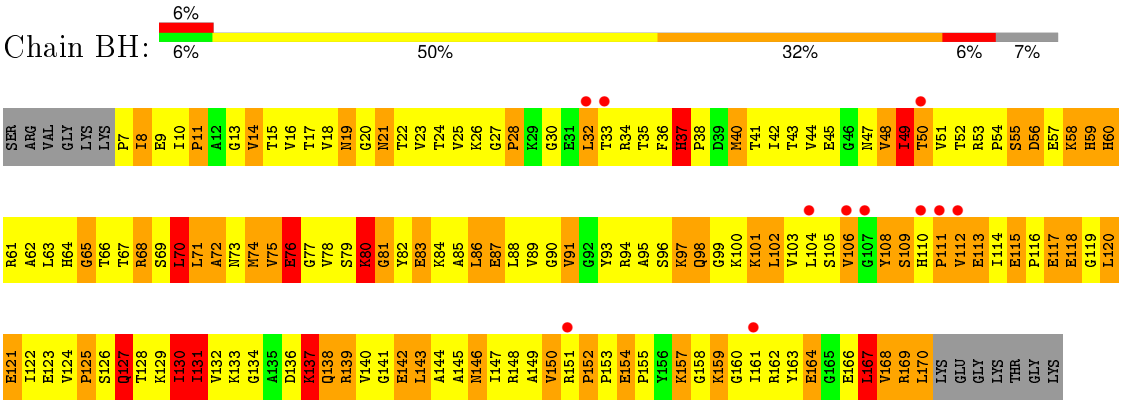


• Molecule 31: 50S ribosomal protein L5

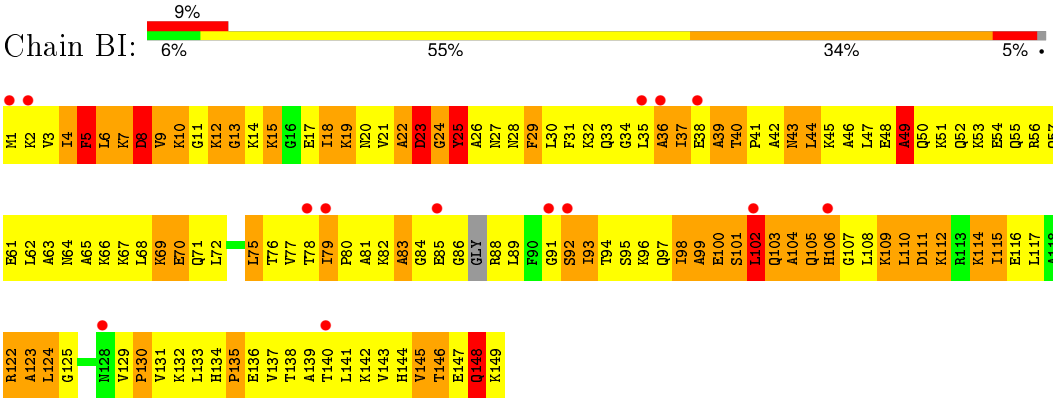
Chain BG:



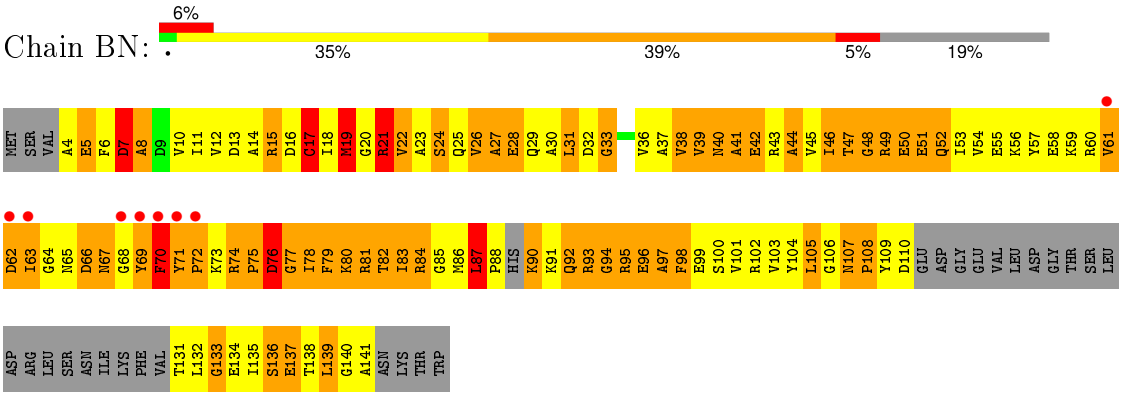
• Molecule 32: 50S ribosomal protein L6



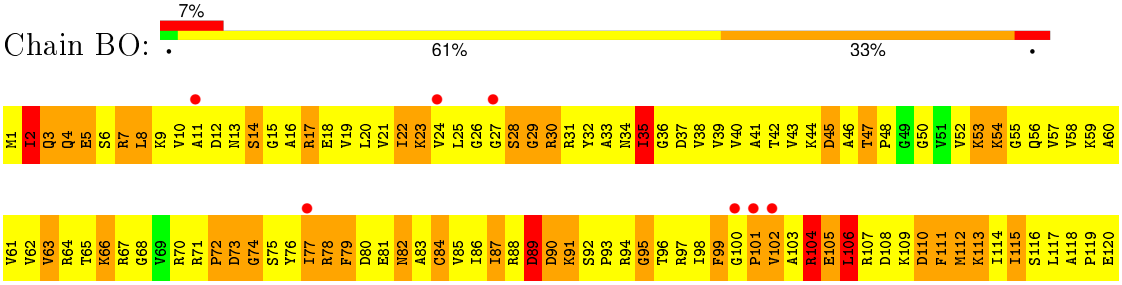
- Molecule 33: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L13

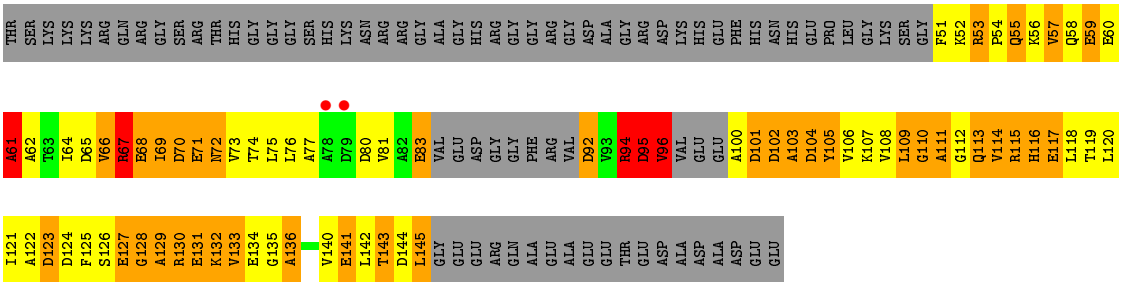


- Molecule 35: 50S ribosomal protein L14



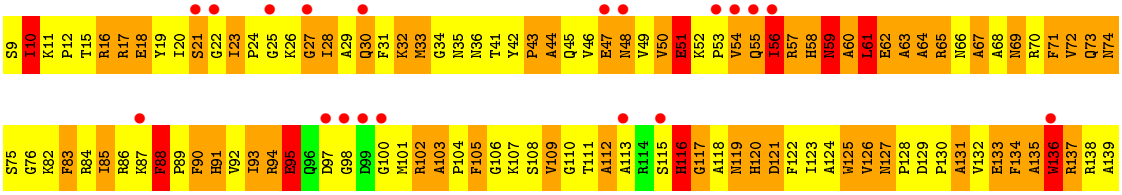
• Molecule 36: 50S ribosomal protein L15

Chain BP:



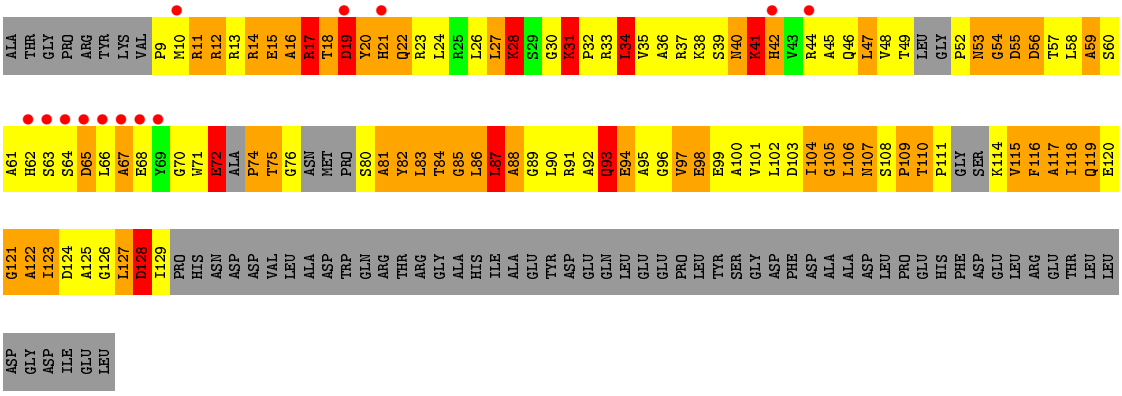
• Molecule 37: 50S ribosomal protein L16

Chain BQ:



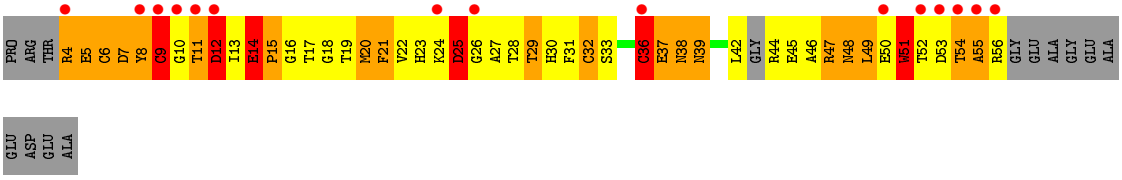
• Molecule 38: 50S ribosomal protein L18

Chain BS:



• Molecule 39: 50S ribosomal protein L19

Chain BT:

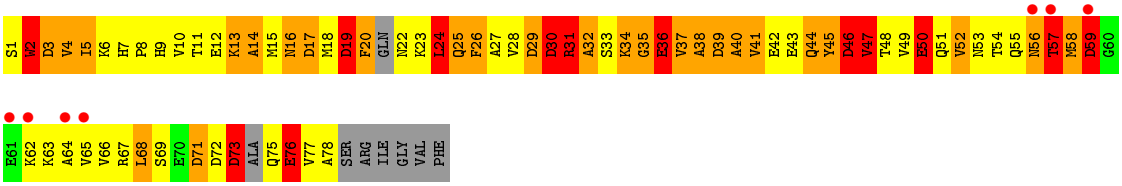


• Molecule 40: 50S ribosomal protein L22

Chain BW:

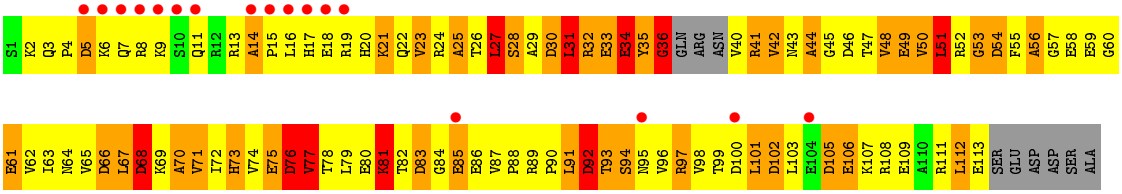
• Molecule 41: 50S ribosomal protein L23

Chain BX:



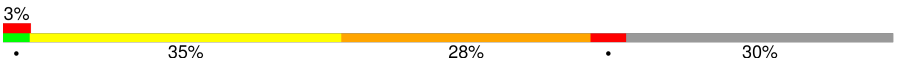
• Molecule 42: 50S ribosomal protein 24

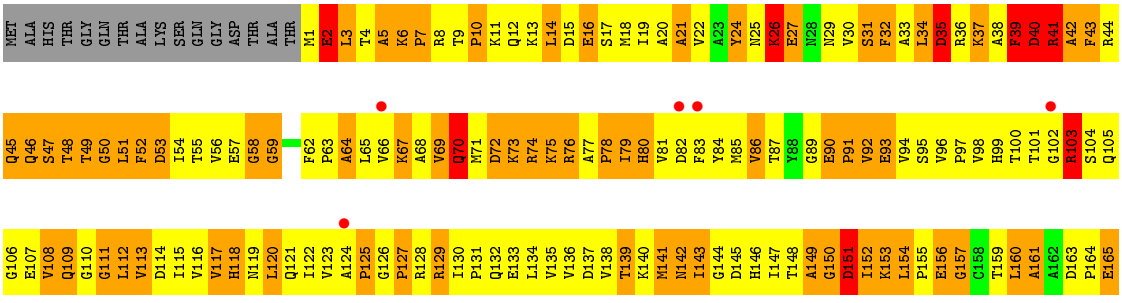
Chain BY:

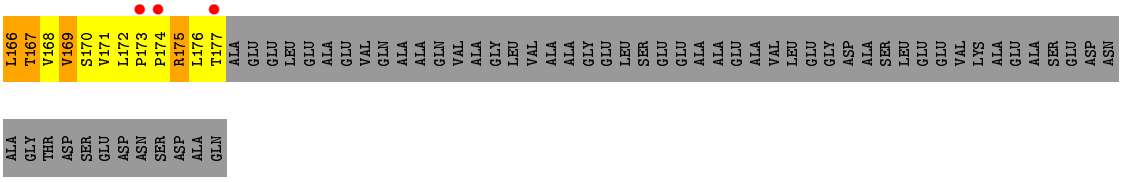


• Molecule 43: 50S ribosomal protein CTC

Chain BZ:

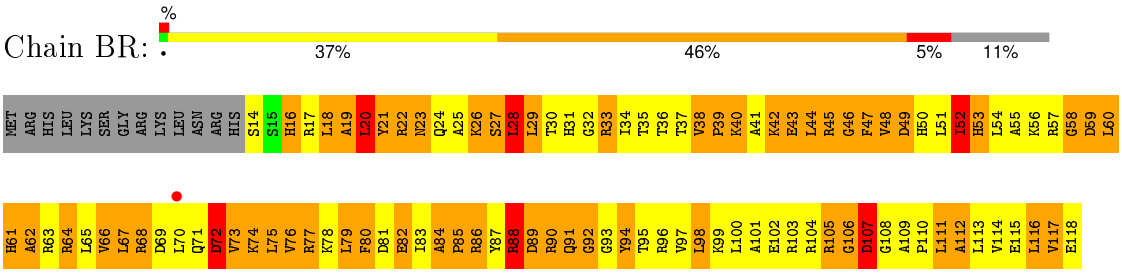






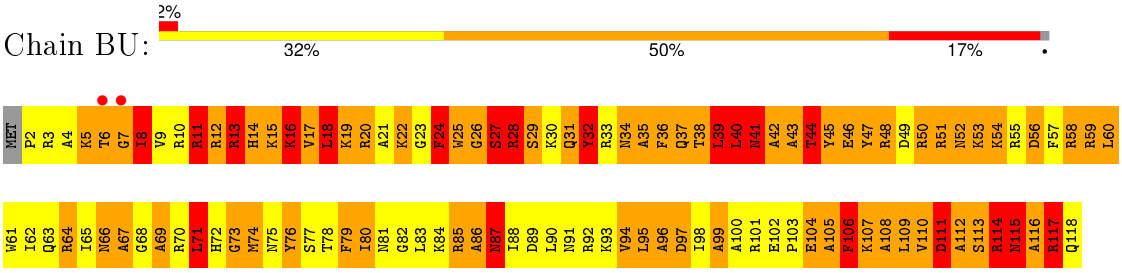
- Molecule 44: 50S ribosomal protein L17

Chain BR:



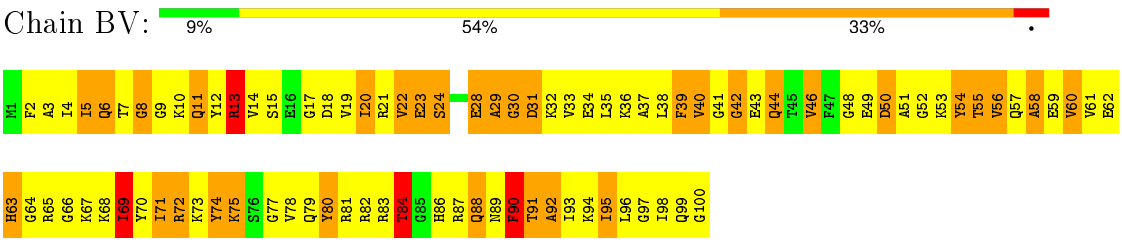
- Molecule 45: 50S ribosomal protein L20

Chain BU:



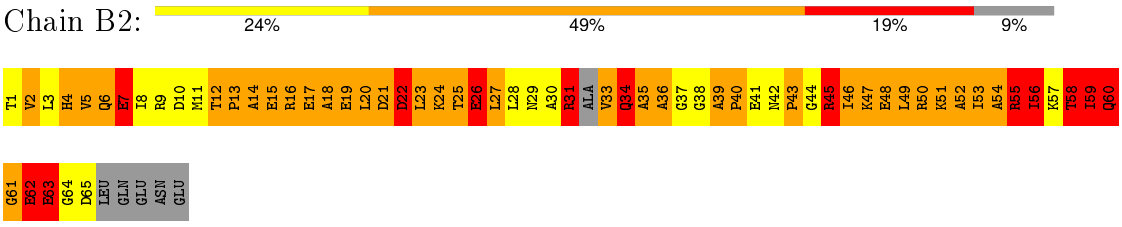
- Molecule 46: 50S ribosomal protein L21

Chain BV:



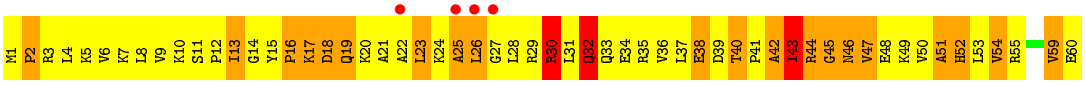
- Molecule 47: 50S ribosomal protein L29

Chain B2:



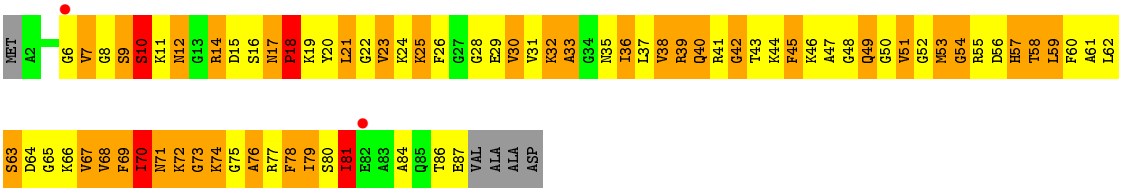
- Molecule 48: 50S ribosomal protein L30

Chain B3:



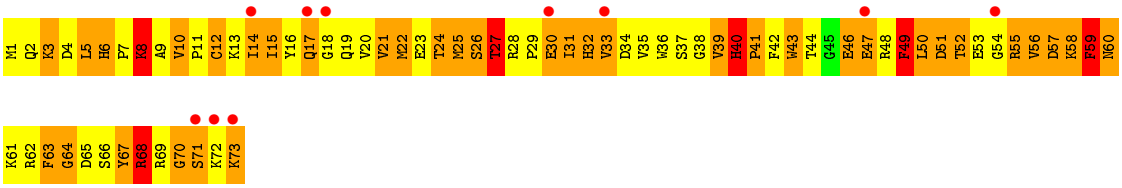
• Molecule 49: 50S ribosomal protein L27

Chain B0:



• Molecule 50: 50S ribosomal protein L31

Chain B4:

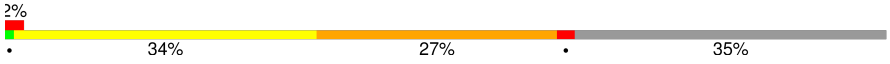


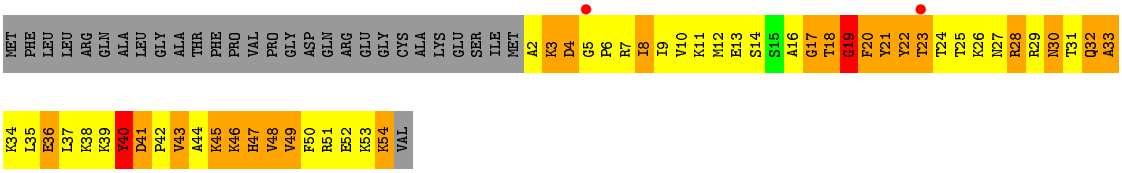
• Molecule 51: 50S ribosomal protein L32

Chain B5:

• Molecule 52: 50S ribosomal protein L33

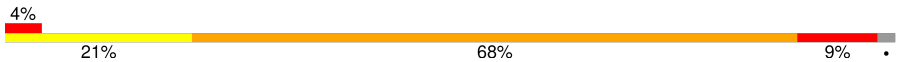
Chain B6:

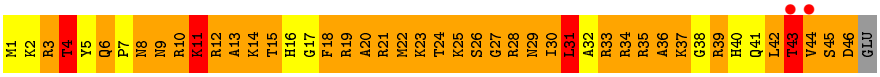




• Molecule 53: 50S ribosomal protein L34

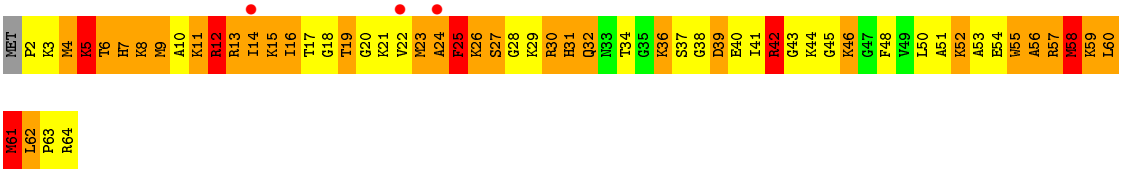
Chain B7:





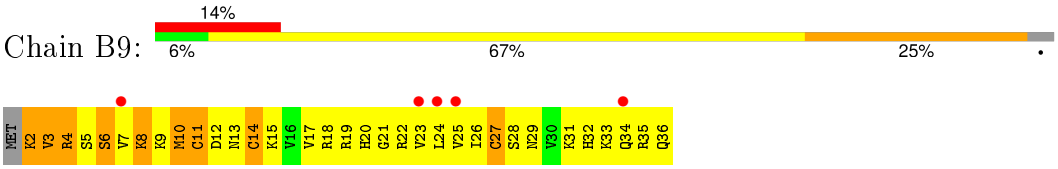
• Molecule 54: 50S ribosomal protein L35

Chain B8:



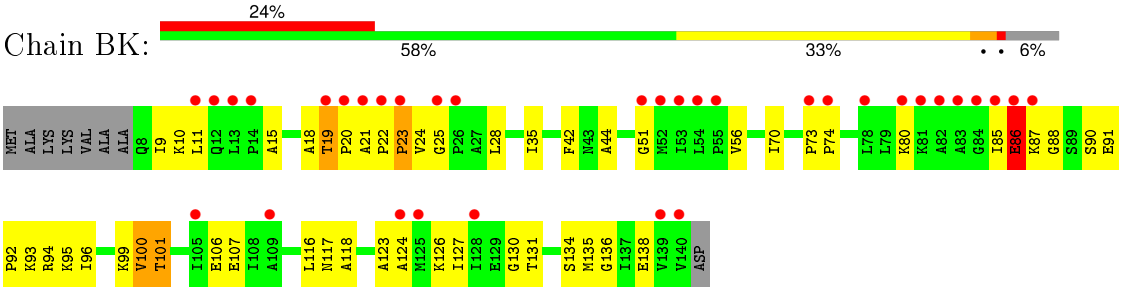
- Molecule 55: 50S ribosomal protein L36

Chain B9:



- Molecule 56: 50S ribosomal protein L11

Chain BK:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	520.21Å 520.21Å 365.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.35 – 6.76 43.35 – 6.02	Depositor EDS
% Data completeness (in resolution range)	96.2 (43.35-6.76) 91.3 (43.35-6.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 6.14Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.341 , 0.356 0.336 , 0.348	Depositor DCC
R_{free} test set	4221 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	233.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 93.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 112763 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	142811	wwPDB-VP
Average B, all atoms (Å^2)	306.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: YYG, PSU

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	1.34	66/36411 (0.2%)	1.47	428/56769 (0.8%)
2	AV	1.58	5/1814 (0.3%)	1.08	11/2827 (0.4%)
3	AW	1.77	16/1737 (0.9%)	1.68	30/2690 (1.1%)
4	AX	0.18	0/139	0.66	0/213
5	AB	0.61	2/1935 (0.1%)	0.61	0/2609
6	AC	0.43	1/1636 (0.1%)	1.10	6/2205 (0.3%)
7	AD	0.79	5/1733 (0.3%)	1.09	11/2318 (0.5%)
8	AE	0.92	1/1162 (0.1%)	0.63	2/1564 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.33	0/1276	0.76	3/1709 (0.2%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.64	1/900 (0.1%)	0.56	0/1213
15	AL	0.99	1/986 (0.1%)	0.70	1/1320 (0.1%)
16	AM	0.35	0/1006	0.56	0/1341
17	AN	0.49	0/501	0.64	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.20	3/870 (0.3%)	1.54	6/1159 (0.5%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.31	0/764	0.57	1/1006 (0.1%)
24	AU	0.34	0/212	0.49	0/277
26	BB	0.79	2/2950 (0.1%)	1.32	17/4602 (0.4%)
27	BA	1.31	147/67834 (0.2%)	1.47	923/105806 (0.9%)
28	BD	0.41	1/1328 (0.1%)	0.65	2/1783 (0.1%)
29	BE	0.67	4/1540 (0.3%)	1.08	8/2078 (0.4%)
30	BF	0.72	3/1444 (0.2%)	0.84	2/1954 (0.1%)
31	BG	0.25	0/971	0.46	0/1304
32	BH	0.45	1/1272 (0.1%)	0.60	3/1721 (0.2%)
33	BI	0.40	1/1156 (0.1%)	0.52	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BN	0.35	0/927	0.55	0/1245
35	BO	0.32	0/946	0.57	0/1269
36	BP	1.44	3/643 (0.5%)	1.31	5/870 (0.6%)
37	BQ	0.32	0/1106	0.52	0/1490
38	BS	1.20	3/877 (0.3%)	0.70	2/1179 (0.2%)
39	BT	0.39	0/412	0.70	0/554
40	BW	0.95	3/869 (0.3%)	0.96	6/1166 (0.5%)
41	BX	0.48	1/608 (0.2%)	1.04	3/820 (0.4%)
42	BY	0.25	0/887	0.83	3/1195 (0.3%)
43	BZ	0.31	1/1385 (0.1%)	0.46	0/1883
44	BR	0.30	0/867	0.49	0/1162
45	BU	0.56	1/994 (0.1%)	0.69	3/1323 (0.2%)
46	BV	0.69	1/796 (0.1%)	0.92	3/1058 (0.3%)
47	B2	0.37	0/497	1.00	2/668 (0.3%)
48	B3	0.31	0/482	0.50	0/646
49	B0	0.40	1/649 (0.2%)	0.82	3/860 (0.3%)
50	B4	1.31	2/620 (0.3%)	0.61	0/831
51	B5	0.38	0/469	1.08	3/629 (0.5%)
52	B6	0.32	0/438	0.55	1/583 (0.2%)
53	B7	0.38	0/387	0.64	0/509
54	B8	0.87	1/503 (0.2%)	0.95	6/657 (0.9%)
55	B9	0.33	0/286	0.59	0/375
56	BK	0.94	1/1010 (0.1%)	0.70	3/1349 (0.2%)
All	All	1.16	278/154788 (0.2%)	1.32	1499/231785 (0.6%)

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
3	AW	1	5
6	AC	0	1
14	AK	0	1
20	AQ	0	1
28	BD	0	1
29	BE	0	3
30	BF	0	4
32	BH	0	1
33	BI	0	1
36	BP	0	1
41	BX	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BY	0	1
47	B2	0	1
49	B0	0	1
51	B5	0	1
All	All	1	24

The worst 5 of 278 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1037	C	O3'-P	-82.19	0.62	1.61
1	AA	1255	G	O3'-P	-72.80	0.73	1.61
27	BA	2199	A	O3'-P	-71.10	0.75	1.61
27	BA	14	A	O3'-P	-50.73	1.00	1.61
27	BA	1924	C	O3'-P	-48.85	1.02	1.61

The worst 5 of 1499 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BA	712(A)	A	P-O3'-C3'	-43.34	67.69	119.70
27	BA	2199	A	O3'-P-O5'	-43.06	22.18	104.00
27	BA	2454	G	P-O3'-C3'	-28.75	85.20	119.70
29	BE	49	THR	O-C-N	-27.49	68.88	121.10
3	AW	33	U	P-O3'-C3'	27.30	152.45	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32551	0	16464	2038	4
2	AV	1622	0	819	182	0
3	AW	1638	0	835	193	0
4	AX	136	0	63	22	0
5	AB	1900	0	1950	92	0
6	AC	1612	0	1675	113	0
7	AD	1703	0	1760	288	0
8	AE	1146	0	1206	59	0
9	AF	843	0	857	49	0
10	AG	1257	0	1295	94	0
11	AH	1116	0	1177	99	0
12	AI	1011	0	1040	89	0
13	AJ	794	0	840	105	0
14	AK	885	0	904	55	0
15	AL	970	0	1056	74	0
16	AM	997	0	1070	186	0
17	AN	492	0	529	95	0
18	AO	734	0	771	30	0
19	AP	700	0	720	78	0
20	AQ	857	0	928	53	0
21	AR	597	0	668	52	0
22	AS	647	0	672	215	0
23	AT	762	0	859	33	0
24	AU	208	0	221	75	0
25	AY	365	0	0	14	0
26	BB	2637	0	1338	187	1
27	BA	60599	0	30523	10794	127
28	BD	1308	0	1346	1071	0
29	BE	1507	0	1475	1137	4
30	BF	1430	0	1357	1068	0
31	BG	957	0	950	687	0
32	BH	1251	0	1291	749	0
33	BI	1145	0	1224	627	4
34	BN	917	0	896	761	0
35	BO	937	0	992	621	0
36	BP	639	0	606	487	0
37	BQ	1081	0	1047	934	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BS	866	0	868	691	0
39	BT	406	0	359	164	0
40	BW	860	0	909	568	0
41	BX	602	0	559	448	0
42	BY	879	0	859	751	0
43	BZ	1360	0	1377	897	0
44	BR	855	0	904	561	0
45	BU	978	0	1001	880	0
46	BV	787	0	784	643	0
47	B2	494	0	504	396	0
48	B3	477	0	528	441	0
49	B0	641	0	658	517	0
50	B4	604	0	586	493	0
51	B5	457	0	455	288	0
52	B6	431	0	454	288	0
53	B7	383	0	411	393	0
54	B8	496	0	539	359	0
55	B9	285	0	312	150	0
56	BK	999	0	1065	119	0
All	All	142811	0	94556	28242	136

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 120.

The worst 5 of 28242 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)
51:B5:33:CYS:SG	51:B5:36:CYS:HB2	1.24	1.69
27:BA:2470:G:C2	27:BA:2471:C:C5	1.81	1.69
27:BA:2712:U:C6	27:BA:712(A):A:C8	1.76	1.68
53:B7:30:ILE:HA	53:B7:33:ARG:CD	1.21	1.67
27:BA:2580:U:C6	27:BA:2581:G:C8	1.82	1.66

The worst 5 of 136 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	Interatomic distance (Å)	Clash overlap (Å)
27:BA:6:A:O4'	27:BA:2902:C:C1'[8_554]	0.64	1.56
27:BA:6:A:C4'	27:BA:2902:C:O2'[8_554]	0.74	1.46
27:BA:6:A:C4'	27:BA:2902:C:C2'[8_554]	0.77	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:5:A:N7	27:BA:2901:C:N1[8_554]	0.83	1.37
27:BA:6:A:O4'	27:BA:2902:C:C2'[8_554]	0.90	1.30

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
5	AB	232/256 (91%)	183 (79%)	34 (15%)	15 (6%)	1 25
6	AC	204/239 (85%)	165 (81%)	23 (11%)	16 (8%)	1 20
7	AD	206/209 (99%)	156 (76%)	33 (16%)	17 (8%)	1 18
8	AE	148/162 (91%)	115 (78%)	29 (20%)	4 (3%)	6 45
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	4 35
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	7 45
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1 21
12	AI	125/128 (98%)	87 (70%)	30 (24%)	8 (6%)	2 25
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1 16
14	AK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2 26
15	AL	122/135 (90%)	92 (75%)	13 (11%)	17 (14%)	0 6
16	AM	119/126 (94%)	95 (80%)	19 (16%)	5 (4%)	3 34
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1 23
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16 61
19	AP	81/88 (92%)	64 (79%)	10 (12%)	7 (9%)	1 17
20	AQ	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	2 27
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1 17
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	4 37
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1 17
28	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0 0
29	BE	183/338 (54%)	90 (49%)	34 (19%)	59 (32%)	0 0
30	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0 0
31	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0 0
32	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0 0
33	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0 0
34	BN	111/145 (77%)	34 (31%)	20 (18%)	57 (51%)	0 0
35	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0 1
36	BP	82/164 (50%)	29 (35%)	19 (23%)	34 (42%)	0 0
37	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0 0
38	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0 0
39	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0 0
40	BW	104/113 (92%)	41 (39%)	16 (15%)	47 (45%)	0 0
41	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0 0
42	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0 0
43	BZ	175/253 (69%)	53 (30%)	52 (30%)	70 (40%)	0 0
44	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0 0
45	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0 0
46	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0 0
47	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0 0
48	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0 0
49	B0	84/91 (92%)	33 (39%)	17 (20%)	34 (40%)	0 0
50	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0 0
51	B5	56/60 (93%)	16 (29%)	17 (30%)	23 (41%)	0 0
52	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0 0
53	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0 0
54	B8	61/64 (95%)	22 (36%)	9 (15%)	30 (49%)	0 0
55	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0 0
56	BK	124/141 (88%)	92 (74%)	26 (21%)	6 (5%)	3 32
All	All	5318/6250 (85%)	2968 (56%)	1014 (19%)	1336 (25%)	0 2

5 of 1336 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	ALA

5.3.2 Protein sidechains (i)

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
5	AB	202/220 (92%)	173 (86%)	29 (14%)	4 25
6	AC	160/188 (85%)	146 (91%)	14 (9%)	12 45
7	AD	180/181 (99%)	162 (90%)	18 (10%)	9 38
8	AE	115/123 (94%)	94 (82%)	21 (18%)	2 14
9	AF	90/90 (100%)	83 (92%)	7 (8%)	16 51
10	AG	126/127 (99%)	116 (92%)	10 (8%)	15 51
11	AH	119/119 (100%)	91 (76%)	28 (24%)	1 7
12	AI	98/99 (99%)	90 (92%)	8 (8%)	14 49
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	6 30
14	AK	90/99 (91%)	85 (94%)	5 (6%)	26 62
15	AL	104/111 (94%)	93 (89%)	11 (11%)	8 36
16	AM	100/101 (99%)	87 (87%)	13 (13%)	5 28
17	AN	49/50 (98%)	43 (88%)	6 (12%)	6 31
18	AO	79/80 (99%)	70 (89%)	9 (11%)	7 32
19	AP	72/74 (97%)	62 (86%)	10 (14%)	4 26
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	11 42
21	AR	64/77 (83%)	57 (89%)	7 (11%)	8 35
22	AS	71/80 (89%)	64 (90%)	7 (10%)	10 39
23	AT	76/82 (93%)	68 (90%)	8 (10%)	8 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	AU	19/22 (86%)	19 (100%)	0	100 100
28	BD	135/135 (100%)	99 (73%)	36 (27%)	0 5
29	BE	156/284 (55%)	128 (82%)	28 (18%)	2 15
30	BF	152/193 (79%)	124 (82%)	28 (18%)	2 14
31	BG	102/147 (69%)	93 (91%)	9 (9%)	12 45
32	BH	137/147 (93%)	111 (81%)	26 (19%)	2 13
33	BI	119/119 (100%)	98 (82%)	21 (18%)	2 16
34	BN	95/121 (78%)	80 (84%)	15 (16%)	3 21
35	BO	101/101 (100%)	81 (80%)	20 (20%)	1 12
36	BP	67/126 (53%)	56 (84%)	11 (16%)	3 20
37	BQ	110/110 (100%)	83 (76%)	27 (24%)	1 6
38	BS	89/149 (60%)	73 (82%)	16 (18%)	2 15
39	BT	44/52 (85%)	30 (68%)	14 (32%)	0 2
40	BW	88/92 (96%)	74 (84%)	14 (16%)	3 21
41	BX	67/73 (92%)	44 (66%)	23 (34%)	0 2
42	BY	97/105 (92%)	80 (82%)	17 (18%)	2 16
43	BZ	151/203 (74%)	130 (86%)	21 (14%)	4 26
44	BR	89/101 (88%)	71 (80%)	18 (20%)	1 11
45	BU	96/97 (99%)	68 (71%)	28 (29%)	0 3
46	BV	79/79 (100%)	69 (87%)	10 (13%)	5 29
47	B2	51/56 (91%)	37 (72%)	14 (28%)	0 4
48	B3	52/52 (100%)	47 (90%)	5 (10%)	10 40
49	B0	64/67 (96%)	57 (89%)	7 (11%)	8 35
50	B4	66/66 (100%)	54 (82%)	12 (18%)	2 15
51	B5	51/53 (96%)	43 (84%)	8 (16%)	3 21
52	B6	46/69 (67%)	39 (85%)	7 (15%)	3 22
53	B7	39/40 (98%)	31 (80%)	8 (20%)	1 10
54	B8	50/51 (98%)	39 (78%)	11 (22%)	1 9
55	B9	34/35 (97%)	30 (88%)	4 (12%)	6 31
56	BK	108/113 (96%)	105 (97%)	3 (3%)	51 78
All	All	4533/5148 (88%)	3841 (85%)	692 (15%)	3 22

5 of 692 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	BF	107	ARG
34	BN	79	PHE
50	B4	5	LEU
30	BF	245	GLU
32	BH	131	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
29	BE	259	HIS
33	BI	64	ASN
49	B0	71	ASN
29	BE	318	ASN
30	BF	219	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1496/1522 (98%)	518 (34%)	159 (10%)
2	AV	75/76 (98%)	17 (22%)	2 (2%)
26	BB	122/123 (99%)	44 (36%)	3 (2%)
27	BA	2779/2916 (95%)	1485 (53%)	361 (12%)
3	AW	68/76 (89%)	13 (19%)	4 (5%)
4	AX	5/18 (27%)	0	0
All	All	4545/4731 (96%)	2077 (45%)	529 (11%)

5 of 2077 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 529 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	669	G

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Mol	Chain	Res	Type
27	BA	1128	A
27	BA	2612	C
27	BA	729	G
27	BA	830	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	YYG	AW	37	10,3	27,42,43	1.04	2 (7%)	29,62,65	2.22	8 (27%)
3	PSU	AW	39	3	13,21,22	1.33	2 (15%)	18,30,33	6.13	4 (22%)
3	PSU	AW	55	3	13,21,22	1.52	2 (15%)	18,30,33	6.00	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YYG	AW	37	10,3	1/1/8/9	0/20/42/43	0/4/4/4
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	39	PSU	C6-C5	-3.32	1.33	1.38
3	AW	55	PSU	C6-C5	-2.79	1.34	1.38
3	AW	37	YYG	C2-N2	2.00	1.38	1.35
3	AW	37	YYG	C6-N1	2.86	1.42	1.37
3	AW	39	PSU	C4-N3	2.99	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AW	39	PSU	N1-C2-N3	-21.97	114.31	128.33
3	AW	55	PSU	N1-C2-N3	-21.69	114.49	128.33
3	AW	37	YYG	C13-C12-C11	-4.14	123.54	130.59
3	AW	37	YYG	O23-C21-O22	-3.84	119.70	124.70
3	AW	55	PSU	C4-C5-C1'	-2.39	116.87	121.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	37	YYG	31	0
3	AW	39	PSU	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	BA	76

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Mol	Chain	Number of breaks
1	AA	47
3	AW	8
56	BK	6
2	AV	4
37	BQ	3
50	B4	2
40	BW	2
46	BV	2
20	AQ	2
16	AM	2
45	BU	1
14	AK	1
8	AE	1
5	AB	1
28	BD	1
38	BS	1
7	AD	1
15	AL	1

The worst 5 of 162 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	70:ILE	C	71:LYS	N	5.81
1	BK	71:LYS	C	72:THR	N	5.77
1	AW	73:A	O3'	74:C	P	5.46
1	BK	73:PRO	C	74:PRO	N	5.30
1	BK	72:THR	C	73:PRO	N	5.11

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1515/1522 (99%)	0.76	190 (12%) 5 11	208, 348, 400, 400	0
2	AV	76/76 (100%)	0.71	9 (11%) 6 12	208, 360, 393, 393	0
3	AW	73/76 (96%)	1.21	22 (30%) 1 5	342, 400, 400, 400	0
4	AX	17/18 (94%)	3.91	13 (76%) 0 2	399, 399, 399, 399	0
5	AB	234/256 (91%)	0.07	6 (2%) 59 55	400, 400, 400, 400	0
6	AC	206/239 (86%)	0.41	24 (11%) 6 12	398, 400, 400, 400	0
7	AD	208/209 (99%)	0.34	19 (9%) 11 16	311, 385, 400, 400	0
8	AE	150/162 (92%)	0.38	15 (10%) 9 14	335, 400, 400, 400	0
9	AF	101/101 (100%)	0.21	7 (6%) 20 22	400, 400, 400, 400	0
10	AG	155/156 (99%)	0.51	15 (9%) 10 14	376, 395, 395, 395	0
11	AH	138/138 (100%)	0.08	11 (7%) 15 19	389, 389, 389, 389	0
12	AI	127/128 (99%)	0.95	25 (19%) 1 7	400, 400, 400, 400	0
13	AJ	98/105 (93%)	1.48	20 (20%) 1 7	399, 399, 399, 399	0
14	AK	119/129 (92%)	-0.23	3 (2%) 61 56	250, 250, 400, 400	0
15	AL	124/135 (91%)	0.49	18 (14%) 3 9	383, 383, 397, 397	0
16	AM	125/126 (99%)	0.96	20 (16%) 3 8	400, 400, 400, 400	0
17	AN	60/61 (98%)	0.64	8 (13%) 4 10	398, 398, 398, 398	0
18	AO	88/89 (98%)	0.84	15 (17%) 2 8	392, 392, 392, 392	0
19	AP	83/88 (94%)	1.46	21 (25%) 1 5	394, 394, 394, 394	0
20	AQ	104/105 (99%)	0.73	7 (6%) 21 23	397, 397, 400, 400	0
21	AR	73/88 (82%)	0.67	11 (15%) 3 9	400, 400, 400, 400	0
22	AS	80/93 (86%)	1.14	19 (23%) 1 6	395, 395, 395, 395	0
23	AT	99/106 (93%)	0.38	12 (12%) 6 11	400, 400, 400, 400	0
24	AU	24/27 (88%)	0.59	3 (12%) 5 11	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	AY	365/365 (100%)	0.85	76 (20%) 1 7	340, 396, 400, 400	0
26	BB	123/123 (100%)	0.29	3 (2%) 62 58	242, 265, 342, 342	0
27	BA	2814/2916 (96%)	0.39	138 (4%) 33 33	67, 222, 387, 400	0
28	BD	173/173 (100%)	0.07	8 (4%) 36 35	398, 398, 400, 400	0
29	BE	191/338 (56%)	0.36	18 (9%) 11 15	388, 400, 400, 400	0
30	BF	189/246 (76%)	0.13	7 (3%) 45 42	398, 398, 399, 399	0
31	BG	122/176 (69%)	0.66	18 (14%) 3 9	400, 400, 400, 400	0
32	BH	164/177 (92%)	0.08	11 (6%) 21 23	399, 399, 400, 400	0
33	BI	148/149 (99%)	0.41	14 (9%) 10 15	400, 400, 400, 400	0
34	BN	117/145 (80%)	0.25	8 (6%) 20 23	388, 388, 388, 388	0
35	BO	122/122 (100%)	0.19	8 (6%) 22 23	400, 400, 400, 400	0
36	BP	84/164 (51%)	0.10	2 (2%) 62 58	400, 400, 400, 400	0
37	BQ	138/138 (100%)	0.77	19 (13%) 4 10	391, 391, 391, 391	0
38	BS	113/186 (60%)	0.28	13 (11%) 6 12	275, 370, 400, 400	0
39	BT	52/66 (78%)	1.29	15 (28%) 1 5	400, 400, 400, 400	0
40	BW	108/113 (95%)	-0.19	0 100 100	275, 277, 400, 400	0
41	BX	76/84 (90%)	0.20	7 (9%) 11 16	400, 400, 400, 400	0
42	BY	110/119 (92%)	0.77	17 (15%) 3 9	400, 400, 400, 400	0
43	BZ	177/253 (69%)	-0.05	8 (4%) 37 36	376, 376, 379, 379	0
44	BR	105/118 (88%)	-0.23	1 (0%) 84 79	345, 345, 345, 345	0
45	BU	117/118 (99%)	-0.36	2 (1%) 73 67	356, 356, 392, 392	0
46	BV	100/100 (100%)	-0.27	0 100 100	385, 385, 400, 400	0
47	B2	64/70 (91%)	-0.61	0 100 100	287, 287, 287, 287	0
48	B3	60/60 (100%)	0.22	4 (6%) 21 23	343, 343, 343, 343	0
49	B0	86/91 (94%)	-0.09	2 (2%) 64 59	400, 400, 400, 400	0
50	B4	73/73 (100%)	0.69	10 (13%) 4 10	400, 400, 400, 400	0
51	B5	58/60 (96%)	0.08	2 (3%) 49 46	400, 400, 400, 400	0
52	B6	53/82 (64%)	-0.19	2 (3%) 44 42	400, 400, 400, 400	0
53	B7	46/47 (97%)	-0.04	2 (4%) 39 37	400, 400, 400, 400	0
54	B8	63/64 (98%)	0.13	3 (4%) 34 33	400, 400, 400, 400	0
55	B9	35/36 (97%)	0.71	5 (14%) 4 9	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
56	BK	133/141 (94%)	1.17	34 (25%)	1	5	397, 400, 400, 400	0
All	All	10456/11346 (92%)	0.46	970 (9%)	11	16	67, 388, 400, 400	0

The worst 5 of 970 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AJ	73	ASP	13.9
12	AI	15	ALA	12.9
16	AM	123	ALA	11.2
27	BA	546	C	11.0
25	AY	31	ARG	10.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	PSU	AW	55	20/21	0.86	0.20	-	400,400,400,400	0
3	YYG	AW	37	39/40	0.35	0.68	-	400,400,400,400	0
3	PSU	AW	39	20/21	0.53	0.52	-	400,400,400,400	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.