wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:26 PM GMT

PDB ID	:	4V4P
Title	:	Crystal structure of 70S ribosome with thrS operator and tRNAs.
Authors	:	Jenner, L.; Romby, P.; Rees, B.; Schulze-Briese, C.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.; Yusupova, G.; Yusupov, M.
Deposited on	:	2005-01-19
Resolution	:	5.50 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:

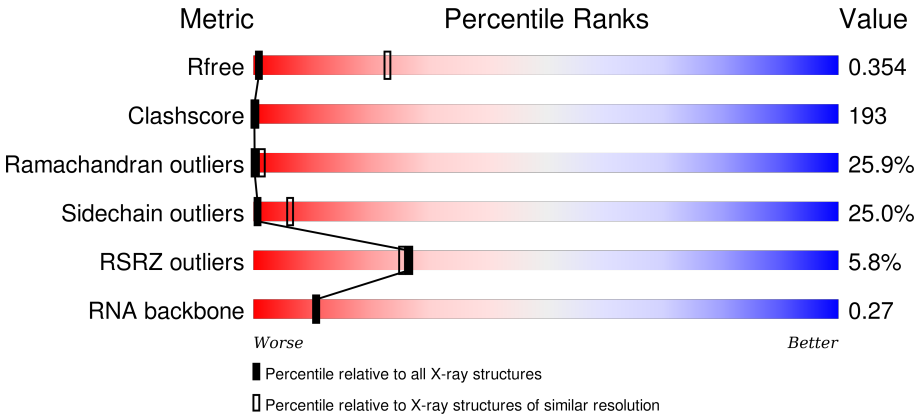
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 5.50 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}	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)
RNA backbone	2183	1101 (7.80-2.80)

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	AB	123	52% 41% 7%
2	AA	2915	% 41% 39% 18%
3	AC	228	2% 9% 64% 19%
4	AD	178	8% 39% 40% 16%

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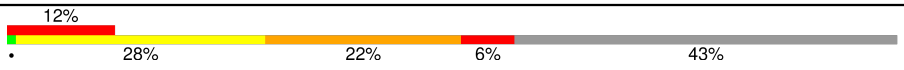
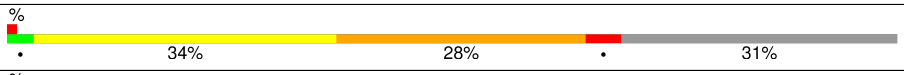
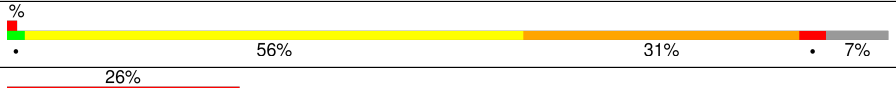
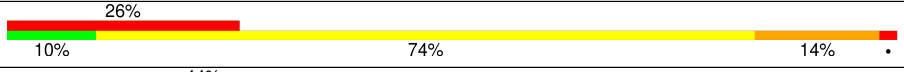
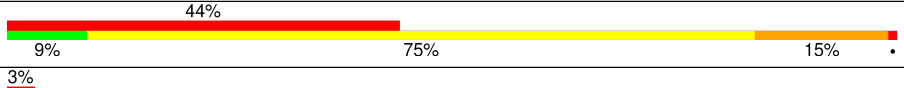
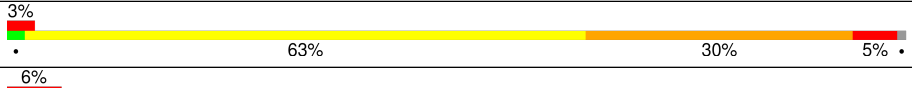
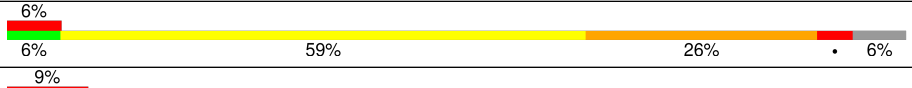
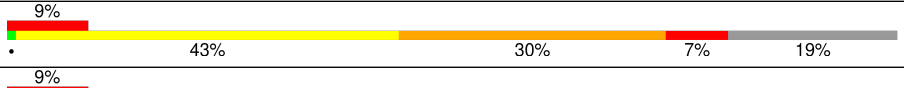
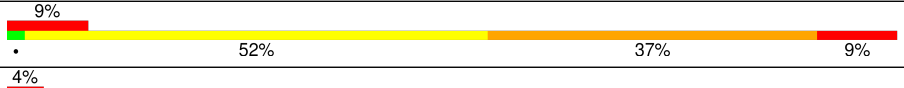
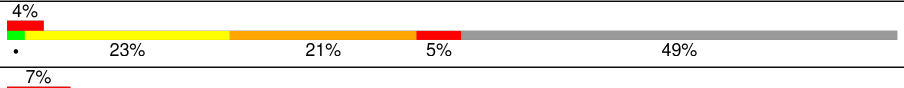
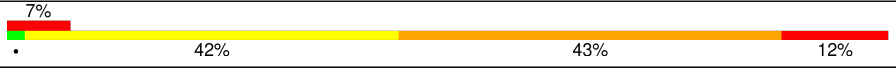
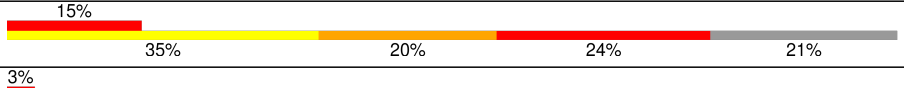
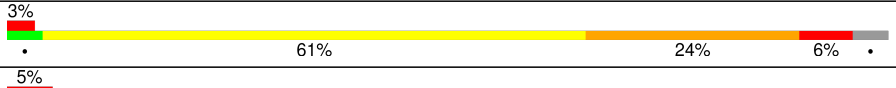
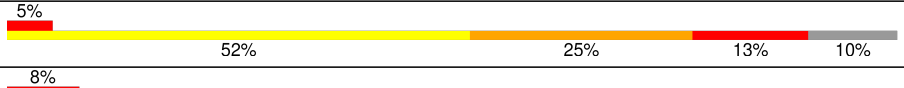
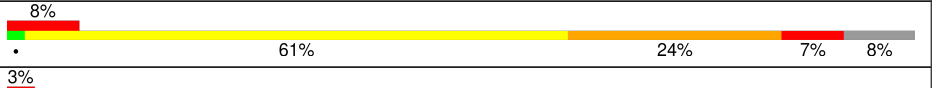
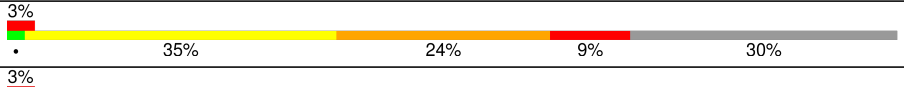
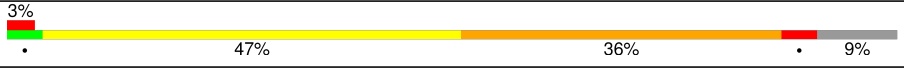
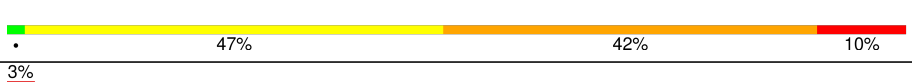
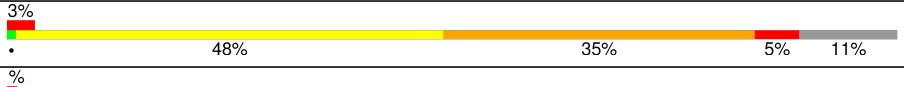
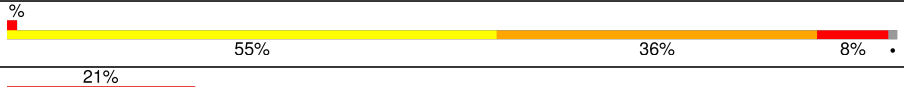
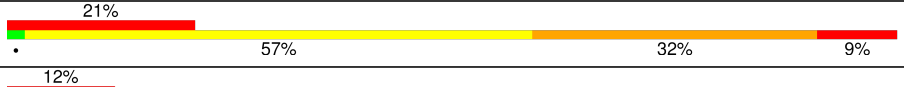
Mol	Chain	Length	Quality of chain
5	AE	338	
6	AF	246	
7	AG	176	
8	AH	177	
9	AI	128	
9	AJ	128	
10	AK	149	
11	AL	141	
12	AM	145	
13	AN	122	
14	AO	164	
15	AP	138	
16	AQ	186	
17	AR	66	
18	AS	113	
19	AT	84	
20	AU	119	
21	AV	253	
22	AW	70	
23	AX	60	
24	A0	118	
25	A1	118	
26	A2	100	
27	A3	91	
28	A4	73	

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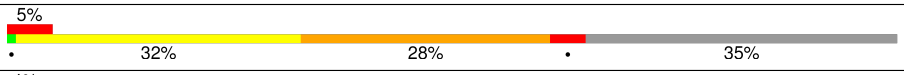
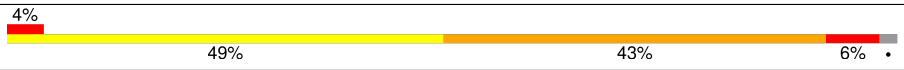
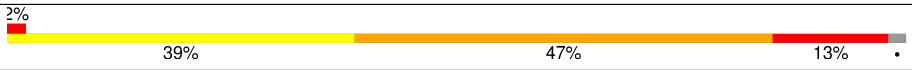
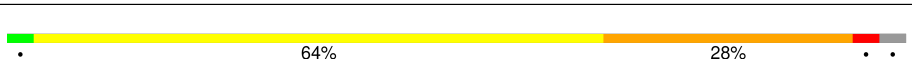
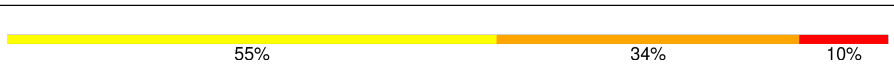
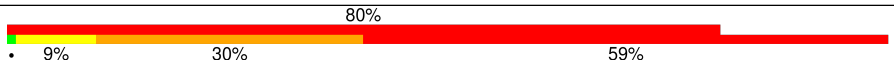
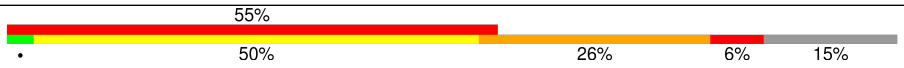
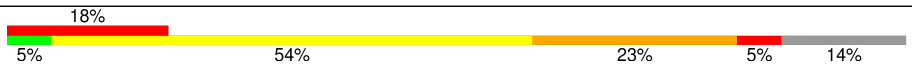
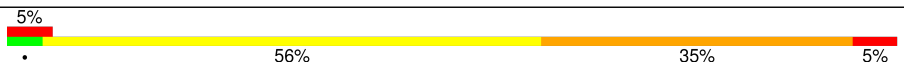
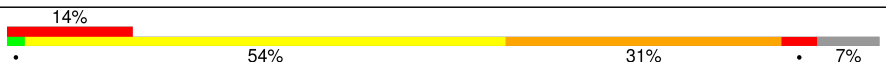
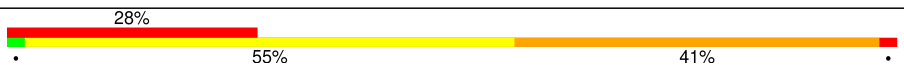
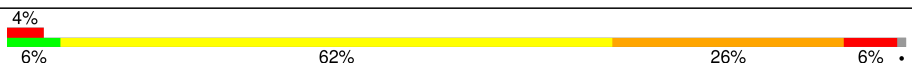
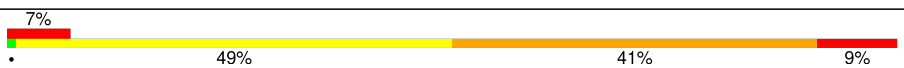
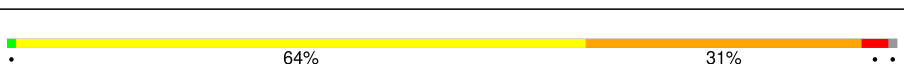
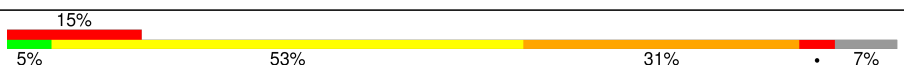
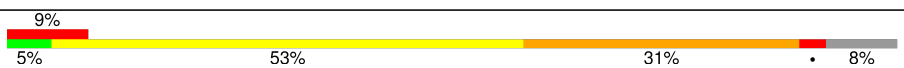
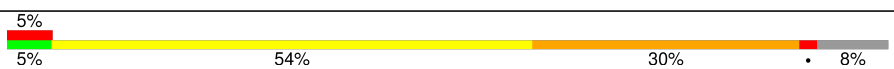
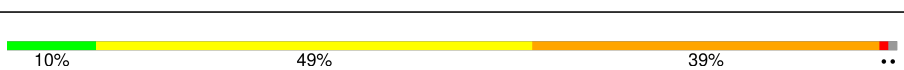
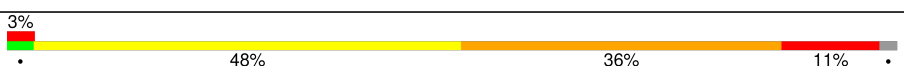
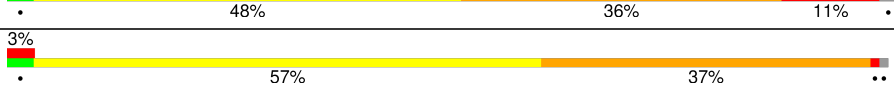
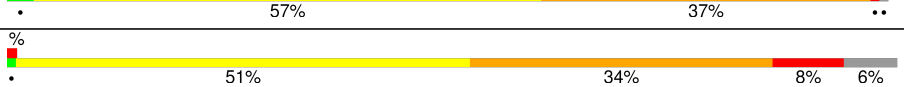
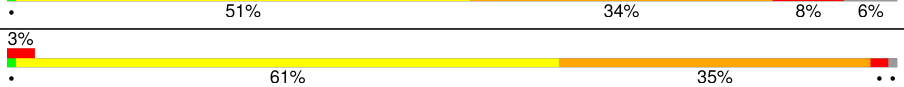
Mol	Chain	Length	Quality of chain
29	A5	60	
30	A6	82	
31	A7	47	
32	A8	64	
33	A9	36	
34	BA	1522	
35	BB	76	
35	BC	76	
36	B1	78	
37	BE	256	
38	BF	239	
39	BG	209	
40	BH	162	
41	BI	101	
42	BJ	156	
43	BK	138	
44	BL	128	
45	BM	105	
46	BN	129	
47	BO	135	
48	BP	126	
49	BQ	61	
50	BR	89	
51	BS	88	
52	BT	105	

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Mol	Chain	Length	Quality of chain
53	BU	88	
54	BV	93	
55	BW	106	
56	BX	27	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 148539 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AB	123	2641	1175	488	855	123	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	-1	A	-	INSERTION	GB 48271
AB	120	U	-	INSERTION	GB 48271

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AA	2872	61847	27526	11556	19893	2872	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	494	G	-	INSERTION	GB 48268

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	221	1687	1066	306	312	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0	0
			945	599	152	193	1			
9	AJ	128	Total	C	N	O	S	0	0	0
			945	599	152	193	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L11.

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

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S general stress protein CTC (L25).

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	A0	105	Total	C	N	O	0	0	0
			855	536	174	145			

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 35 is a RNA chain called tRNA Phe (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	76	Total	C	N	O	P	0	0	0
			1626	725	293	532	76			
35	BC	76	Total	C	N	O	P	0	0	0
			1626	725	293	532	76			

- Molecule 36 is a RNA chain called thrS mRNA operator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B1	66	Total	C	N	O	P	0	0	0
			1405	629	247	463	66			

- Molecule 37 is a protein called 30S ribosomal protein S2.

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

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	25	ASP	GLU	CONFLICT	UNP Q5SHQ2
BK	37	ARG	LYS	CONFLICT	UNP Q5SHQ2
BK	52	ASP	GLU	CONFLICT	UNP Q5SHQ2
BK	61	VAL	ILE	CONFLICT	UNP Q5SHQ2
BK	62	TYR	HIS	CONFLICT	UNP Q5SHQ2
BK	81	HIS	LYS	CONFLICT	UNP Q5SHQ2
BK	88	LYS	ARG	CONFLICT	UNP Q5SHQ2
BK	115	SER	PRO	CONFLICT	UNP Q5SHQ2

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

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

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	96	GLN	GLU	CONFLICT	UNP Q5SHP7

- Molecule 53 is a protein called 30S ribosomal protein S18.

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

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	41	VAL	ILE	CONFLICT	UNP Q5SIH2

- Molecule 56 is a protein called 30S ribosomal protein Thx.

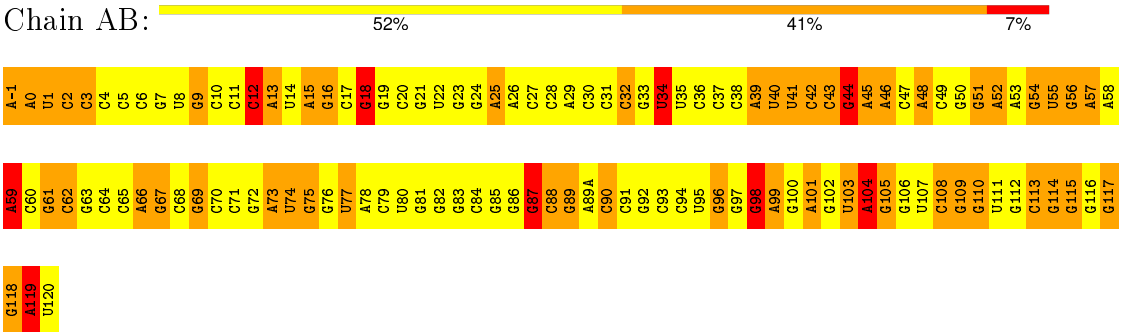
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	24	Total	C	N	O	0	0	0
			208	128	50	30			

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.

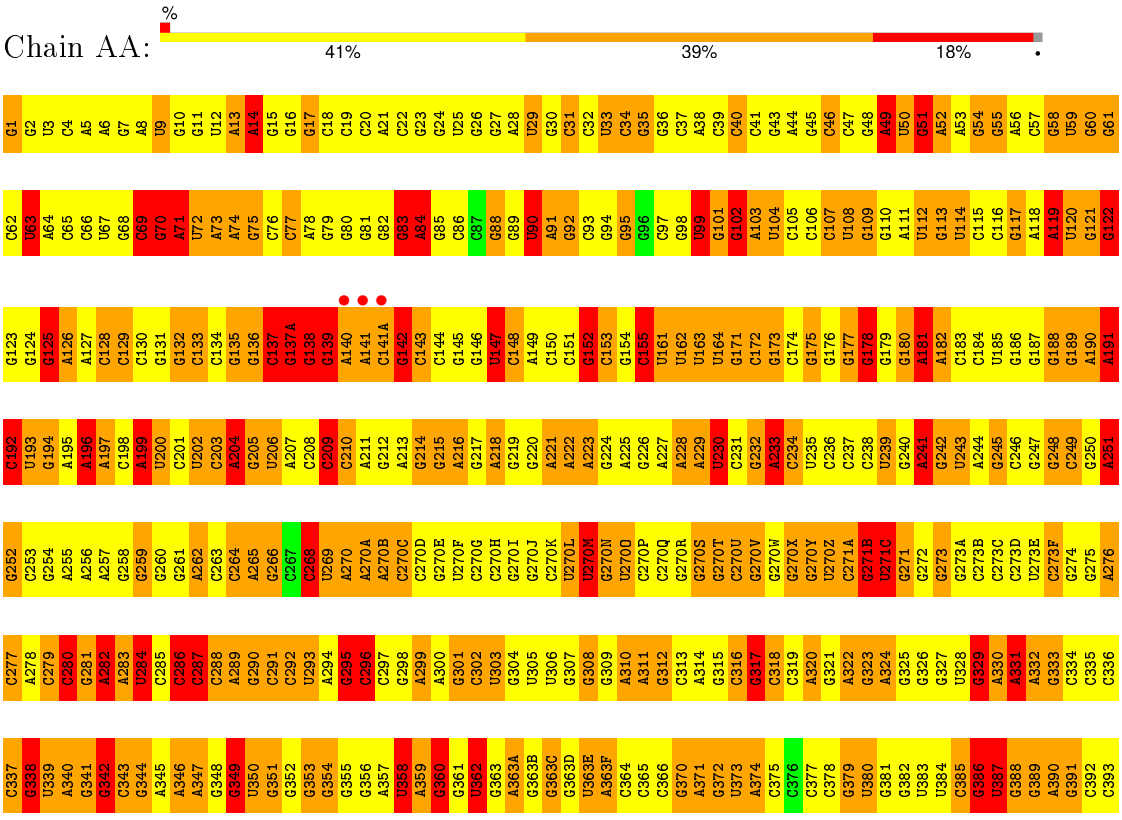
- Molecule 1: 5S ribosomal RNA

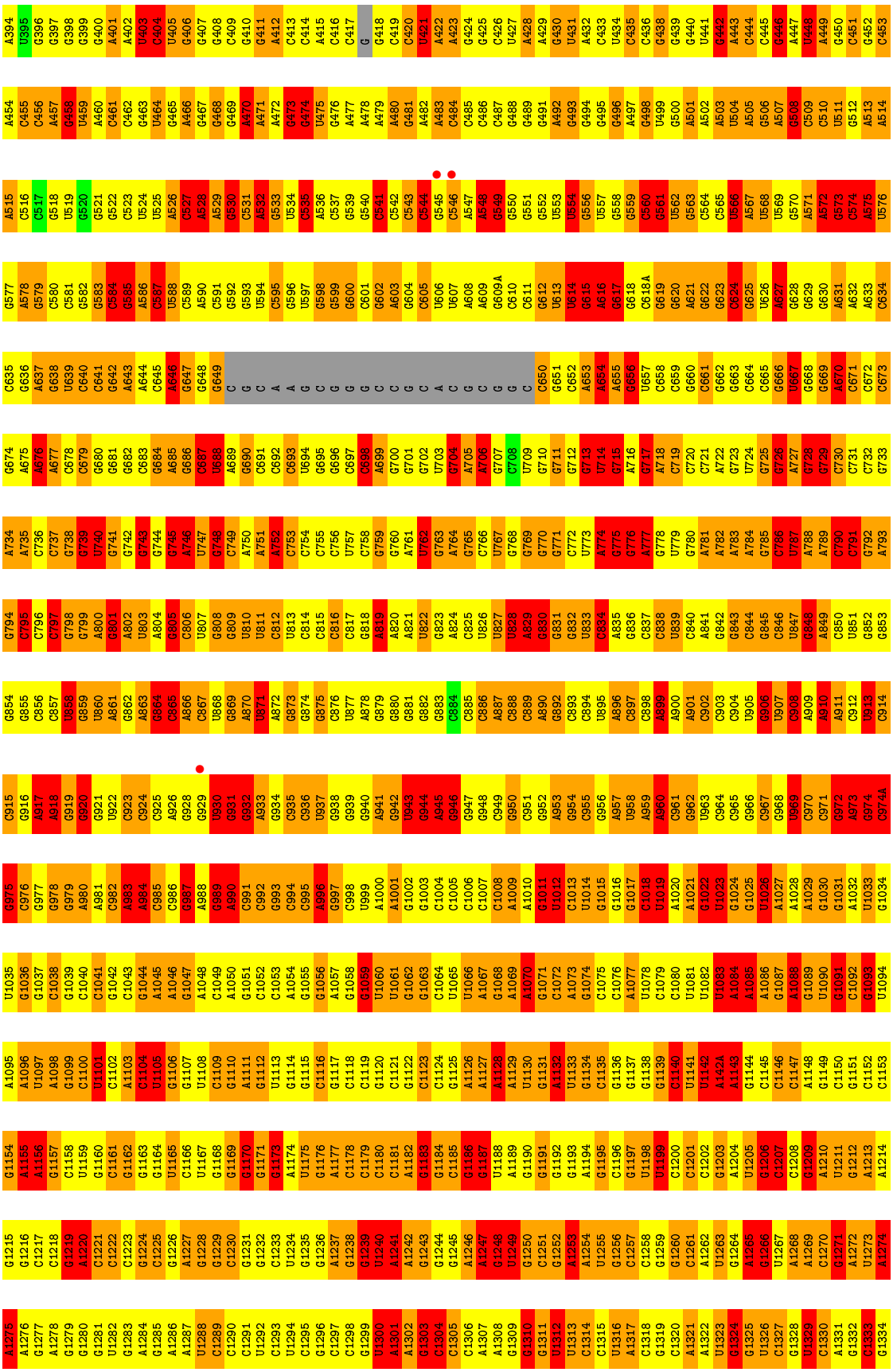
Chain AB:

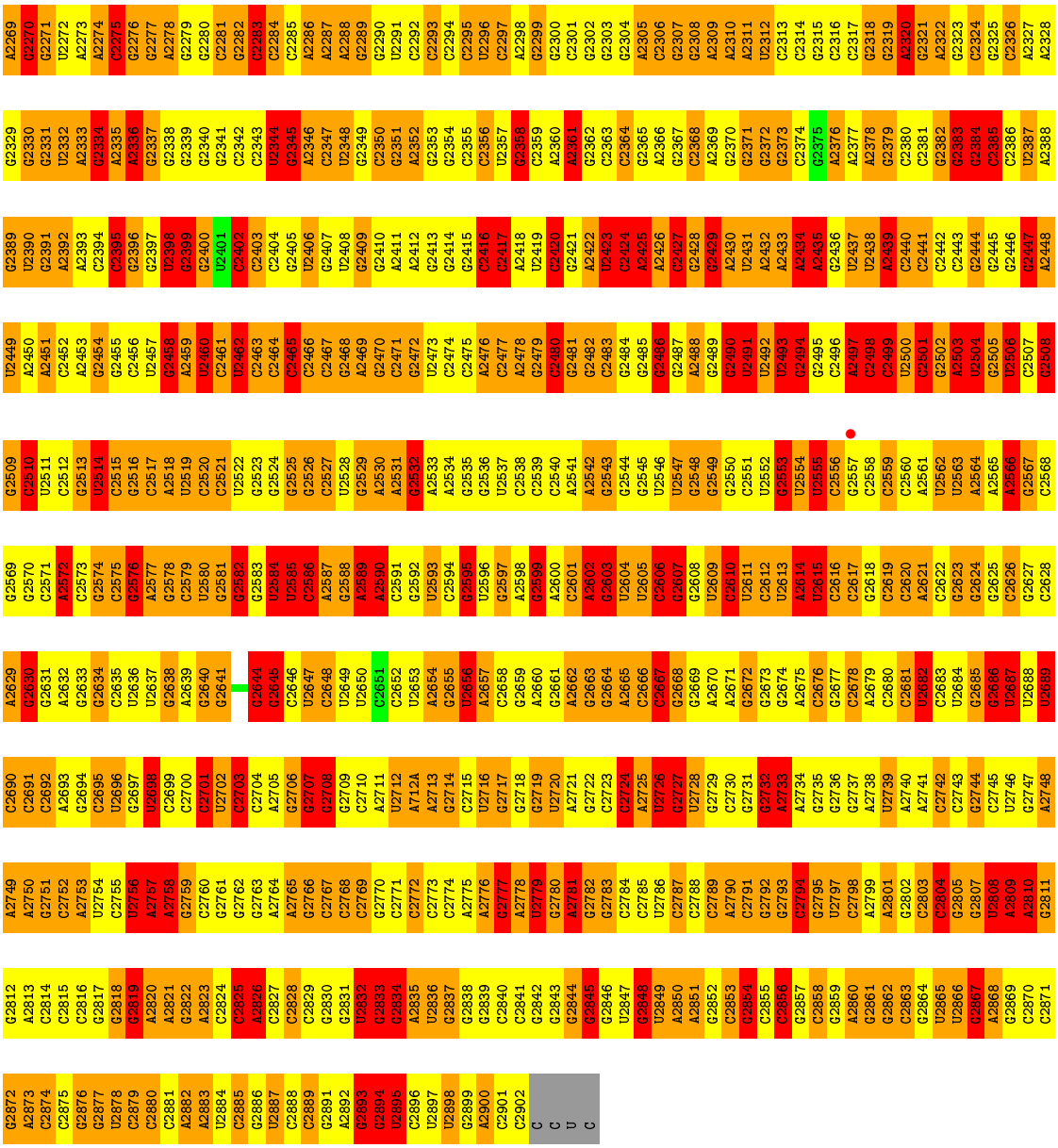


- Molecule 2: 23S ribosomal RNA

Chain AA:

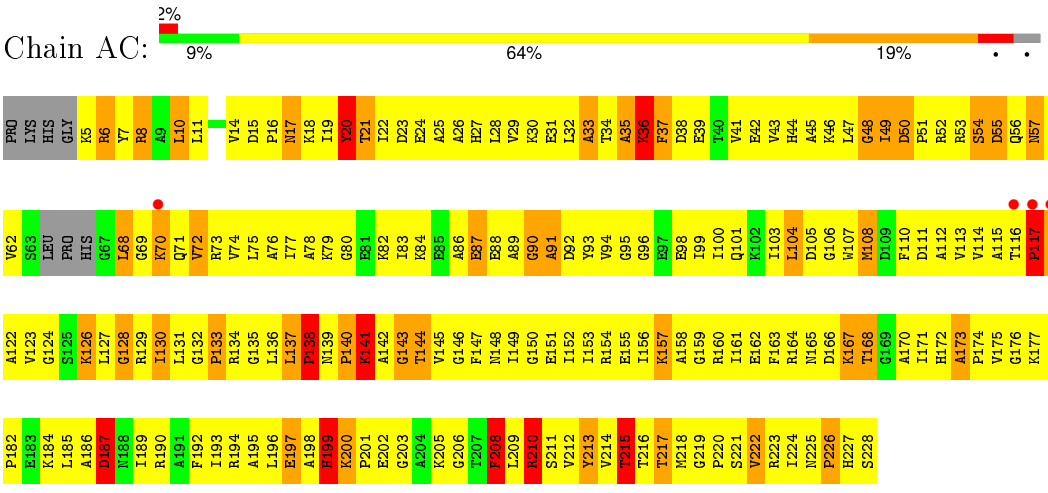






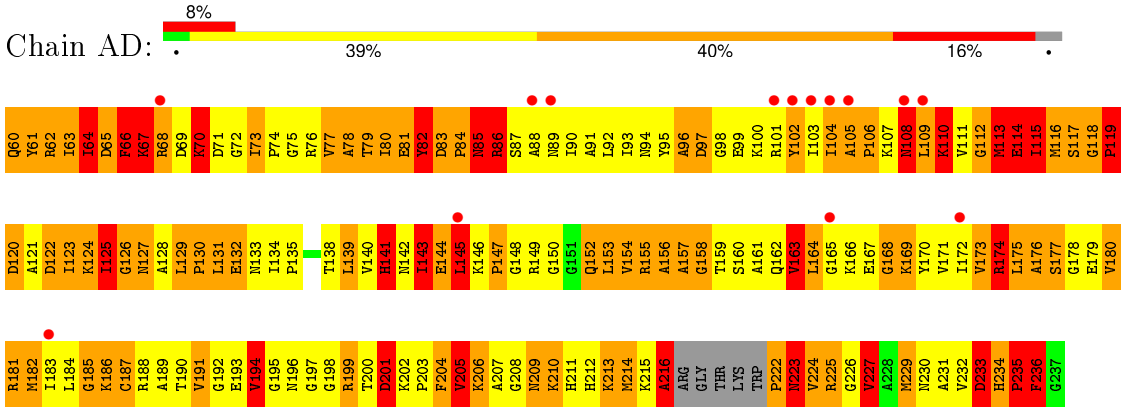
• Molecule 3: 50S ribosomal protein L1

Chain AC:



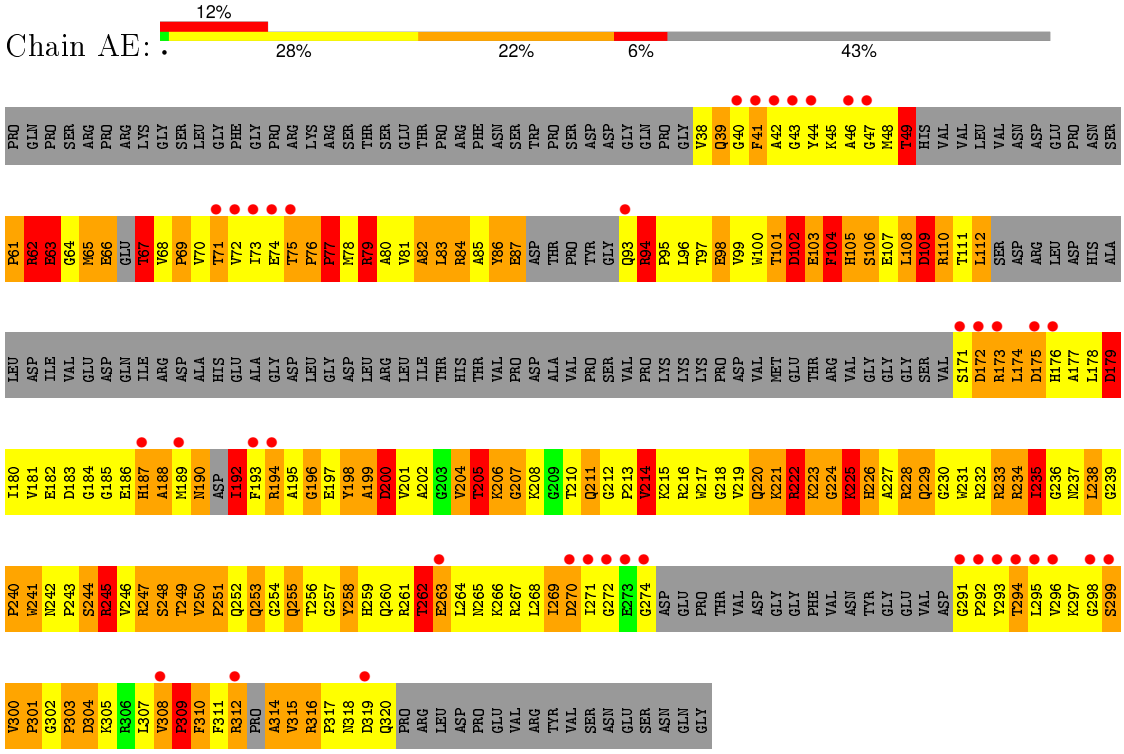
- Molecule 4: 50S ribosomal protein L2

Chain AD:



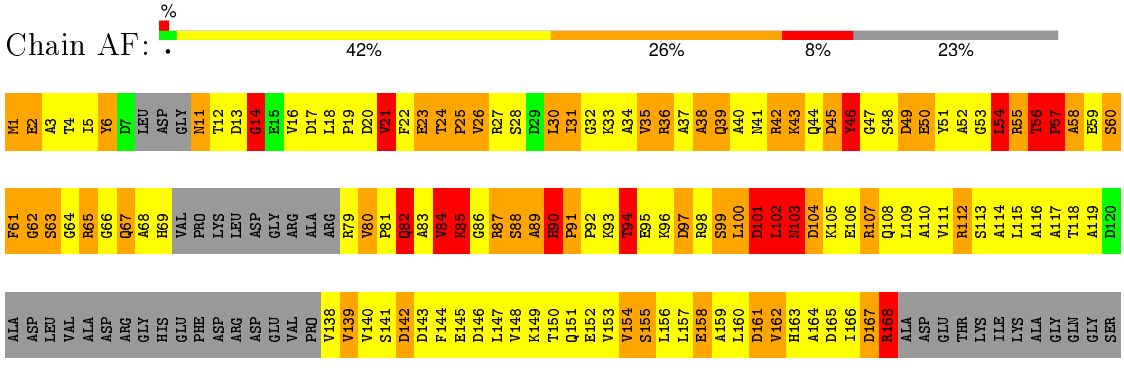
- Molecule 5: 50S ribosomal protein L3

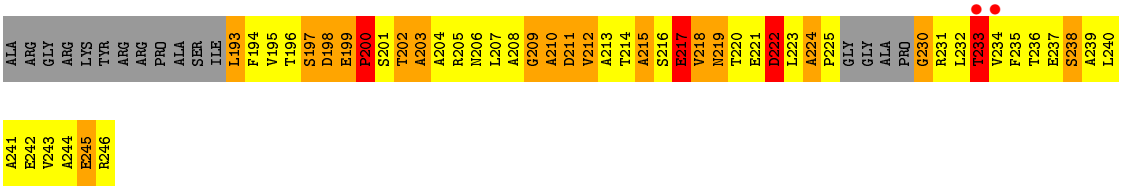
Chain AE:



- Molecule 6: 50S ribosomal protein L4

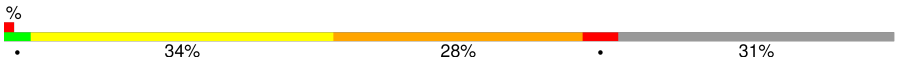
Chain AF:

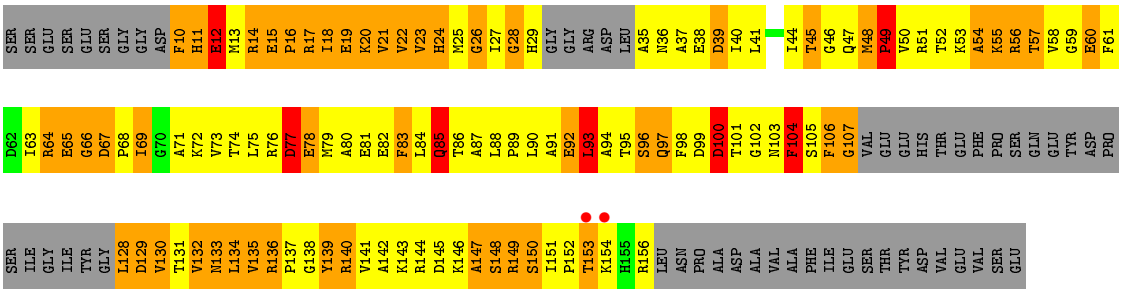




• Molecule 7: 50S ribosomal protein L5

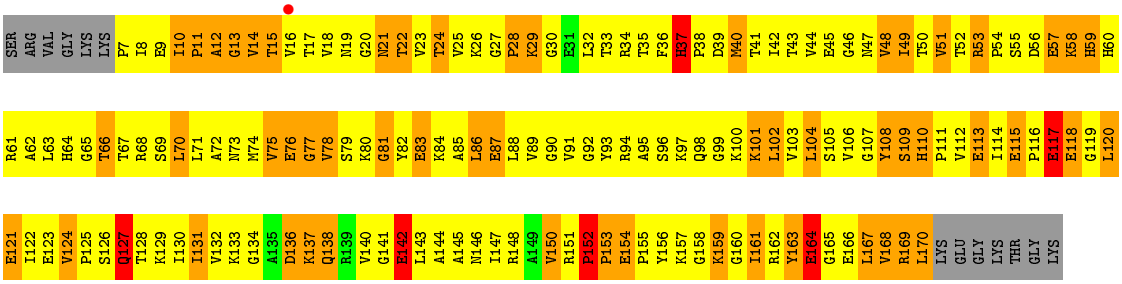
Chain AG:





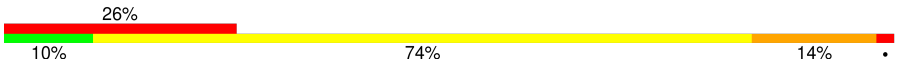
• Molecule 8: 50S ribosomal protein L6

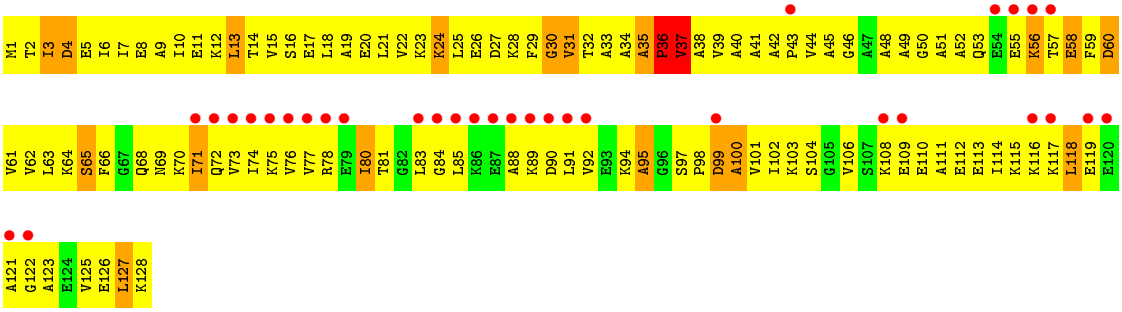
Chain AH:



• Molecule 9: 50S ribosomal protein L7/L12

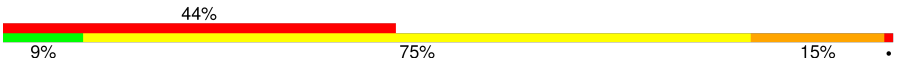
Chain AI:

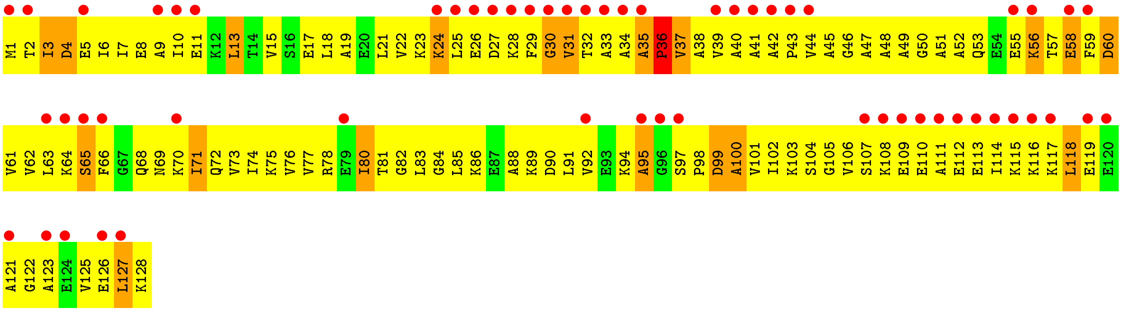




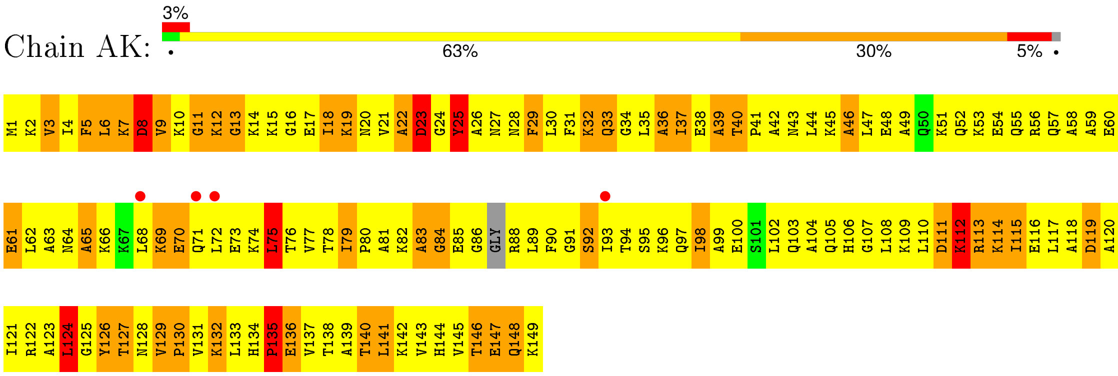
• Molecule 9: 50S ribosomal protein L7/L12

Chain AJ:

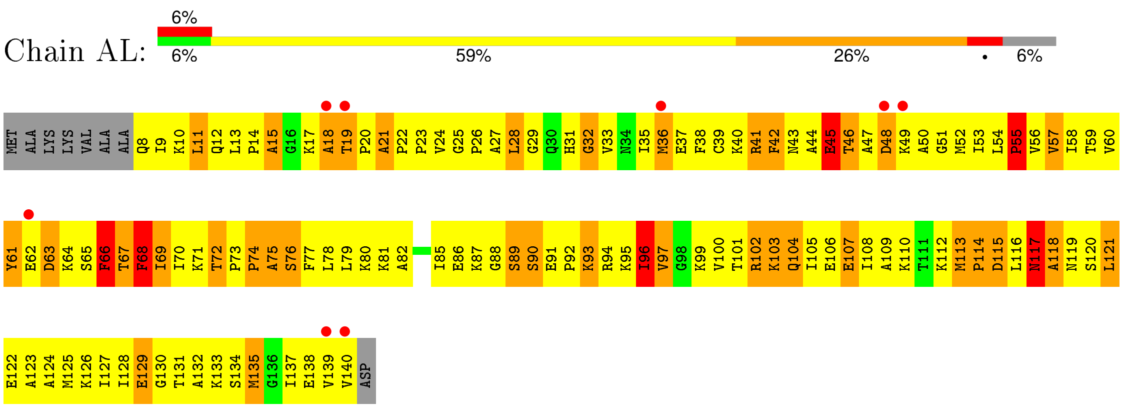




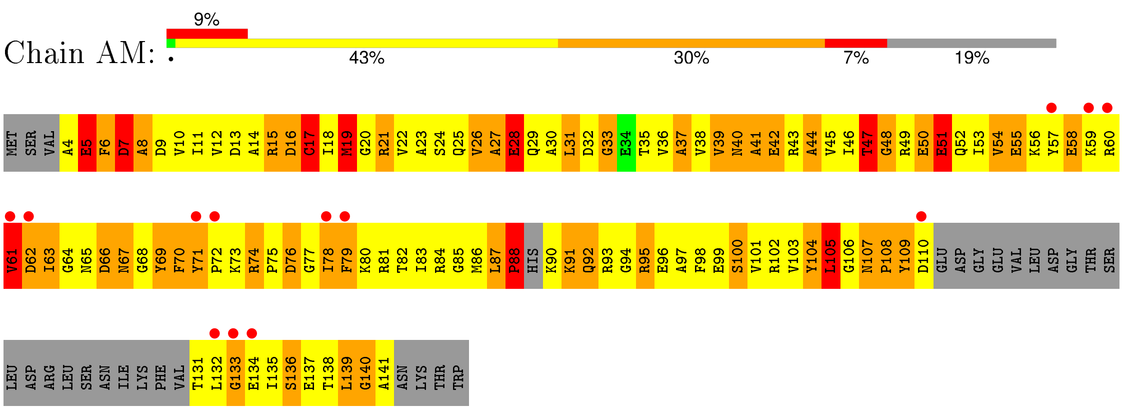
• Molecule 10: 50S ribosomal protein L9



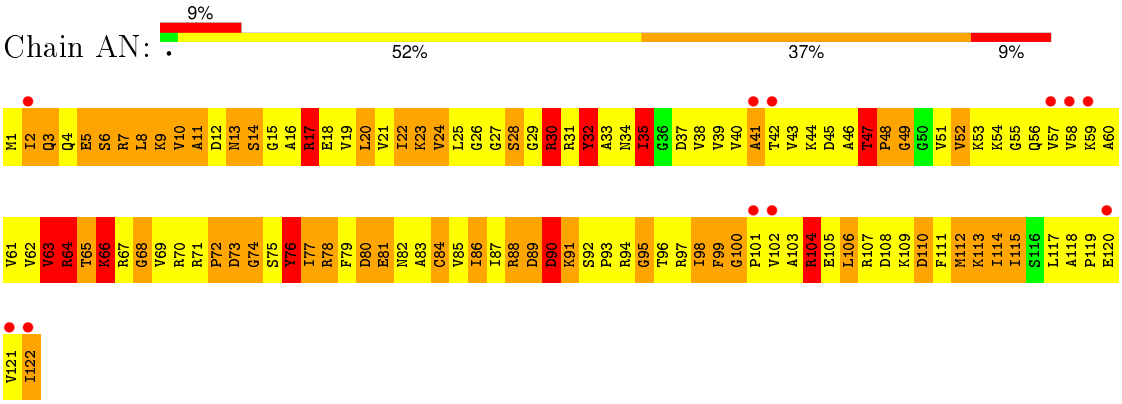
• Molecule 11: 50S ribosomal protein L11



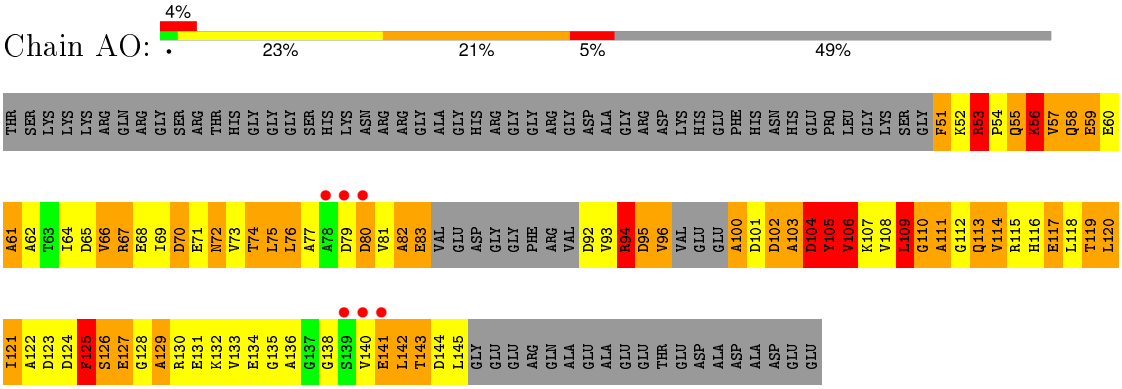
• Molecule 12: 50S ribosomal protein L13



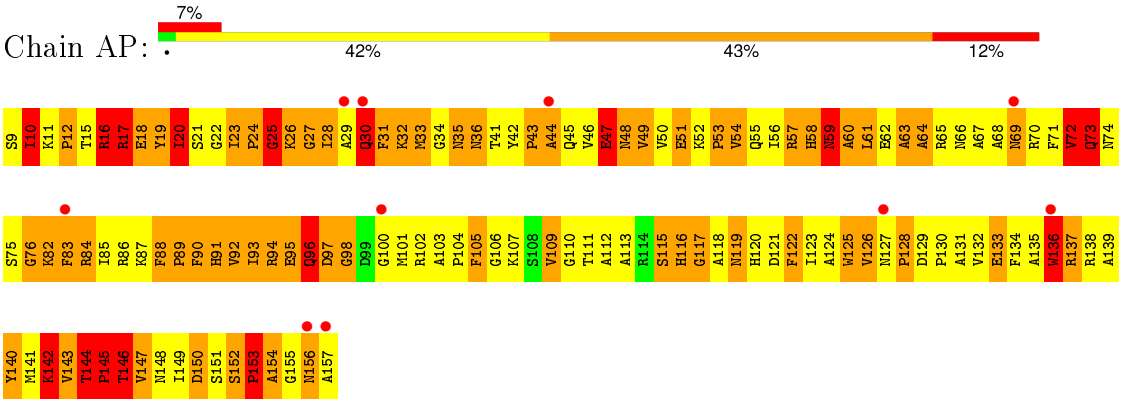
• Molecule 13: 50S ribosomal protein L14



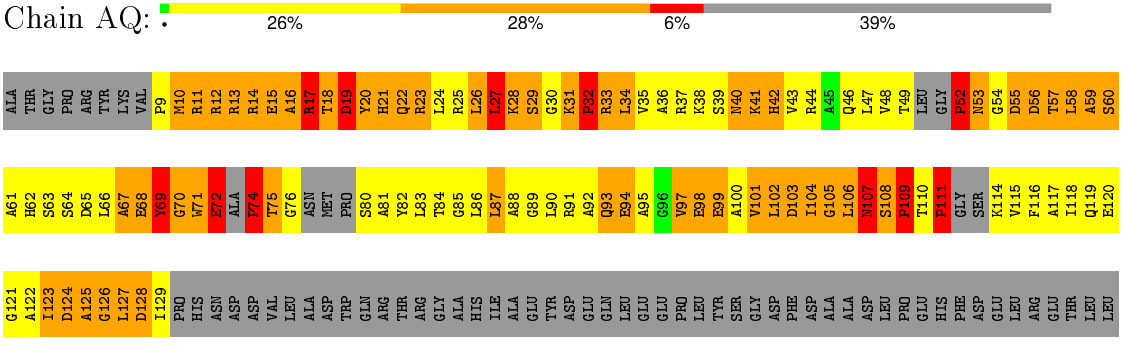
- Molecule 14: 50S ribosomal protein L15



- Molecule 15: 50S ribosomal protein L16

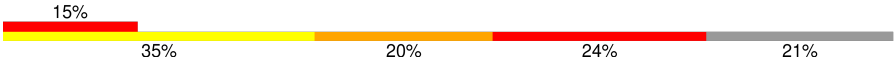


- Molecule 16: 50S ribosomal protein L18



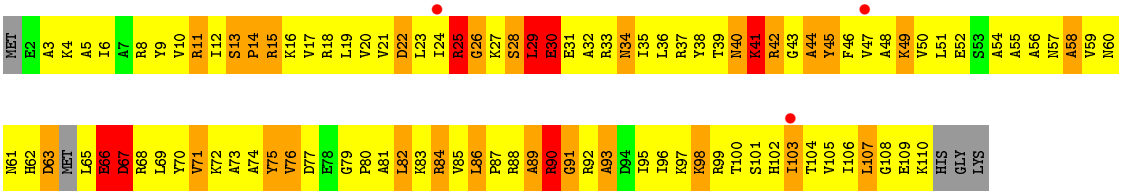
• Molecule 17: 50S ribosomal protein L19

Chain AR:



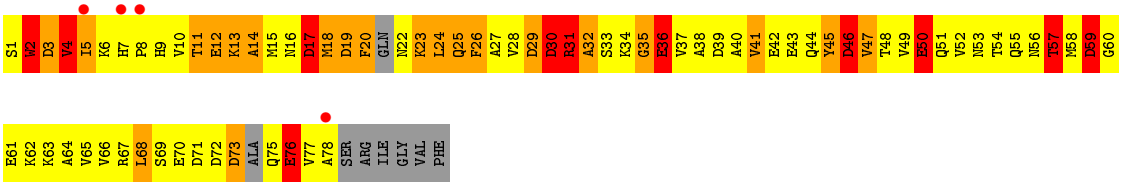
• Molecule 18: 50S ribosomal protein L22

Chain AS:



• Molecule 19: 50S ribosomal protein L23

Chain AT:

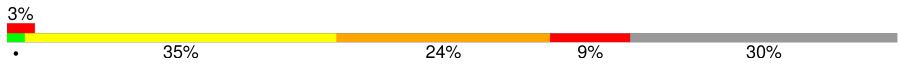


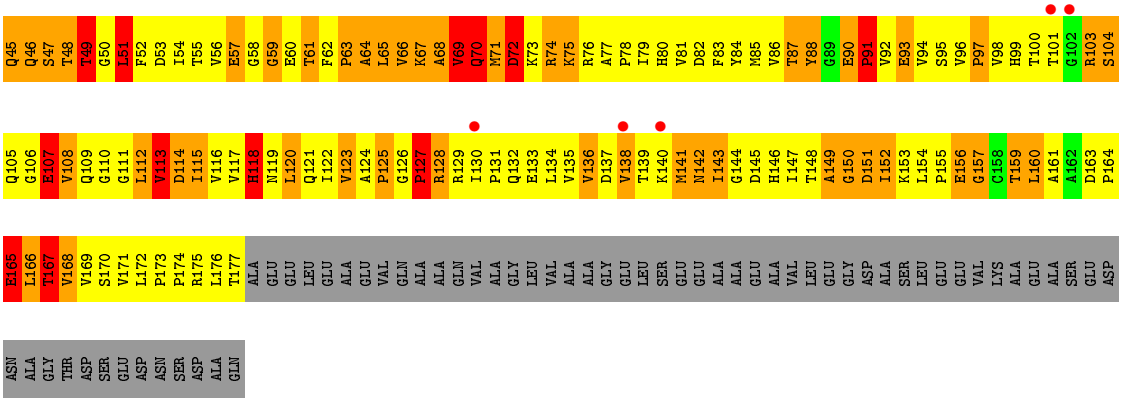
• Molecule 20: 50S ribosomal protein L24

Chain AU:

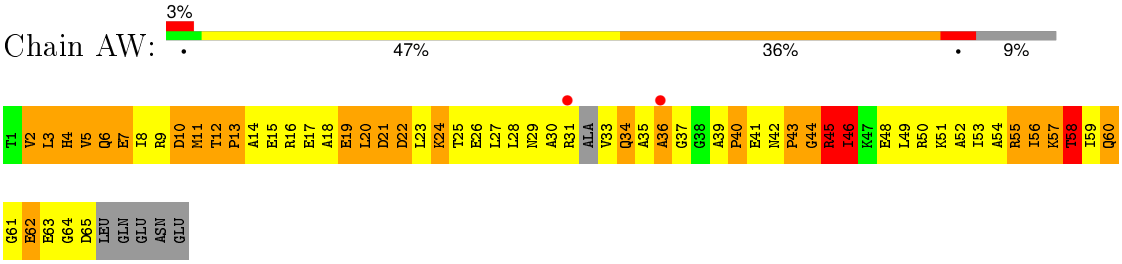
• Molecule 21: 50S general stress protein CTC (L25)

Chain AV:

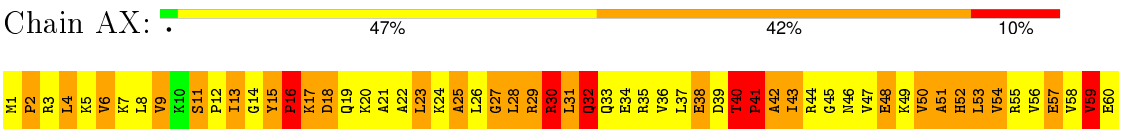




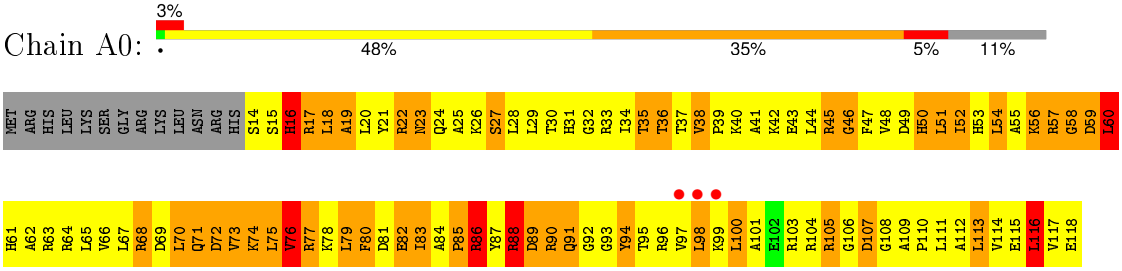
• Molecule 22: 50S ribosomal protein L29



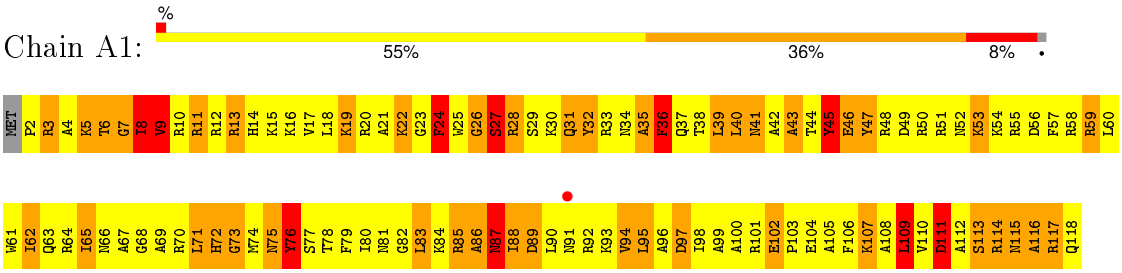
• Molecule 23: 50S ribosomal protein L30



• Molecule 24: 50S ribosomal protein L17

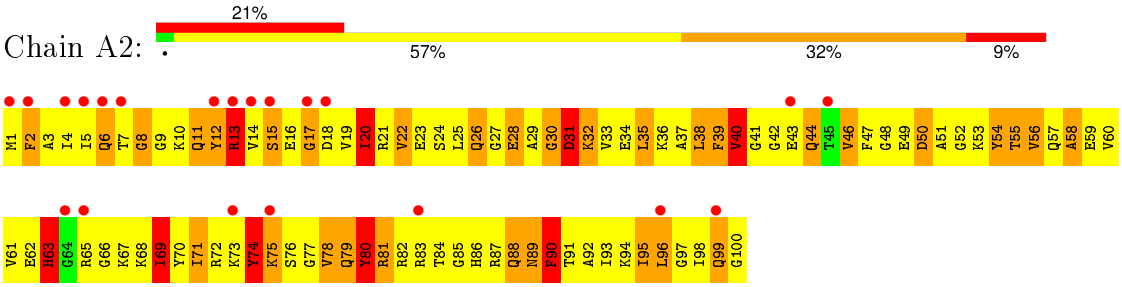


• Molecule 25: 50S ribosomal protein L20



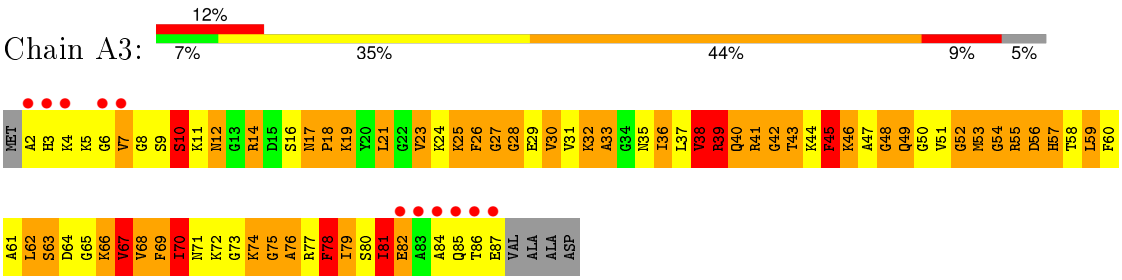
• Molecule 26: 50S ribosomal protein L21

Chain A2:



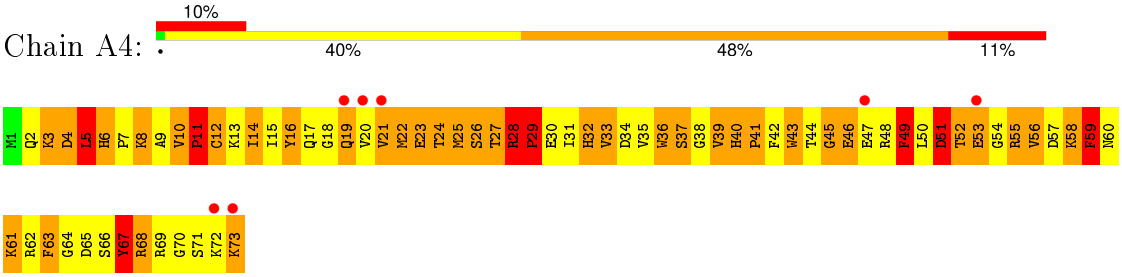
• Molecule 27: 50S ribosomal protein L27

Chain A3:



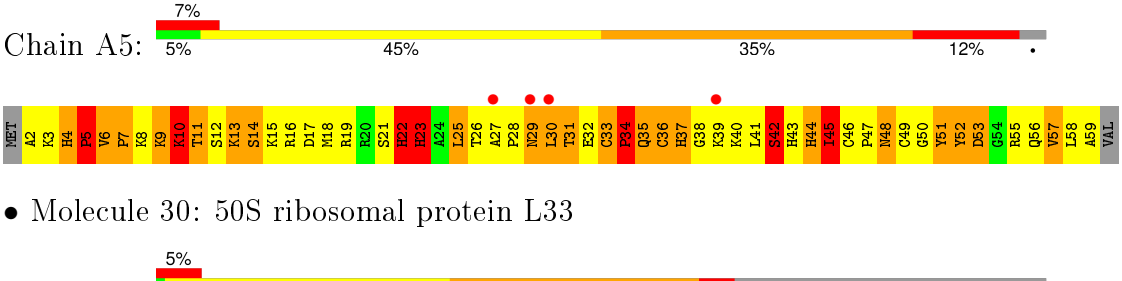
• Molecule 28: 50S ribosomal protein L31

Chain A4:



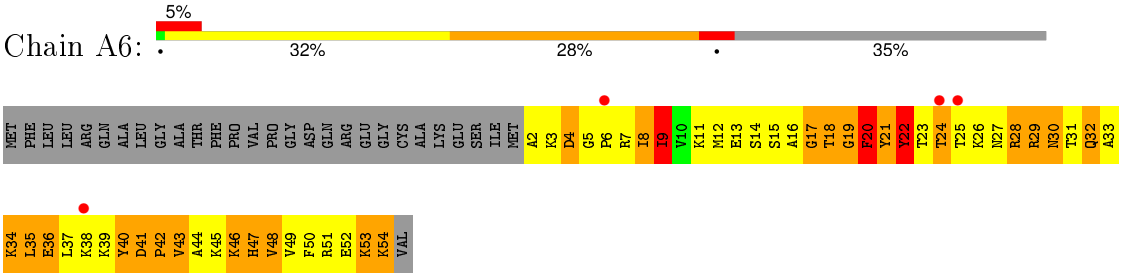
• Molecule 29: 50S ribosomal protein L32

Chain A5:



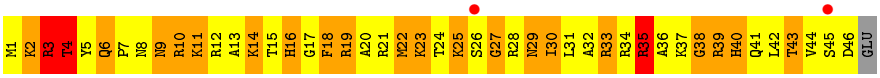
• Molecule 30: 50S ribosomal protein L33

Chain A6:



• Molecule 31: 50S ribosomal protein L34

Chain A7:

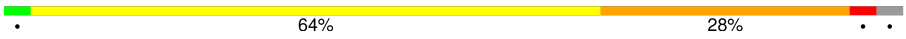


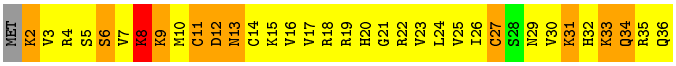
- Molecule 32: 50S ribosomal protein L35

Chain A8:

- Molecule 33: 50S ribosomal protein L36

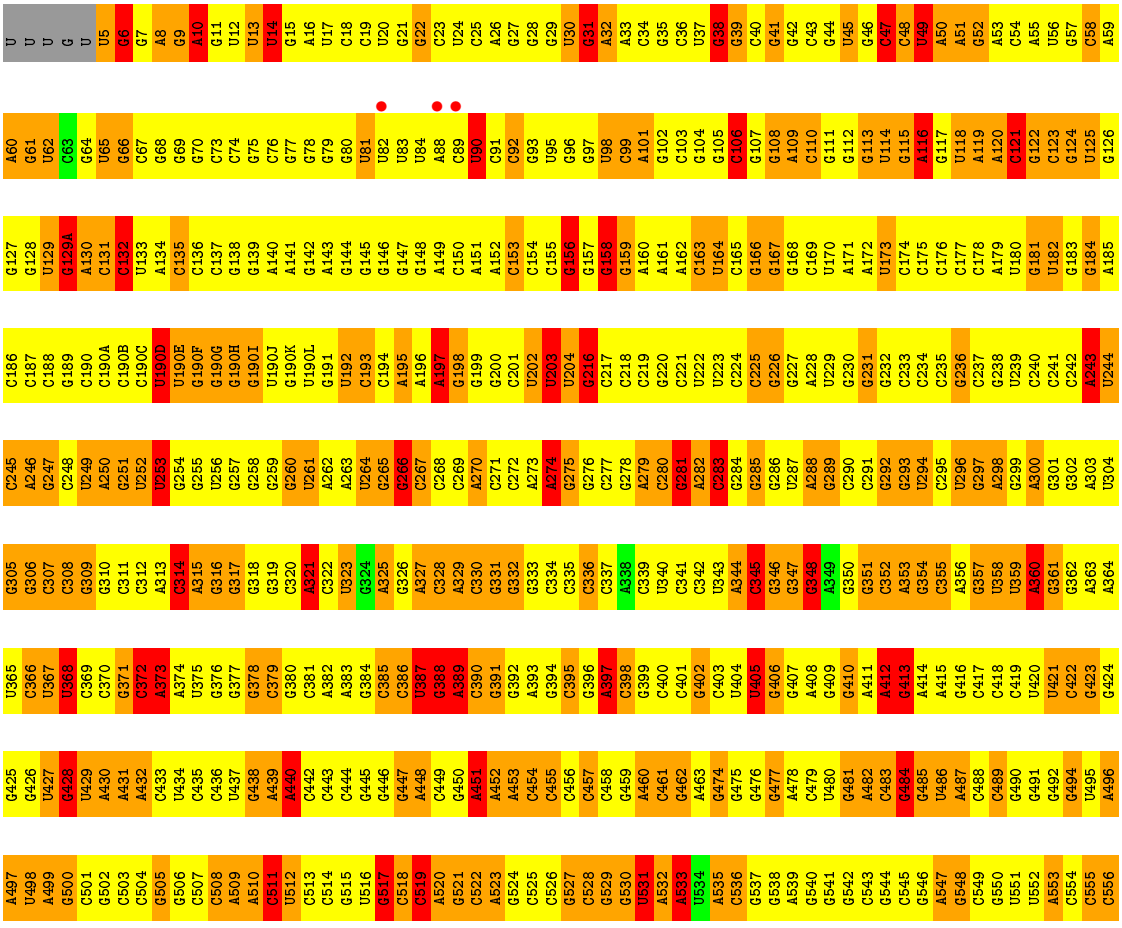
Chain A9:

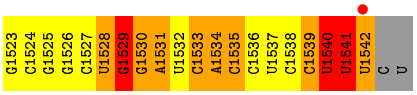




- Molecule 34: 16S rRNA

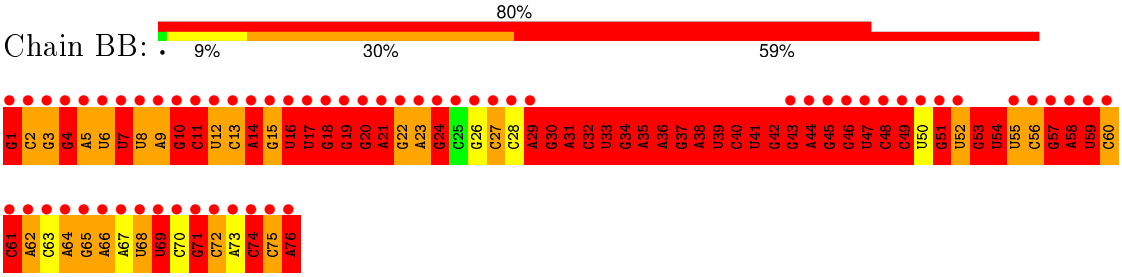
Chain BA:





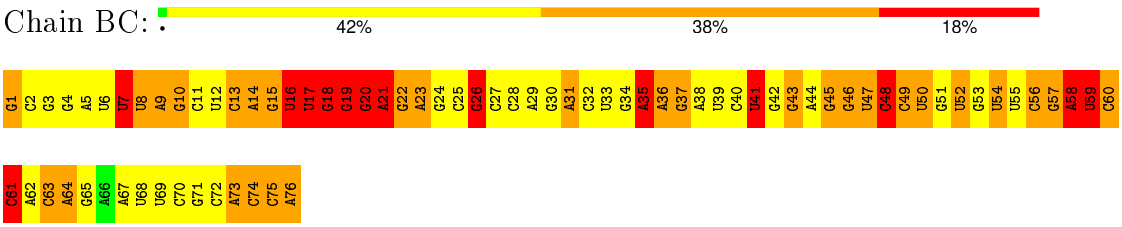
- Molecule 35: tRNA Phe (unmodified bases)

Chain BB:



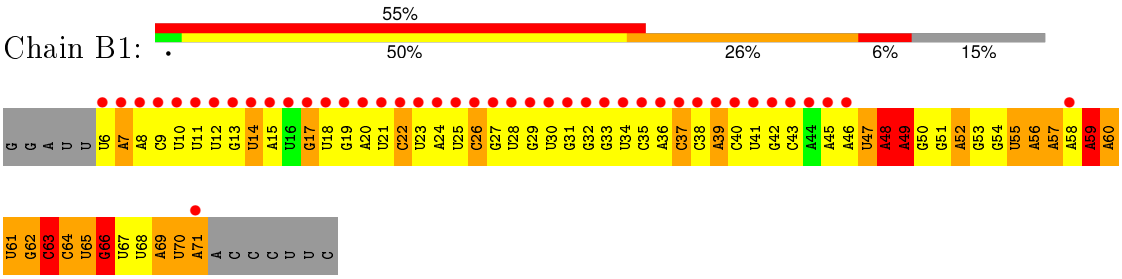
- Molecule 35: tRNA Phe (unmodified bases)

Chain BC:



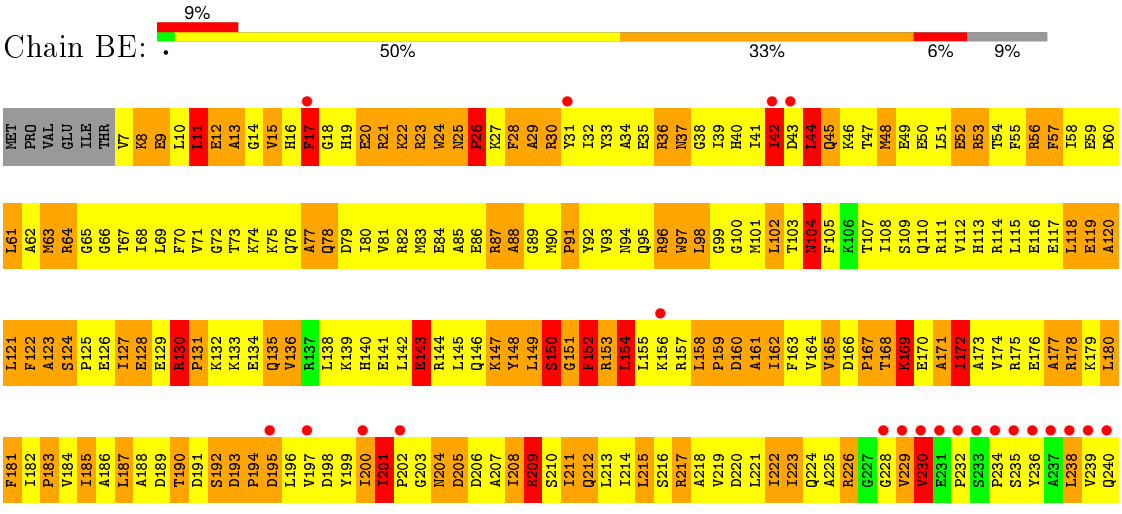
- Molecule 36: thrS mRNA operator

Chain B1:



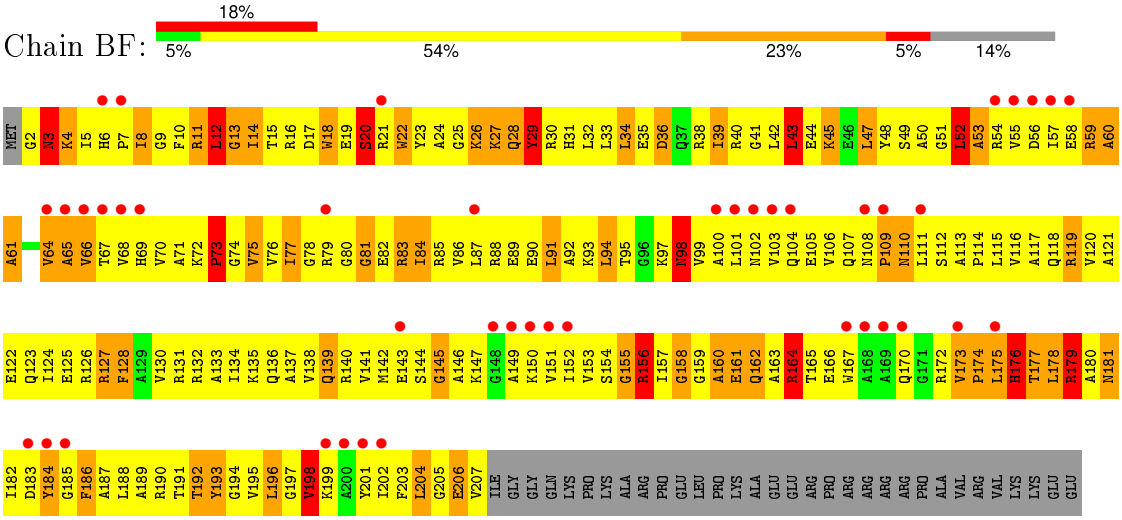
- Molecule 37: 30S ribosomal protein S2

Chain BE:



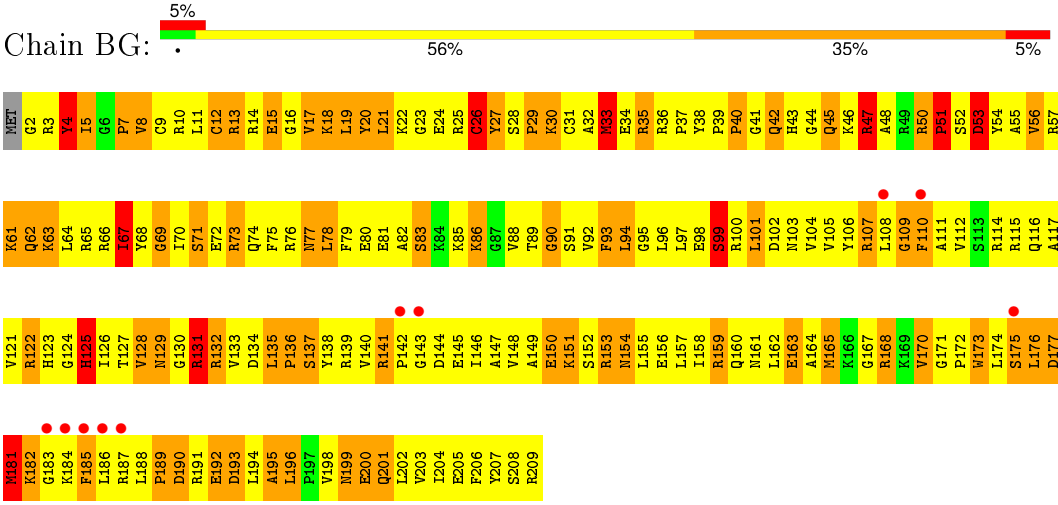
- Molecule 38: 30S ribosomal protein S3

Chain BF:



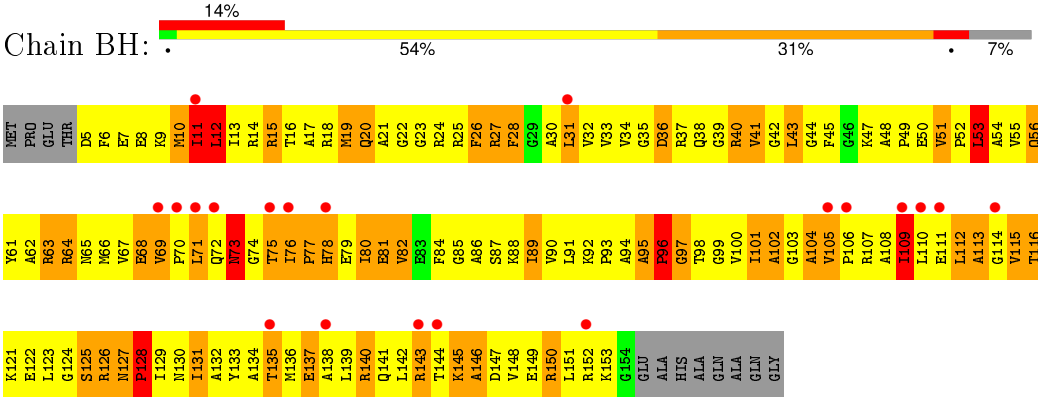
- Molecule 39: 30S ribosomal protein S4

Chain BG:



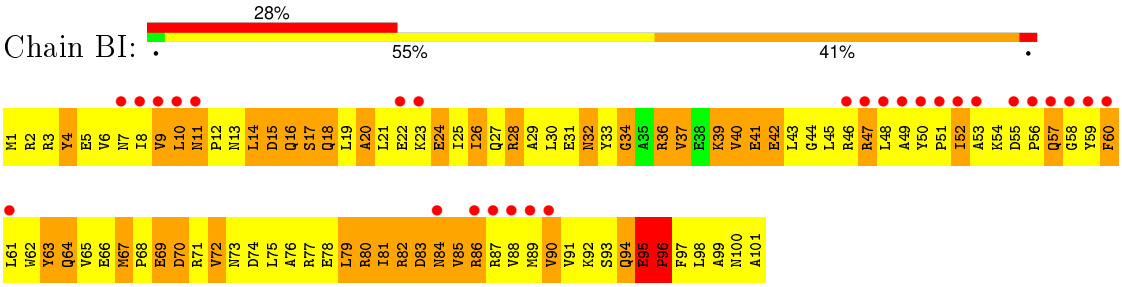
- Molecule 40: 30S ribosomal protein S5

Chain BH:



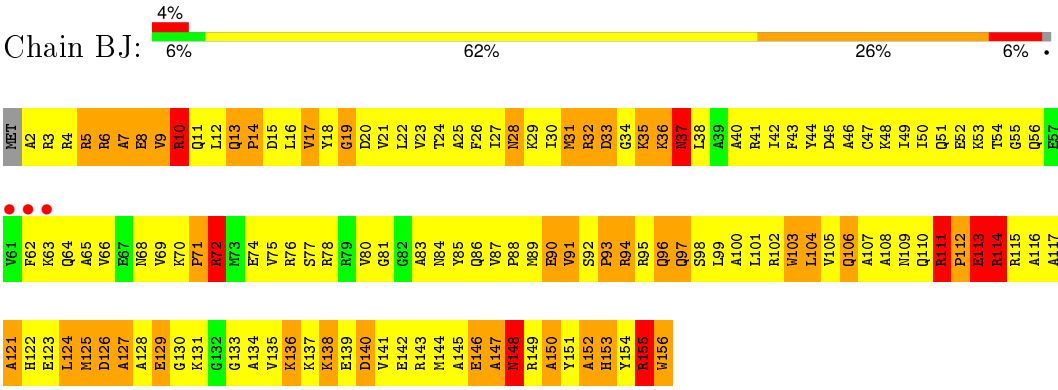
- Molecule 41: 30S ribosomal protein S6

Chain BI:



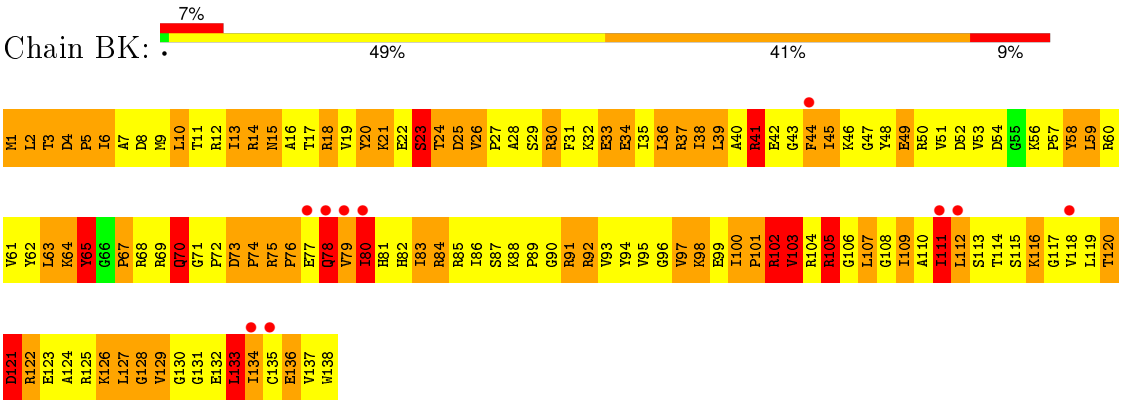
- Molecule 42: 30S ribosomal protein S7

Chain BJ:



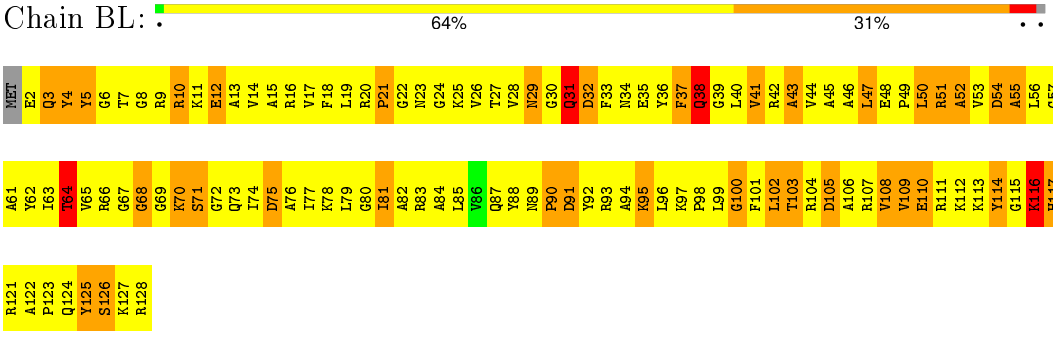
- Molecule 43: 30S ribosomal protein S8

Chain BK:



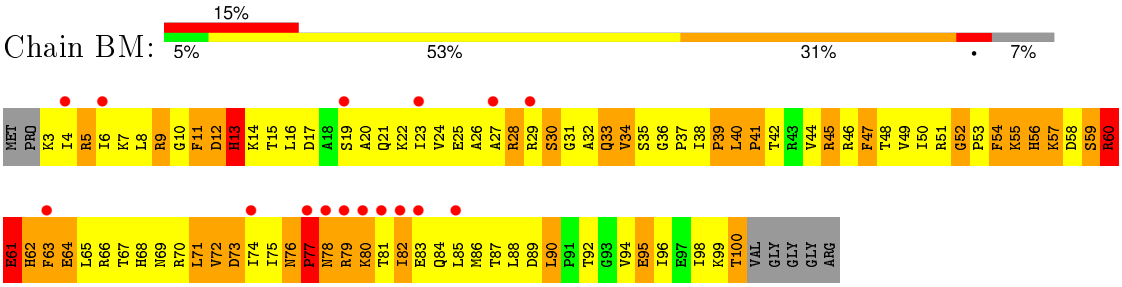
- Molecule 44: 30S ribosomal protein S9

Chain BL:



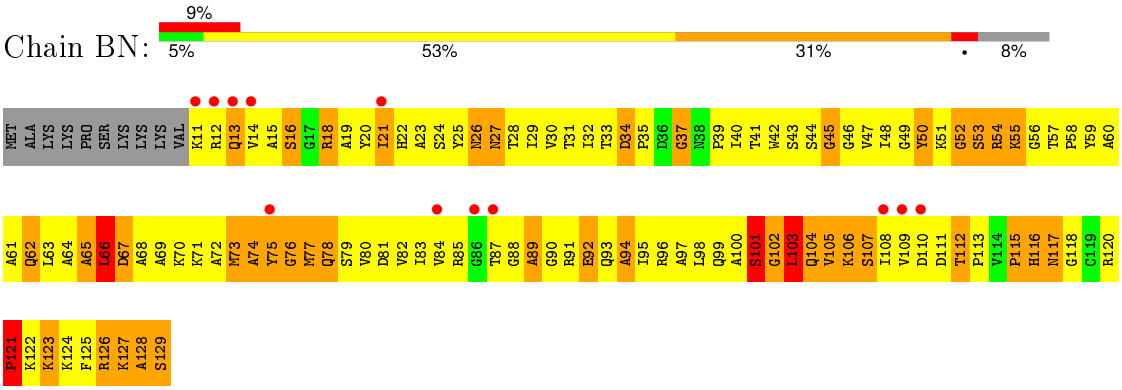
- Molecule 45: 30S ribosomal protein S10

Chain BM:



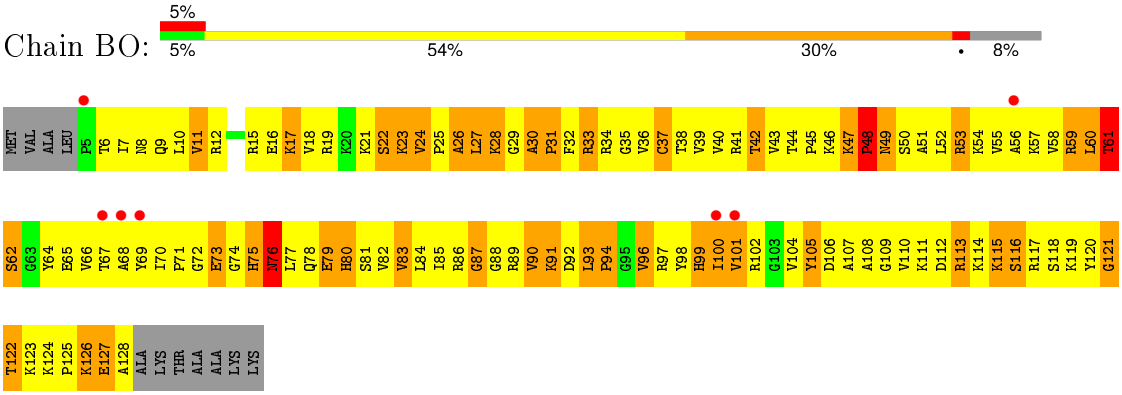
• Molecule 46: 30S ribosomal protein S11

Chain BN:



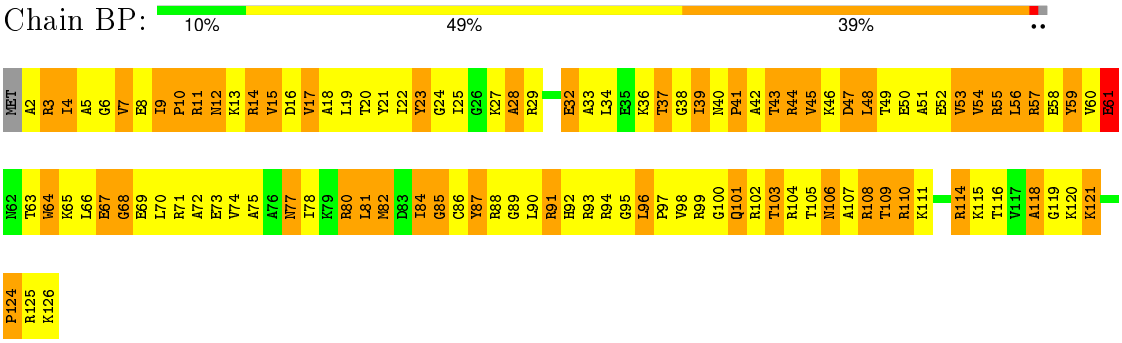
• Molecule 47: 30S ribosomal protein S12

Chain BO:



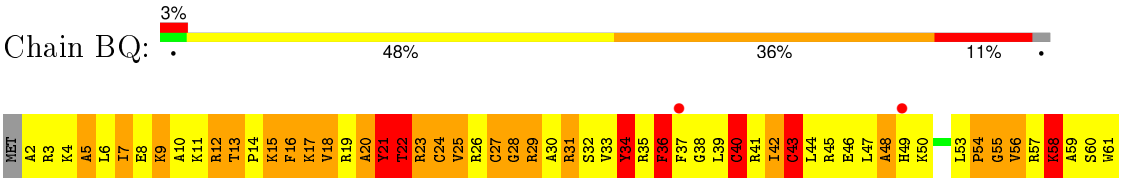
• Molecule 48: 30S ribosomal protein S13

Chain BP:



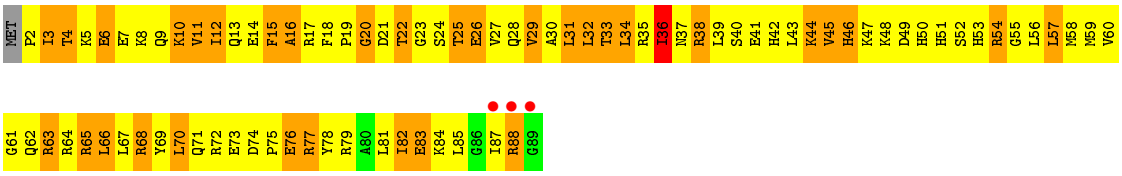
• Molecule 49: 30S ribosomal protein S14

Chain BQ:



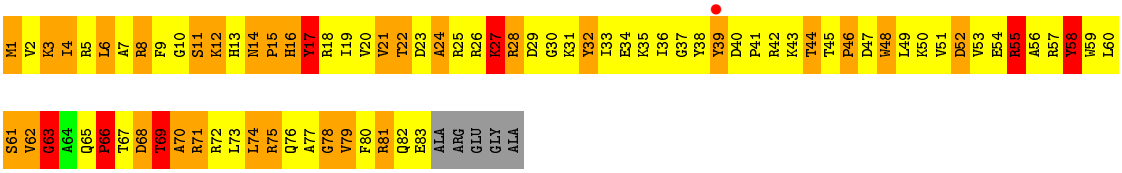
- Molecule 50: 30S ribosomal protein S15

Chain BR:



- Molecule 51: 30S ribosomal protein S16

Chain BS:

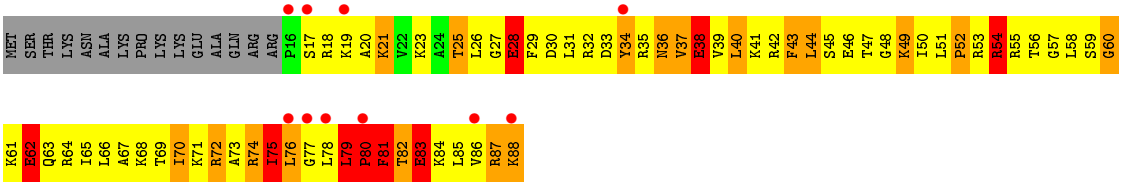


- Molecule 52: 30S ribosomal protein S17

Chain BT:

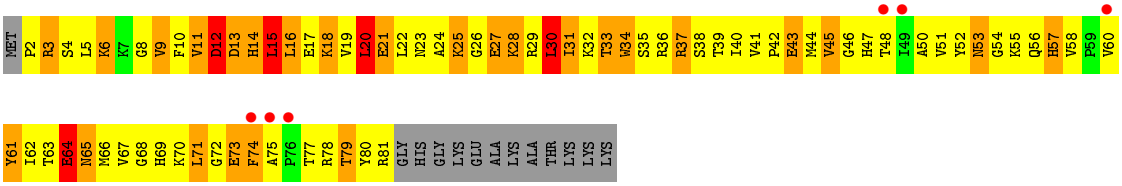
- Molecule 53: 30S ribosomal protein S18

Chain BU:



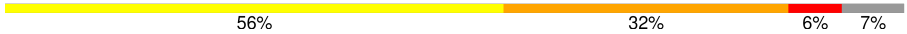
- Molecule 54: 30S ribosomal protein S19

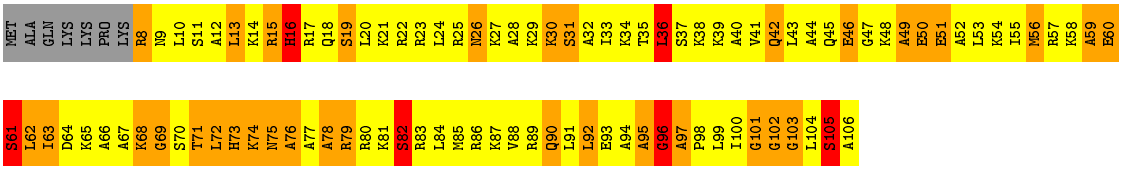
Chain BV:



- Molecule 55: 30S ribosomal protein S20

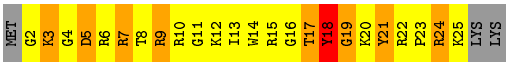
Chain BW:





- Molecule 56: 30S ribosomal protein Thx

Chain BX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	508.64Å 508.64Å 806.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 268.38 – 5.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (300.00-5.50) 97.5 (268.38-5.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 5.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.307 , 0.356 0.308 , 0.354	Depositor DCC
R_{free} test set	7724 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	206.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.11 , 178.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 169564 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	148539	wwPDB-VP
Average B, all atoms (Å^2)	338.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AB	0.95	1/2954 (0.0%)	1.06	7/4606 (0.2%)
2	AA	1.16	181/69267 (0.3%)	1.22	549/108130 (0.5%)
3	AC	0.62	0/1715	0.94	2/2310 (0.1%)
4	AD	1.11	6/1329 (0.5%)	1.52	22/1787 (1.2%)
5	AE	1.04	3/1542 (0.2%)	1.41	21/2084 (1.0%)
6	AF	0.82	0/1446	1.26	14/1960 (0.7%)
7	AG	0.83	0/972	1.20	6/1307 (0.5%)
8	AH	0.76	0/1272	1.13	1/1721 (0.1%)
9	AI	0.48	0/950	0.72	0/1275
9	AJ	0.43	0/950	0.68	0/1275
10	AK	0.73	0/1157	1.17	8/1547 (0.5%)
11	AL	0.48	0/1015	0.91	4/1366 (0.3%)
12	AM	1.04	2/928 (0.2%)	1.23	2/1248 (0.2%)
13	AN	1.06	2/946 (0.2%)	1.43	14/1269 (1.1%)
14	AO	0.67	0/643	1.30	9/870 (1.0%)
15	AP	1.04	1/1109 (0.1%)	1.43	16/1499 (1.1%)
16	AQ	0.71	0/880	1.23	5/1189 (0.4%)
17	AR	1.37	4/413 (1.0%)	2.01	18/557 (3.2%)
18	AS	0.81	0/869	1.19	3/1166 (0.3%)
19	AT	0.76	0/609	1.05	0/823
20	AU	0.46	0/887	0.89	0/1195
21	AV	0.71	0/1385	1.10	7/1883 (0.4%)
22	AW	0.73	0/497	1.05	1/668 (0.1%)
23	AX	0.81	0/482	1.18	2/646 (0.3%)
24	A0	0.86	0/867	1.24	3/1162 (0.3%)
25	A1	1.03	0/994	1.33	6/1323 (0.5%)
26	A2	0.71	0/797	1.14	4/1061 (0.4%)
27	A3	0.72	0/649	1.14	3/860 (0.3%)
28	A4	0.97	1/620 (0.2%)	1.18	4/831 (0.5%)
29	A5	0.79	0/469	1.41	5/629 (0.8%)
30	A6	0.93	0/438	1.25	4/583 (0.7%)
31	A7	0.78	0/387	1.05	0/509
32	A8	0.98	2/503 (0.4%)	1.48	8/657 (1.2%)
33	A9	1.36	1/286 (0.3%)	1.44	4/375 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BA	1.03	30/36438 (0.1%)	1.17	167/56869 (0.3%)
35	BB	2.33	76/1818 (4.2%)	2.48	157/2831 (5.5%)
35	BC	1.09	5/1818 (0.3%)	1.11	7/2831 (0.2%)
36	B1	1.14	7/1571 (0.4%)	0.96	7/2445 (0.3%)
37	BE	0.75	0/1935	1.06	3/2609 (0.1%)
38	BF	0.62	0/1636	0.99	5/2205 (0.2%)
39	BG	0.86	2/1733 (0.1%)	1.16	4/2318 (0.2%)
40	BH	0.85	0/1162	1.12	1/1564 (0.1%)
41	BI	0.78	0/856	1.06	1/1154 (0.1%)
42	BJ	0.70	1/1276 (0.1%)	1.00	6/1709 (0.4%)
43	BK	0.81	0/1136	1.18	5/1527 (0.3%)
44	BL	0.52	0/1029	0.86	1/1378 (0.1%)
45	BM	0.58	0/807	0.94	2/1085 (0.2%)
46	BN	0.75	0/900	1.04	0/1213
47	BO	0.78	0/986	1.22	3/1320 (0.2%)
48	BP	0.59	0/1008	0.98	0/1347
49	BQ	0.83	1/501 (0.2%)	1.09	2/664 (0.3%)
50	BR	0.74	0/745	1.05	2/992 (0.2%)
51	BS	0.81	0/716	1.10	3/963 (0.3%)
52	BT	0.82	0/870	1.11	2/1159 (0.2%)
53	BU	0.72	0/603	1.18	2/799 (0.3%)
54	BV	0.59	0/661	0.98	1/890 (0.1%)
55	BW	0.84	0/764	1.12	2/1006 (0.2%)
56	BX	0.45	0/212	0.81	0/277
All	All	1.05	326/161408 (0.2%)	1.21	1135/241526 (0.5%)

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	AB	0	14
2	AA	0	527
4	AD	0	1
5	AE	0	1
6	AF	0	1
7	AG	0	2
12	AM	0	2
13	AN	0	2
14	AO	0	2
16	AQ	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	AX	0	1
25	A1	0	3
26	A2	0	1
28	A4	0	1
30	A6	0	1
34	BA	0	220
35	BB	0	35
35	BC	0	12
36	B1	0	4
38	BF	0	1
39	BG	0	1
41	BI	0	1
43	BK	0	1
48	BP	0	1
51	BS	0	2
All	All	0	838

The worst 5 of 326 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	142	G	C5-C6	27.73	1.70	1.42
36	B1	48	A	C5-C6	27.45	1.65	1.41
35	BB	37	G	C2-N2	18.34	1.52	1.34
34	BA	1541	U	C4-C5	17.23	1.59	1.43
2	AA	142	G	C2-N3	16.69	1.46	1.32

The worst 5 of 1135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	1064	G	N1-C2-N2	-65.61	57.15	116.20
34	BA	1064	G	N3-C2-N2	63.69	164.48	119.90
34	BA	1064	G	N1-C2-N3	-27.38	107.47	123.90
2	AA	1084	A	O5'-P-OP2	-26.59	78.79	110.70
35	BB	36	A	OP1-P-O3'	-18.47	64.57	105.20

There are no chirality outliers.

5 of 838 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	12	C	Sidechain
1	AB	18	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AB	34	U	Sidechain
1	AB	39	A	Sidechain
1	AB	44	G	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	AB	2641	0	1337	635	1
2	AA	61847	0	31165	17729	1
3	AC	1687	0	1737	723	0
4	AD	1308	0	1355	898	0
5	AE	1507	0	1494	986	0
6	AF	1430	0	1386	832	0
7	AG	957	0	959	519	0
8	AH	1251	0	1298	612	0
9	AI	945	0	999	497	0
9	AJ	945	0	999	362	0
10	AK	1145	0	1227	630	0
11	AL	999	0	1071	497	0
12	AM	917	0	904	616	0
13	AN	937	0	1000	549	0
14	AO	639	0	615	373	0
15	AP	1081	0	1062	743	0
16	AQ	866	0	875	512	0
17	AR	406	0	361	160	0
18	AS	860	0	919	442	0
19	AT	602	0	563	332	0
20	AU	879	0	868	477	0
21	AV	1360	0	1390	788	0
22	AW	494	0	506	240	0
23	AX	477	0	529	309	0
24	A0	855	0	906	492	0
25	A1	978	0	1020	685	0
26	A2	787	0	804	571	0
27	A3	641	0	668	421	0
28	A4	604	0	595	365	0
29	A5	457	0	462	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A6	431	0	456	224	0
31	A7	383	0	414	260	0
32	A8	496	0	549	296	0
33	A9	285	0	312	125	0
34	BA	32554	0	16429	7563	1
35	BB	1626	0	817	629	0
35	BC	1626	0	820	429	0
36	B1	1405	0	706	258	1
37	BE	1900	0	1951	930	0
38	BF	1612	0	1677	662	0
39	BG	1703	0	1763	719	0
40	BH	1146	0	1207	489	1
41	BI	843	0	857	398	0
42	BJ	1257	0	1296	527	0
43	BK	1116	0	1177	677	0
44	BL	1011	0	1043	442	0
45	BM	794	0	840	332	0
46	BN	885	0	904	409	0
47	BO	970	0	1057	459	0
48	BP	997	0	1072	493	0
49	BQ	492	0	529	258	0
50	BR	734	0	771	330	0
51	BS	700	0	720	318	0
52	BT	857	0	930	423	0
53	BU	597	0	668	334	0
54	BV	647	0	673	254	0
55	BW	762	0	859	366	0
56	BX	208	0	221	103	0
All	All	148539	0	99792	47710	3

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 193.

The worst 5 of 47710 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)
2:AA:2515:C:N4	2:AA:2569:G:H1	1.08	1.45
34:BA:292:G:H1	34:BA:308:C:N4	1.08	1.45
34:BA:144:G:H1	34:BA:178:C:N4	1.13	1.45
2:AA:447:A:H1'	2:AA:449:A:N6	1.28	1.44
33:A9:11:CYS:SG	33:A9:11:CYS:CB	2.06	1.44

All (3) 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)
1:AB:-1:A:O2'	1:AB:-1:A:O2'[15_545]	1.59	0.61
2:AA:2153:G:O2'	34:BA:423:G:OP2[3_655]	2.16	0.04
36:B1:29:G:O3'	40:BH:5:ASP:OD2[3_655]	2.17	0.03

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	
3	AC	217/228 (95%)	143 (66%)	36 (17%)	38 (18%)	0	4
4	AD	171/178 (96%)	71 (42%)	38 (22%)	62 (36%)	0	0
5	AE	187/338 (55%)	89 (48%)	41 (22%)	57 (30%)	0	0
6	AF	183/246 (74%)	83 (45%)	40 (22%)	60 (33%)	0	0
7	AG	118/176 (67%)	57 (48%)	29 (25%)	32 (27%)	0	0
8	AH	162/177 (92%)	89 (55%)	39 (24%)	34 (21%)	0	3
9	AI	126/128 (98%)	87 (69%)	24 (19%)	15 (12%)	0	8
9	AJ	126/128 (98%)	86 (68%)	25 (20%)	15 (12%)	0	8
10	AK	146/149 (98%)	83 (57%)	34 (23%)	29 (20%)	0	3
11	AL	131/141 (93%)	66 (50%)	33 (25%)	32 (24%)	0	2
12	AM	113/145 (78%)	48 (42%)	26 (23%)	39 (34%)	0	0
13	AN	120/122 (98%)	60 (50%)	33 (28%)	27 (22%)	0	2
14	AO	82/164 (50%)	40 (49%)	17 (21%)	25 (30%)	0	0
15	AP	136/138 (99%)	50 (37%)	43 (32%)	43 (32%)	0	0
16	AQ	111/186 (60%)	41 (37%)	32 (29%)	38 (34%)	0	0
17	AR	50/66 (76%)	19 (38%)	17 (34%)	14 (28%)	0	0
18	AS	104/113 (92%)	70 (67%)	18 (17%)	16 (15%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	74/84 (88%)	33 (45%)	17 (23%)	24 (32%)	0	0
20	AU	108/119 (91%)	60 (56%)	25 (23%)	23 (21%)	0	3
21	AV	175/253 (69%)	69 (39%)	46 (26%)	60 (34%)	0	0
22	AW	62/70 (89%)	21 (34%)	25 (40%)	16 (26%)	0	1
23	AX	58/60 (97%)	29 (50%)	13 (22%)	16 (28%)	0	0
24	A0	103/118 (87%)	50 (48%)	33 (32%)	20 (19%)	0	3
25	A1	115/118 (98%)	48 (42%)	40 (35%)	27 (24%)	0	2
26	A2	98/100 (98%)	54 (55%)	18 (18%)	26 (26%)	0	1
27	A3	84/91 (92%)	32 (38%)	16 (19%)	36 (43%)	0	0
28	A4	71/73 (97%)	21 (30%)	19 (27%)	31 (44%)	0	0
29	A5	56/60 (93%)	25 (45%)	11 (20%)	20 (36%)	0	0
30	A6	51/82 (62%)	26 (51%)	8 (16%)	17 (33%)	0	0
31	A7	44/47 (94%)	14 (32%)	12 (27%)	18 (41%)	0	0
32	A8	61/64 (95%)	24 (39%)	16 (26%)	21 (34%)	0	0
33	A9	33/36 (92%)	19 (58%)	8 (24%)	6 (18%)	0	4
37	BE	232/256 (91%)	107 (46%)	58 (25%)	67 (29%)	0	0
38	BF	204/239 (85%)	113 (55%)	46 (22%)	45 (22%)	0	2
39	BG	206/209 (99%)	97 (47%)	63 (31%)	46 (22%)	0	2
40	BH	148/162 (91%)	90 (61%)	38 (26%)	20 (14%)	0	6
41	BI	99/101 (98%)	55 (56%)	24 (24%)	20 (20%)	0	3
42	BJ	153/156 (98%)	63 (41%)	49 (32%)	41 (27%)	0	1
43	BK	136/138 (99%)	67 (49%)	39 (29%)	30 (22%)	0	2
44	BL	125/128 (98%)	64 (51%)	27 (22%)	34 (27%)	0	0
45	BM	96/105 (91%)	54 (56%)	19 (20%)	23 (24%)	0	2
46	BN	117/129 (91%)	54 (46%)	33 (28%)	30 (26%)	0	1
47	BO	122/135 (90%)	65 (53%)	28 (23%)	29 (24%)	0	2
48	BP	123/126 (98%)	59 (48%)	30 (24%)	34 (28%)	0	0
49	BQ	58/61 (95%)	22 (38%)	10 (17%)	26 (45%)	0	0
50	BR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	4
51	BS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	3
52	BT	102/105 (97%)	62 (61%)	20 (20%)	20 (20%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	BU	71/88 (81%)	29 (41%)	24 (34%)	18 (25%)	0 1
54	BV	78/93 (84%)	35 (45%)	17 (22%)	26 (33%)	0 0
55	BW	97/106 (92%)	27 (28%)	46 (47%)	24 (25%)	0 2
56	BX	22/27 (82%)	9 (41%)	5 (23%)	8 (36%)	0 0
All	All	5832/6739 (86%)	2857 (49%)	1467 (25%)	1508 (26%)	0 1

5 of 1508 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	ASN
3	AC	35	ALA
3	AC	54	SER
3	AC	68	LEU
3	AC	87	GLU

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
3	AC	174/180 (97%)	144 (83%)	30 (17%)	2 17
4	AD	135/139 (97%)	90 (67%)	45 (33%)	0 2
5	AE	156/284 (55%)	114 (73%)	42 (27%)	0 5
6	AF	152/193 (79%)	121 (80%)	31 (20%)	1 11
7	AG	102/147 (69%)	74 (72%)	28 (28%)	0 4
8	AH	137/147 (93%)	99 (72%)	38 (28%)	0 4
9	AI	98/98 (100%)	89 (91%)	9 (9%)	11 43
9	AJ	98/98 (100%)	89 (91%)	9 (9%)	11 43
10	AK	119/119 (100%)	96 (81%)	23 (19%)	2 13
11	AL	108/113 (96%)	91 (84%)	17 (16%)	3 22
12	AM	95/121 (78%)	71 (75%)	24 (25%)	1 6
13	AN	101/101 (100%)	74 (73%)	27 (27%)	0 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	AO	67/126 (53%)	51 (76%)	16 (24%)	1 7
15	AP	110/110 (100%)	73 (66%)	37 (34%)	0 2
16	AQ	89/149 (60%)	58 (65%)	31 (35%)	0 2
17	AR	44/52 (85%)	24 (54%)	20 (46%)	0 0
18	AS	88/92 (96%)	65 (74%)	23 (26%)	0 5
19	AT	67/73 (92%)	48 (72%)	19 (28%)	0 3
20	AU	97/105 (92%)	75 (77%)	22 (23%)	1 8
21	AV	151/203 (74%)	109 (72%)	42 (28%)	0 4
22	AW	51/56 (91%)	36 (71%)	15 (29%)	0 3
23	AX	52/52 (100%)	34 (65%)	18 (35%)	0 2
24	A0	89/101 (88%)	59 (66%)	30 (34%)	0 2
25	A1	96/97 (99%)	67 (70%)	29 (30%)	0 3
26	A2	79/79 (100%)	60 (76%)	19 (24%)	1 7
27	A3	64/67 (96%)	46 (72%)	18 (28%)	0 4
28	A4	66/66 (100%)	50 (76%)	16 (24%)	1 7
29	A5	51/53 (96%)	38 (74%)	13 (26%)	1 6
30	A6	46/69 (67%)	35 (76%)	11 (24%)	1 7
31	A7	39/40 (98%)	30 (77%)	9 (23%)	1 8
32	A8	50/51 (98%)	33 (66%)	17 (34%)	0 2
33	A9	34/35 (97%)	30 (88%)	4 (12%)	6 32
37	BE	202/220 (92%)	152 (75%)	50 (25%)	1 6
38	BF	160/188 (85%)	127 (79%)	33 (21%)	1 10
39	BG	180/181 (99%)	136 (76%)	44 (24%)	1 7
40	BH	115/123 (94%)	66 (57%)	49 (43%)	0 0
41	BI	90/90 (100%)	64 (71%)	26 (29%)	0 3
42	BJ	126/127 (99%)	106 (84%)	20 (16%)	3 21
43	BK	119/119 (100%)	73 (61%)	46 (39%)	0 0
44	BL	98/99 (99%)	81 (83%)	17 (17%)	2 17
45	BM	88/92 (96%)	70 (80%)	18 (20%)	1 11
46	BN	90/99 (91%)	70 (78%)	20 (22%)	1 9
47	BO	104/111 (94%)	85 (82%)	19 (18%)	2 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	BP	100/101 (99%)	80 (80%)	20 (20%)	1 12
49	BQ	49/50 (98%)	41 (84%)	8 (16%)	3 20
50	BR	79/80 (99%)	59 (75%)	20 (25%)	1 6
51	BS	72/74 (97%)	44 (61%)	28 (39%)	0 0
52	BT	96/97 (99%)	74 (77%)	22 (23%)	1 8
53	BU	64/77 (83%)	47 (73%)	17 (27%)	0 5
54	BV	71/80 (89%)	59 (83%)	12 (17%)	2 19
55	BW	76/82 (93%)	53 (70%)	23 (30%)	0 3
56	BX	19/22 (86%)	17 (90%)	2 (10%)	8 37
All	All	4903/5528 (89%)	3677 (75%)	1226 (25%)	1 6

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	AX	23	LEU
29	A5	31	THR
51	BS	27	LYS
24	A0	27	SER
25	A1	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
26	A2	79	GLN
31	A7	29	ASN
50	BR	62	GLN
27	A3	17	ASN
28	A4	32	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	122/123 (99%)	47 (38%)	5 (4%)
2	AA	2870/2915 (98%)	1226 (42%)	290 (10%)
34	BA	1515/1522 (99%)	452 (29%)	161 (10%)
35	BB	76/76 (100%)	34 (44%)	16 (21%)
35	BC	75/76 (98%)	31 (41%)	9 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	B1	65/78 (83%)	24 (36%)	4 (6%)
All	All	4723/4790 (98%)	1814 (38%)	485 (10%)

5 of 1814 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	0	A
1	AB	1	U
1	AB	2	C
1	AB	3	C
1	AB	9	G

5 of 485 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AA	1992	G
2	AA	2542	A
34	BA	1498	U
2	AA	2035	G
2	AA	2320	A

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	AB	123/123 (100%)	-0.44	0 100 100	308, 357, 402, 412	0
2	AA	2872/2915 (98%)	-0.45	18 (0%) 90 87	232, 307, 404, 474	0
3	AC	221/228 (96%)	-0.02	4 (1%) 71 66	384, 428, 464, 467	0
4	AD	173/178 (97%)	0.54	14 (8%) 15 17	243, 279, 292, 298	0
5	AE	191/338 (56%)	0.62	39 (20%) 1 5	258, 311, 397, 403	0
6	AF	189/246 (76%)	-0.34	2 (1%) 82 78	233, 399, 427, 434	0
7	AG	122/176 (69%)	-0.32	2 (1%) 74 68	350, 366, 443, 447	0
8	AH	164/177 (92%)	-0.34	1 (0%) 90 87	320, 351, 366, 370	0
9	AI	128/128 (100%)	1.43	33 (25%) 1 4	580, 591, 602, 603	0
9	AJ	128/128 (100%)	2.07	56 (43%) 0 3	569, 582, 594, 596	0
10	AK	148/149 (99%)	-0.08	4 (2%) 58 53	305, 329, 353, 361	0
11	AL	133/141 (94%)	0.16	8 (6%) 25 24	455, 504, 541, 543	0
12	AM	117/145 (80%)	0.31	13 (11%) 7 11	286, 310, 364, 368	0
13	AN	122/122 (100%)	0.35	11 (9%) 12 14	245, 262, 277, 293	0
14	AO	84/164 (51%)	0.28	6 (7%) 19 20	330, 452, 471, 473	0
15	AP	138/138 (100%)	0.49	10 (7%) 18 19	283, 324, 364, 379	0
16	AQ	113/186 (60%)	-0.76	0 100 100	317, 367, 386, 390	0
17	AR	52/66 (78%)	0.71	10 (19%) 2 5	251, 267, 285, 288	0
18	AS	108/113 (95%)	0.21	3 (2%) 56 51	280, 311, 324, 332	0
19	AT	76/84 (90%)	-0.05	4 (5%) 30 29	329, 344, 360, 363	0
20	AU	110/119 (92%)	-0.04	9 (8%) 14 16	647, 661, 722, 724	0
21	AV	177/253 (69%)	-0.02	8 (4%) 37 34	295, 365, 416, 424	0
22	AW	64/70 (91%)	0.16	2 (3%) 52 47	346, 364, 373, 375	0
23	AX	60/60 (100%)	-0.18	0 100 100	291, 306, 315, 316	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
24	A0	105/118 (88%)	-0.12	3 (2%) 55 49	263, 281, 304, 308	0
25	A1	117/118 (99%)	-0.50	1 (0%) 85 81	267, 297, 311, 317	0
26	A2	100/100 (100%)	0.80	21 (21%) 1 5	416, 430, 462, 470	0
27	A3	86/91 (94%)	0.60	11 (12%) 5 9	359, 389, 475, 486	0
28	A4	73/73 (100%)	0.04	7 (9%) 10 13	319, 354, 373, 378	0
29	A5	58/60 (96%)	0.09	4 (6%) 20 20	259, 314, 361, 373	0
30	A6	53/82 (64%)	0.21	4 (7%) 17 19	287, 316, 332, 340	0
31	A7	46/47 (97%)	0.24	2 (4%) 39 35	316, 339, 352, 357	0
32	A8	63/64 (98%)	0.02	1 (1%) 74 68	262, 282, 294, 306	0
33	A9	35/36 (97%)	-0.55	0 100 100	281, 303, 316, 319	0
34	BA	1515/1522 (99%)	-0.46	5 (0%) 94 92	251, 312, 419, 609	0
35	BB	76/76 (100%)	8.23	61 (80%) 0 2	631, 651, 667, 669	0
35	BC	76/76 (100%)	-0.65	0 100 100	273, 310, 328, 337	0
36	B1	66/78 (84%)	6.57	43 (65%) 0 2	337, 829, 918, 922	0
37	BE	234/256 (91%)	0.22	22 (9%) 11 13	293, 321, 364, 385	0
38	BF	206/239 (86%)	0.82	43 (20%) 1 5	301, 349, 377, 382	0
39	BG	208/209 (99%)	0.09	10 (4%) 34 31	276, 299, 318, 329	0
40	BH	150/162 (92%)	0.71	23 (15%) 3 7	277, 295, 315, 324	0
41	BI	101/101 (100%)	1.20	28 (27%) 1 4	299, 318, 330, 336	0
42	BJ	155/156 (99%)	0.07	6 (3%) 43 39	326, 357, 370, 373	0
43	BK	138/138 (100%)	0.22	10 (7%) 18 19	266, 284, 297, 306	0
44	BL	127/128 (99%)	-0.33	0 100 100	385, 487, 499, 500	0
45	BM	98/105 (93%)	0.91	16 (16%) 2 7	337, 394, 423, 424	0
46	BN	119/129 (92%)	0.26	12 (10%) 9 12	288, 307, 330, 334	0
47	BO	124/135 (91%)	0.26	7 (5%) 28 27	265, 282, 319, 328	0
48	BP	125/126 (99%)	-0.89	0 100 100	350, 370, 412, 415	0
49	BQ	60/61 (98%)	-0.04	2 (3%) 50 44	322, 352, 360, 365	0
50	BR	88/89 (98%)	-0.36	3 (3%) 49 44	277, 288, 315, 318	0
51	BS	83/88 (94%)	-0.38	1 (1%) 81 75	271, 284, 303, 316	0
52	BT	104/105 (99%)	-0.18	3 (2%) 55 49	249, 268, 323, 344	0
53	BU	73/88 (82%)	0.32	10 (13%) 4 8	259, 296, 323, 348	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
54	BV	80/93 (86%)	0.23	6 (7%) 17 19	353, 369, 395, 399	0
55	BW	99/106 (93%)	-0.51	0 100 100	264, 281, 292, 300	0
56	BX	24/27 (88%)	-1.09	0 100 100	475, 489, 493, 496	0
All	All	10678/11529 (92%)	0.01	622 (5%) 26 25	232, 322, 533, 922	0

The worst 5 of 622 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	B1	15	A	22.6
35	BB	4	G	21.1
36	B1	42	G	20.4
36	B1	17	G	19.5
35	BB	5	A	18.8

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

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

6.3 Carbohydrates (i)

There are no 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.