wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:24 PM GMT

PDB ID	:	4V4Z
Title	:	70S Thermus thermophilous ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5A.
Authors	:	Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on	:	2006-06-27
Resolution	:	4.51 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:

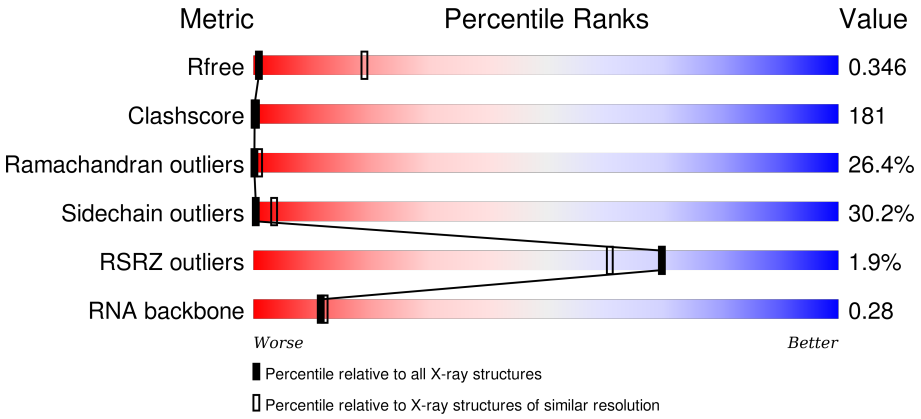
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.51 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	1071 (5.40-3.60)
Clashscore	102246	1004 (5.40-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)
RNA backbone	2183	1091 (6.22-2.80)

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	. 54% 34% 11%
2	AC	76	49% 43% 8%
3	AD	76	. 37% 47% 13%
4	A1	27	26% 7% 52% 22% 19%

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Mol	Chain	Length	Quality of chain
5	AE	256	4% 45% 33% 11% 9%
6	AF	239	6% 5% 51% 25% 5% 14%
7	AG	209	54% 34% 7%
8	AH	162	% 54% 31% 7%
9	AI	101	6% 5% 55% 32% 8%
10	AJ	156	5% 61% 28% 8%
11	AK	138	49% 42% 8%
12	AL	128	66% 28% 5%
13	AM	105	11% 5% 47% 36% 6% 7%
14	AN	129	2% 55% 28% 7% 8%
15	AO	132	6% 44% 37% 7% 6%
16	AP	126	7% 62% 25% 5%
17	AQ	61	54% 39% 5%
18	AR	89	60% 31%
19	AS	88	45% 44% 6%
20	AT	105	57% 33% 5%
21	AU	88	3% 36% 33% 10% 17%
22	AV	93	8% 43% 32% 6% 14%
23	AW	106	53% 37% 7%
24	AX	27	56% 19% 11% 11%
25	BA	2916	42% 39% 18%
26	BB	123	51% 37% 11%
27	BC	229	25% 6% 69% 23%
28	BD	276	3% 44% 43% 11%
29	BE	206	% 43% 43% 12%

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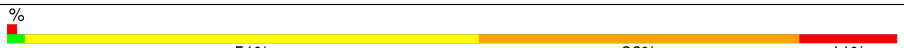
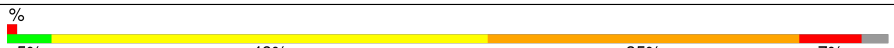
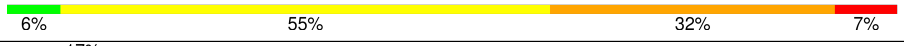
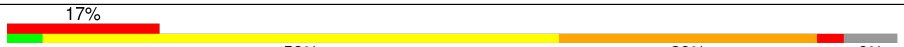
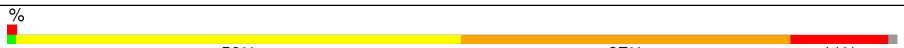
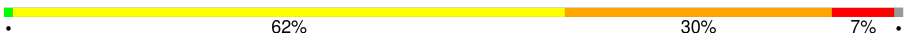
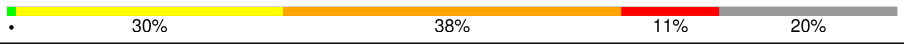
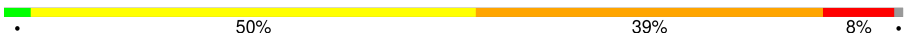
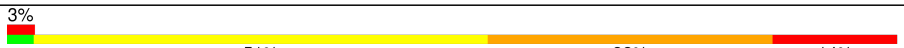
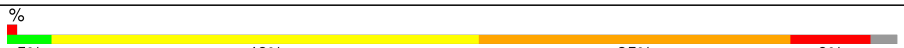
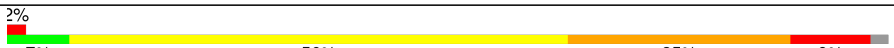
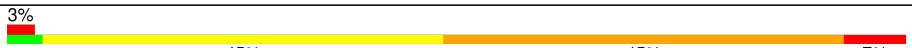
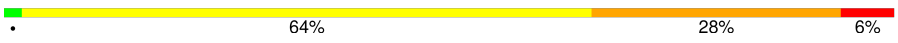
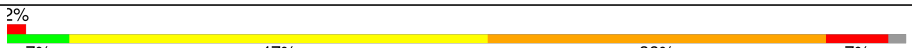
Mol	Chain	Length	Quality of chain
30	BF	210	
31	BG	182	
32	BH	180	
33	BK	148	
34	BL	147	
35	BM	140	
36	BN	122	
37	BO	150	
38	BP	141	
39	BQ	118	
40	BR	112	
41	BS	146	
42	BT	118	
43	BU	101	
44	BV	113	
45	BW	96	
46	BX	110	
47	BY	206	
48	BZ	85	
49	B1	67	
50	B2	60	
51	B3	71	
52	B4	60	
53	B5	54	
54	B6	49	

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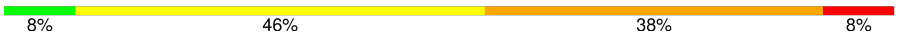
Mol	Chain	Length	Quality of chain
55	B7	65	
56	B8	37	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 149640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a RNA chain called tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AC	76	1624	723	295	530	76	0	0	0

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	AD	76	1623	723	290	534	76	0	0	0

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	A1	27	596	267	127	175	27	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	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	AH	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	AI	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	AJ	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	AK	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	AL	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	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	AN	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	AO	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	AP	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	AQ	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	AR	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	AS	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	AT	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	AU	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	AV	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	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	U	-	INSERTION	GB 48271

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BN	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BR	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	117	Total	C	N	O	S	0	0	0
			976	614	197	164	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BW	94	Total	C	N	O	0	0	0
			742	483	133	126			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BX	110	Total	C	N	O	S	0	0	0
			844	539	158	141	6			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	B2	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

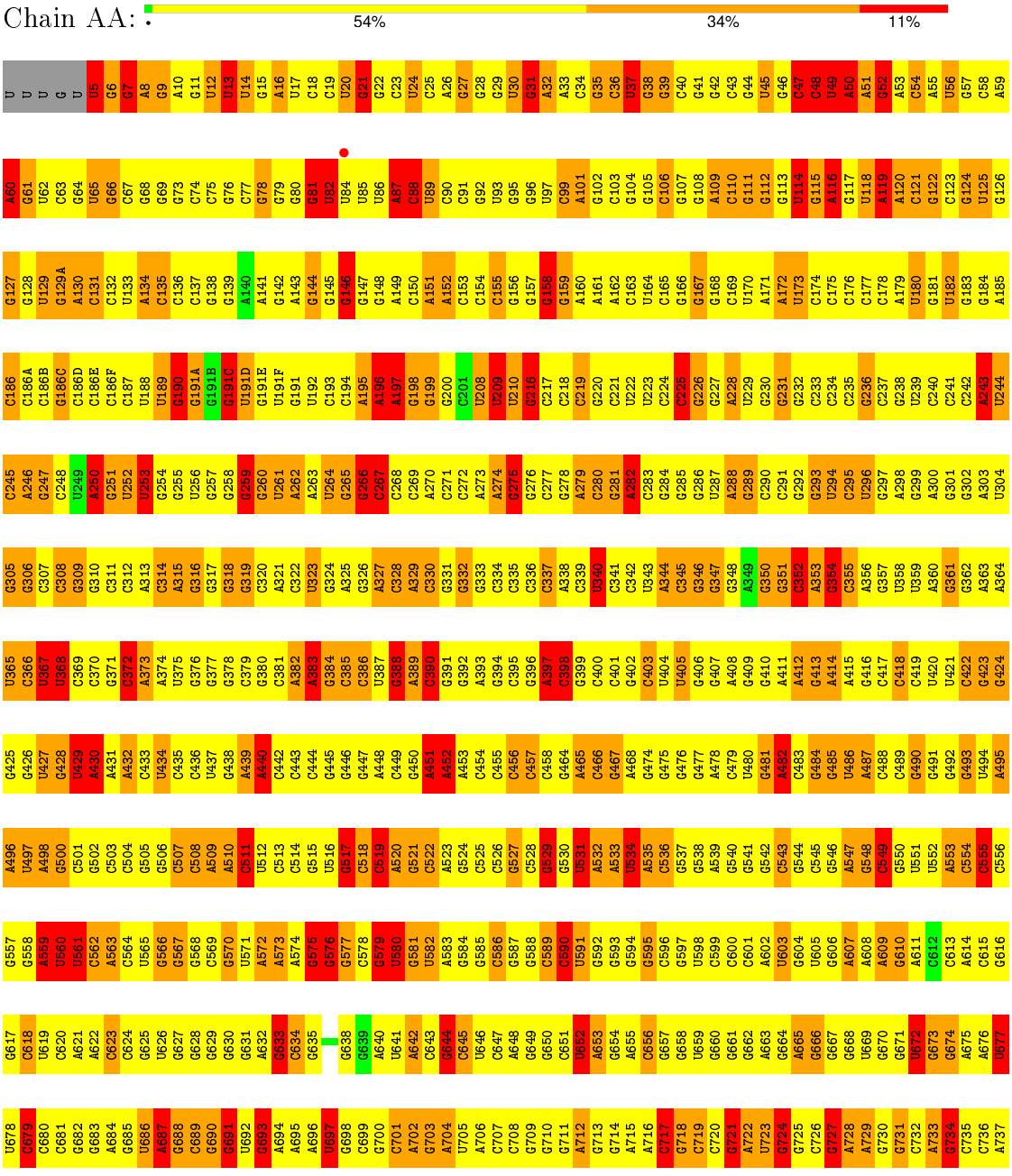
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

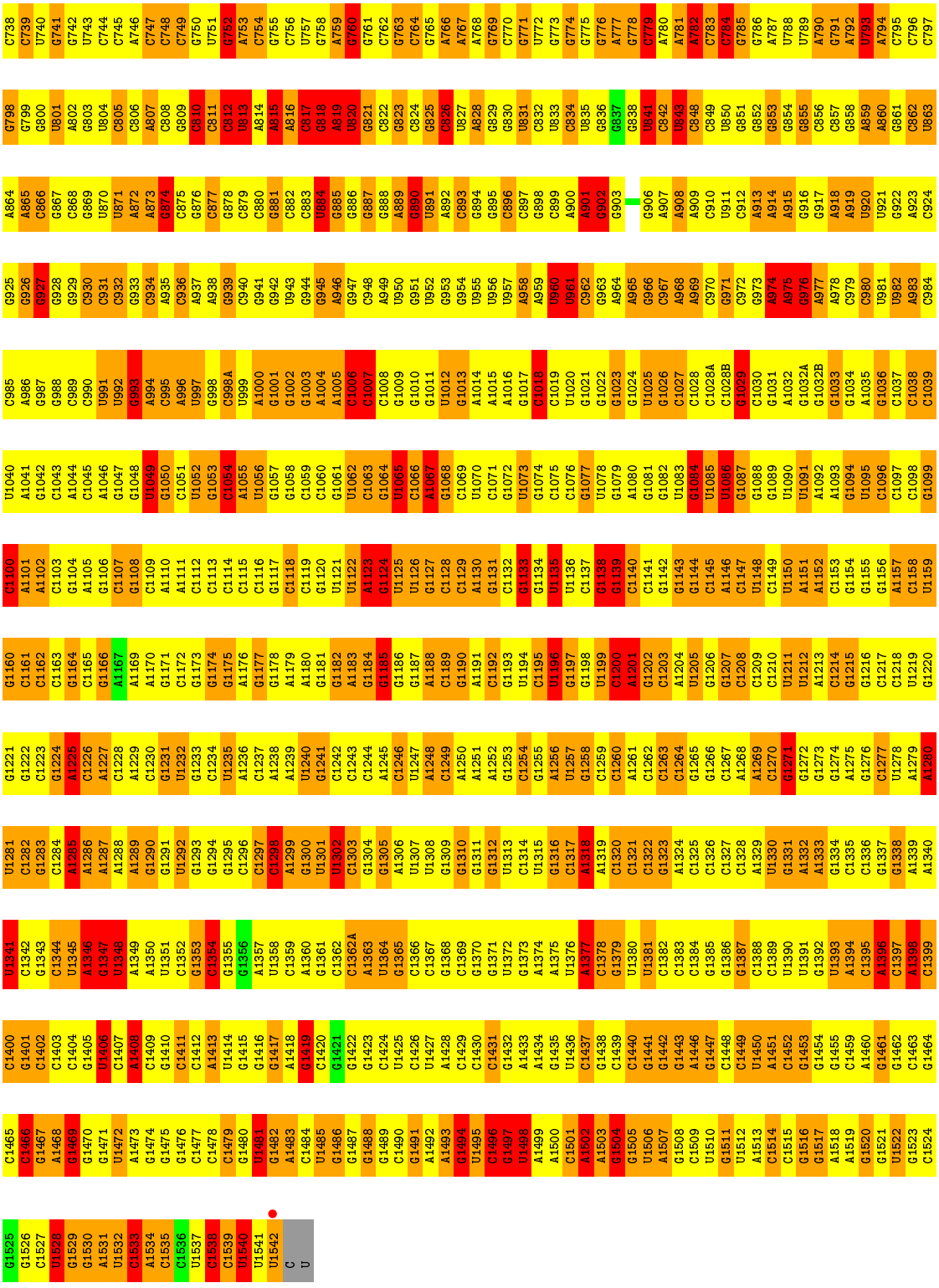
3 Residue-property plots (i)

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 rRNA

Chain AA:



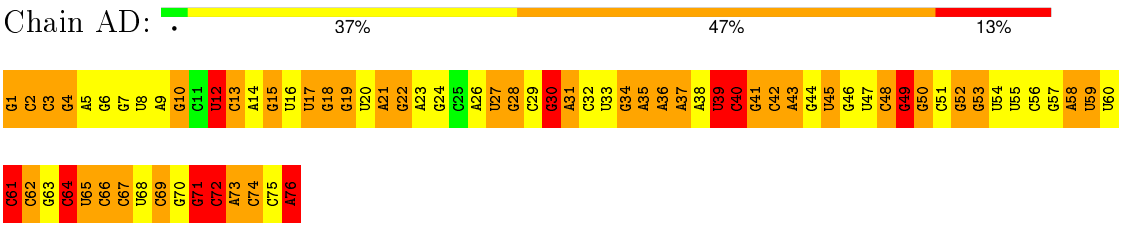


- Molecule 2: tRNA fMET (unmodified bases)

Chain AC:

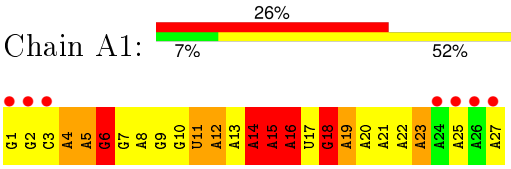
- Molecule 3: tRNA PHE (unmodified bases)

Chain AD:



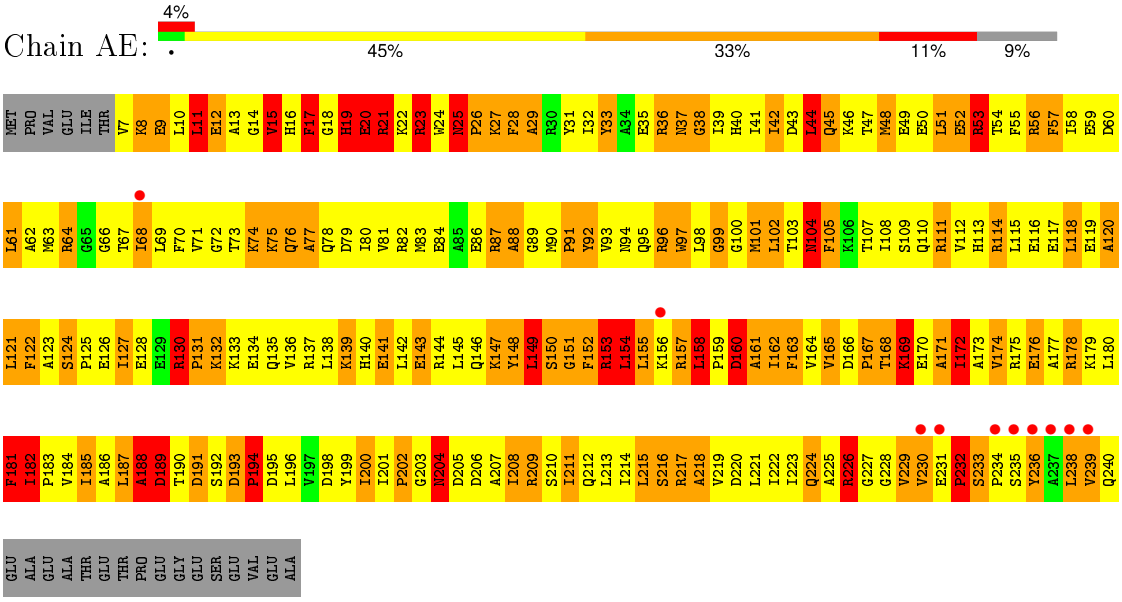
- Molecule 4: mRNA

Chain A1:



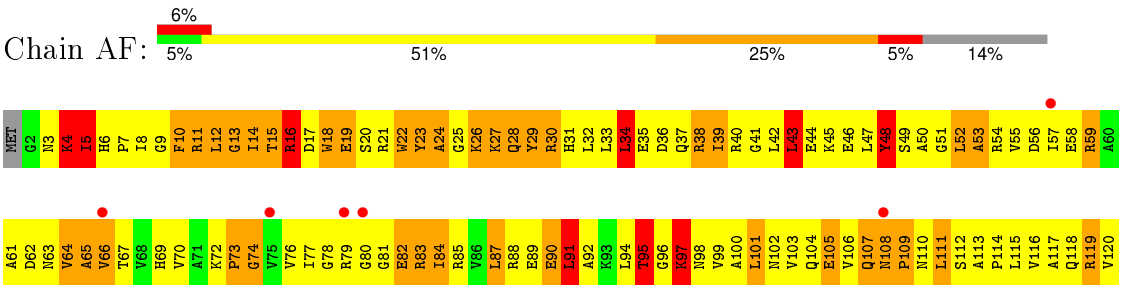
- Molecule 5: 30S ribosomal protein S2

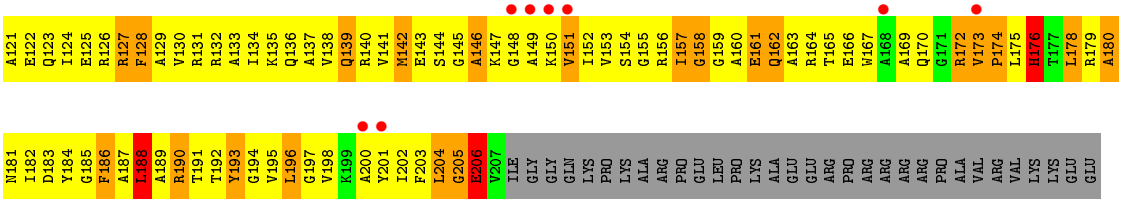
Chain AE:



- Molecule 6: 30S ribosomal protein S3

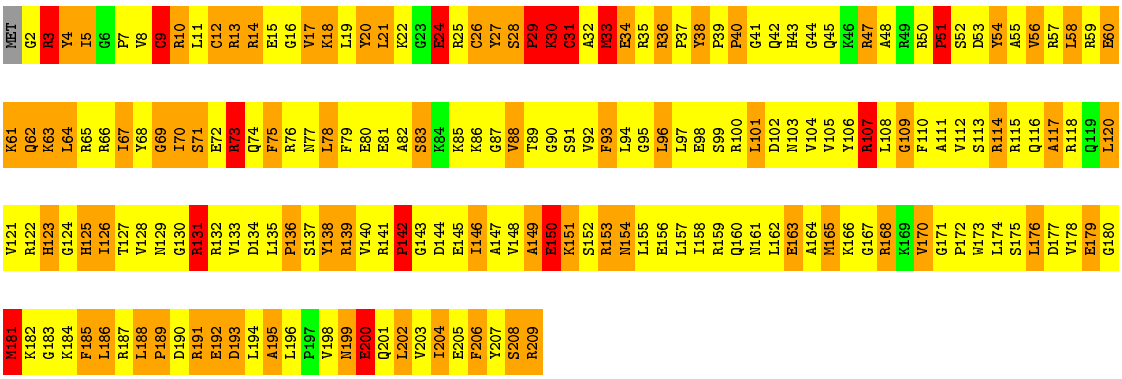
Chain AF:





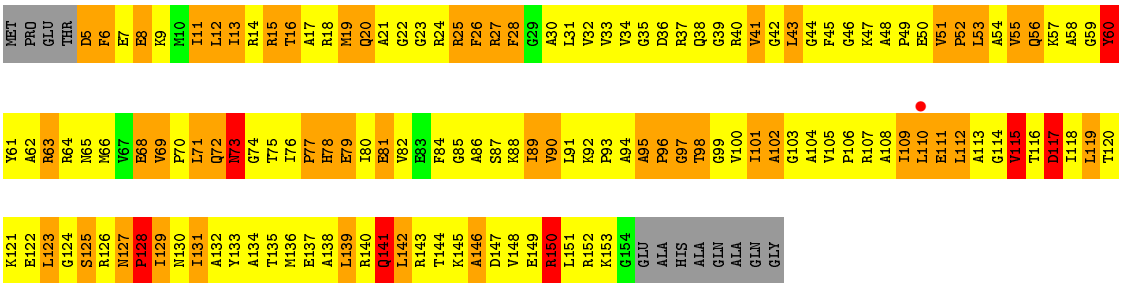
• Molecule 7: 30S ribosomal protein S4

Chain AG:



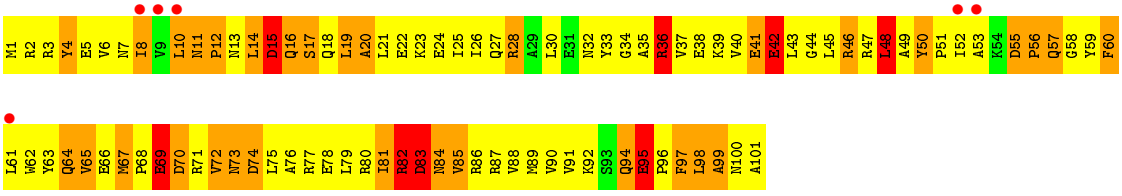
• Molecule 8: 30S ribosomal protein S5

Chain AH:



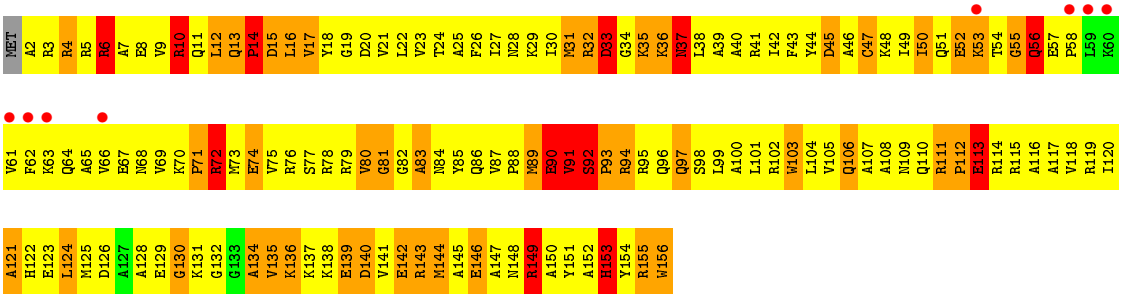
• Molecule 9: 30S ribosomal protein S6

Chain AI:



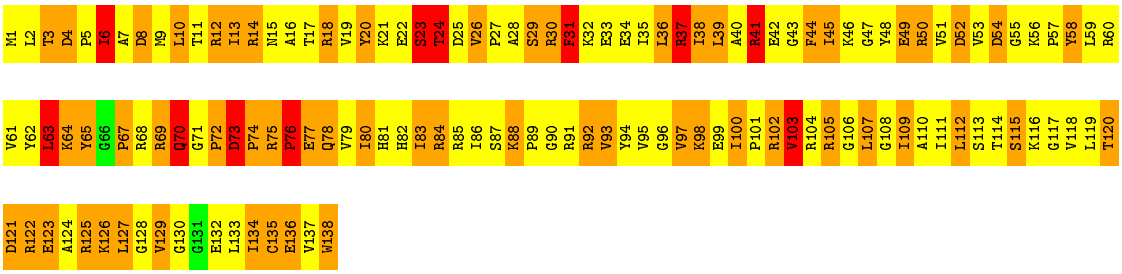
• Molecule 10: 30S ribosomal protein S7

Chain AJ:



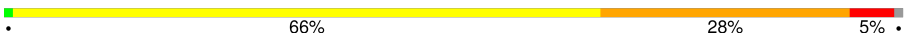
• Molecule 11: 30S ribosomal protein S8

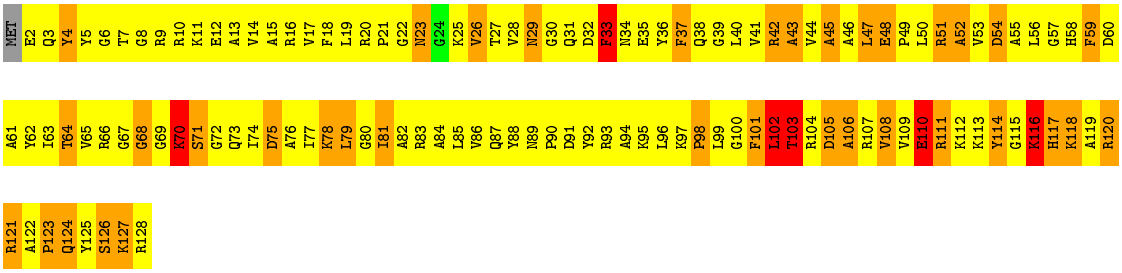
Chain AK:



• Molecule 12: 30S ribosomal protein S9

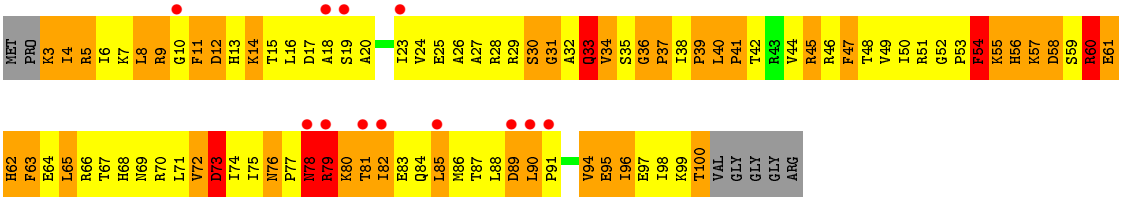
Chain AL:





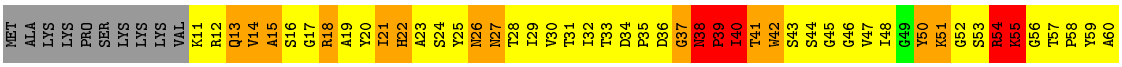
• Molecule 13: 30S ribosomal protein S10

Chain AM:



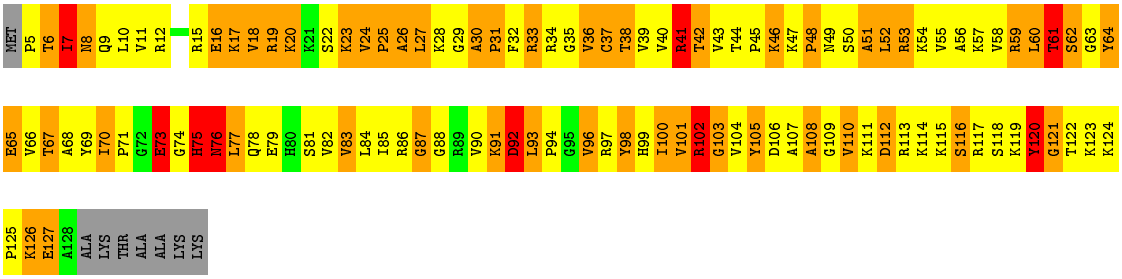
• Molecule 14: 30S ribosomal protein S11

Chain AN:



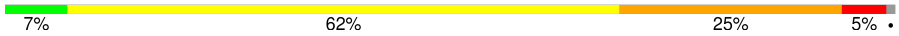
• Molecule 15: 30S ribosomal protein S12

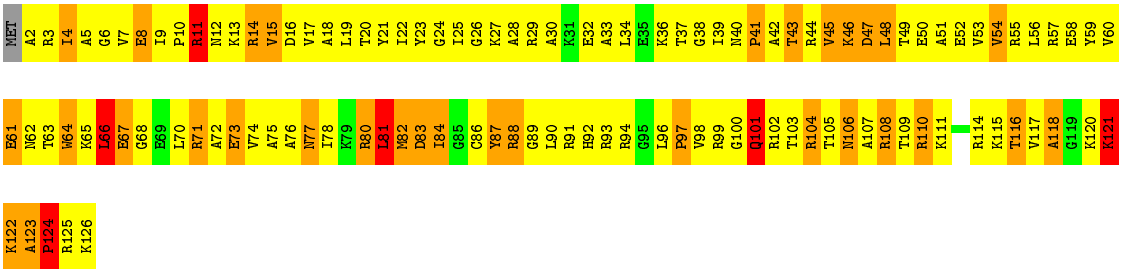
Chain AO:



• Molecule 16: 30S ribosomal protein S13

Chain AP:



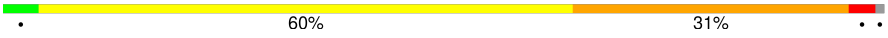


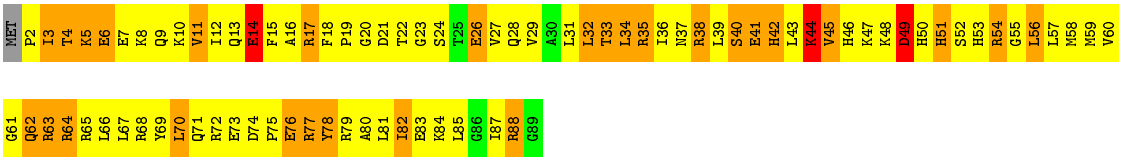
• Molecule 17: 30S ribosomal protein S14

Chain AQ:

• Molecule 18: 30S ribosomal protein S15

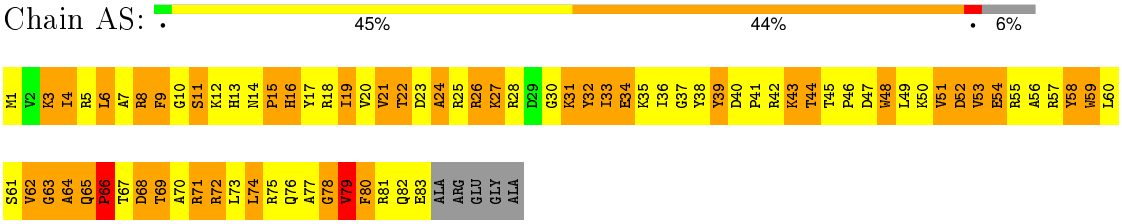
Chain AR:





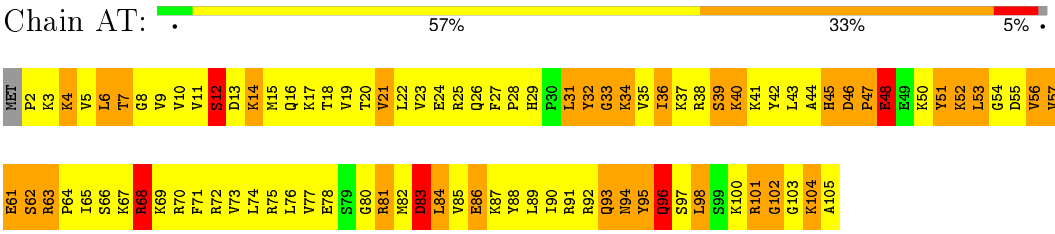
- Molecule 19: 30S ribosomal protein S16

Chain AS:



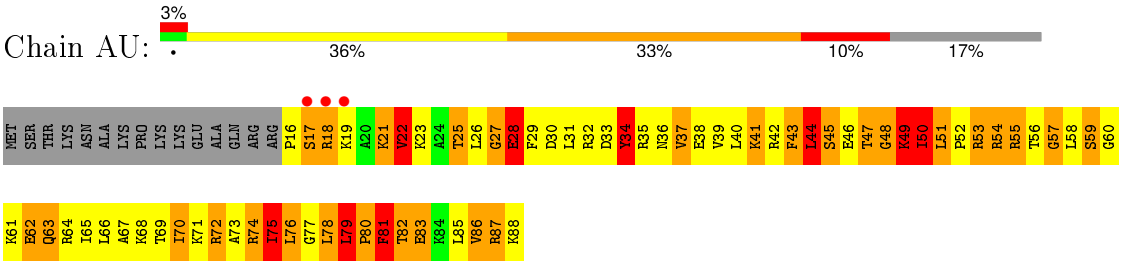
- Molecule 20: 30S ribosomal protein S17

Chain AT:



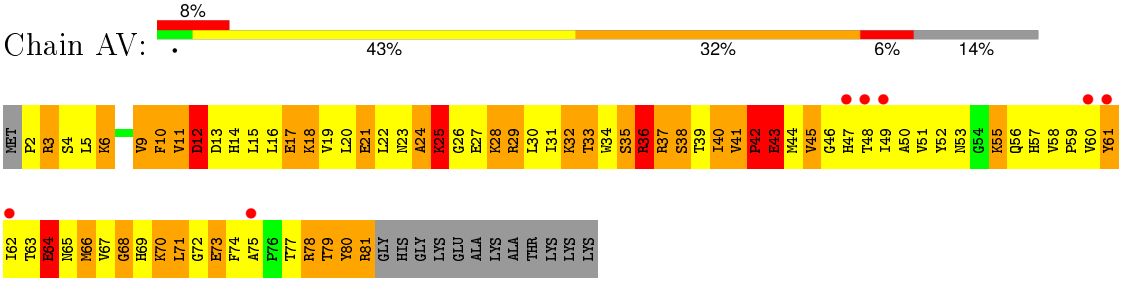
- Molecule 21: 30S ribosomal protein S18

Chain AU:



- Molecule 22: 30S ribosomal protein S19

Chain AV:



- Molecule 23: 30S ribosomal protein S20

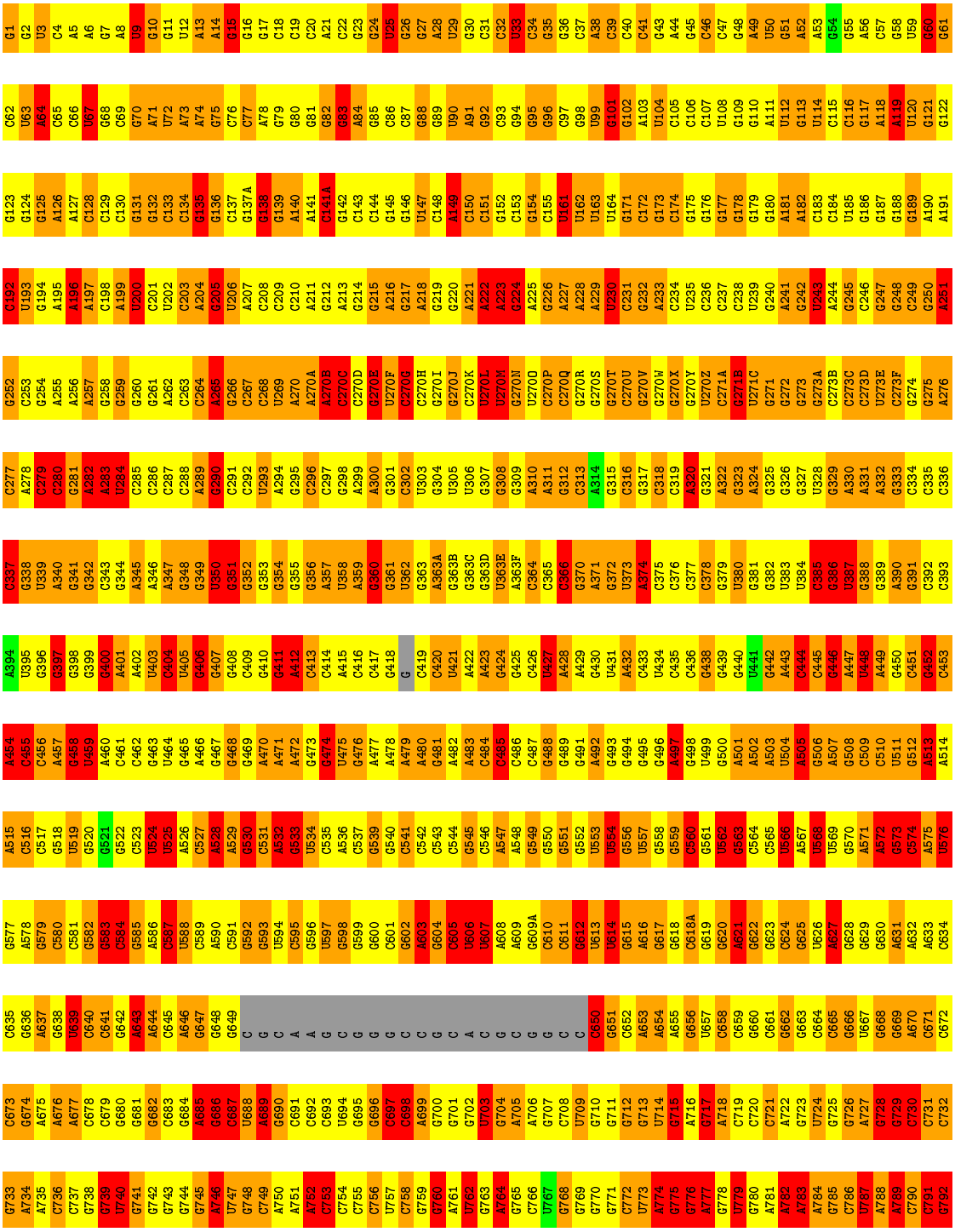
Chain AW:

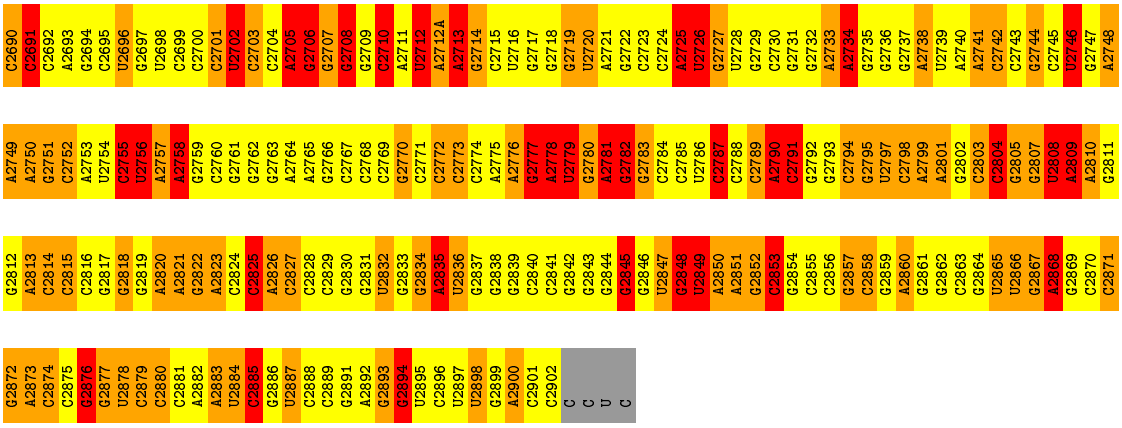
- Molecule 24: 30S ribosomal protein Thx

Chain AX:

- Molecule 25: 23S rRNA

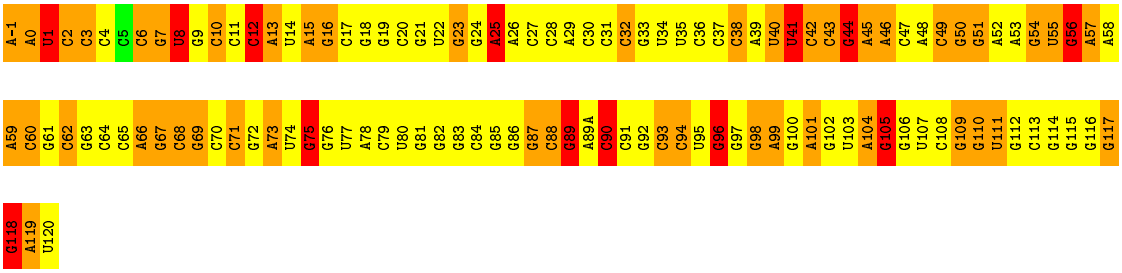
Chain BA:





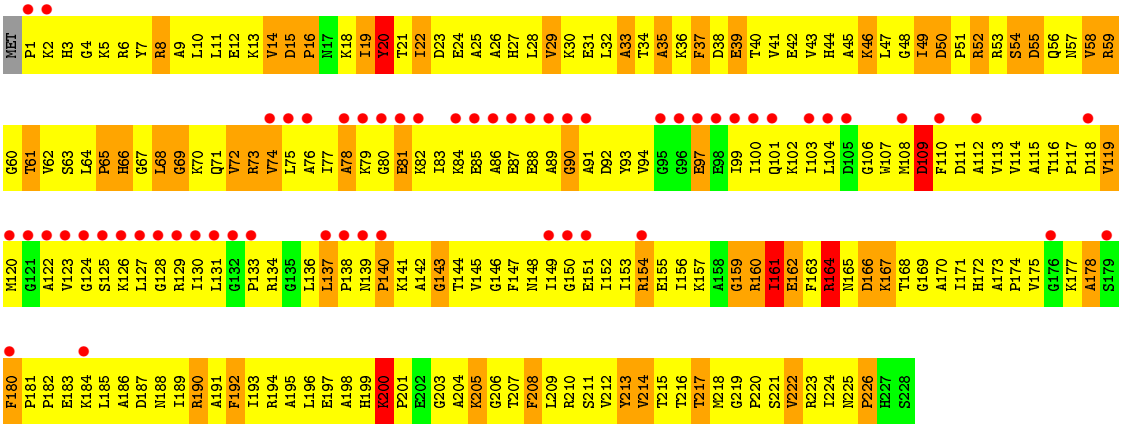
• Molecule 26: 5S rRNA

Chain BB:



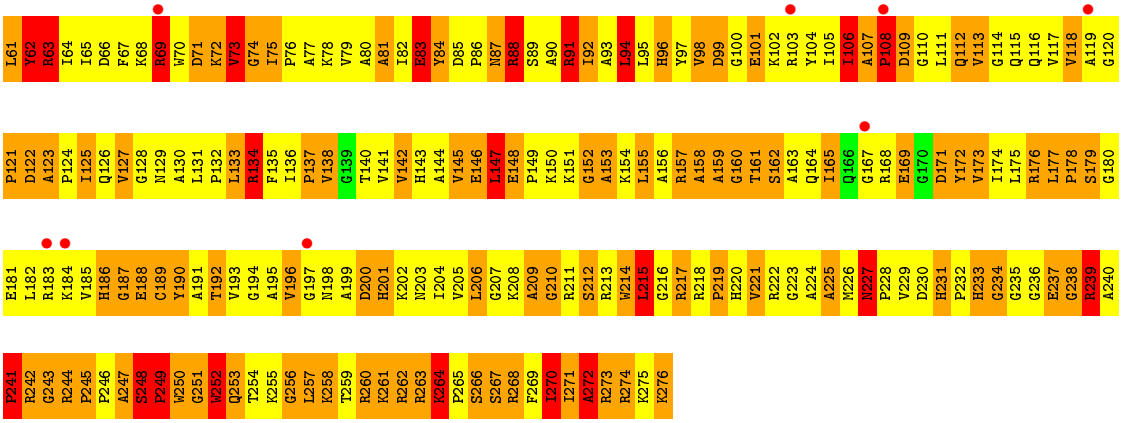
• Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain BC:



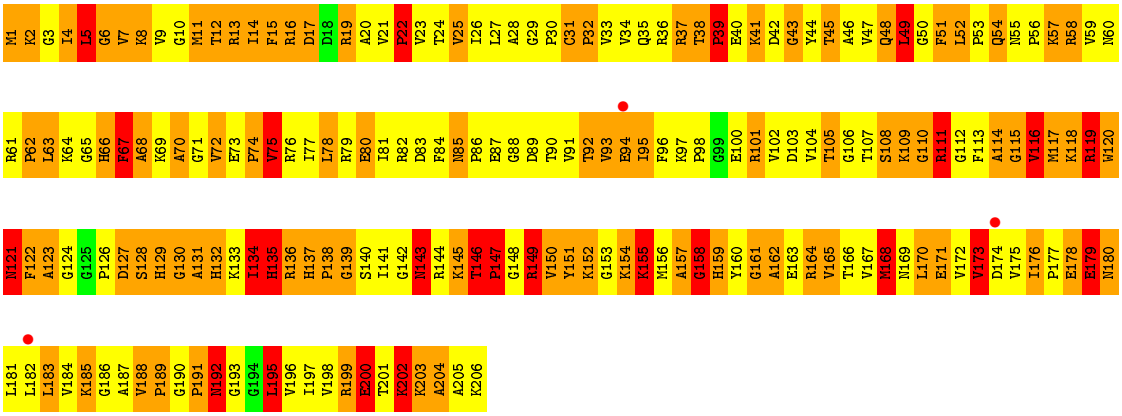
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD:



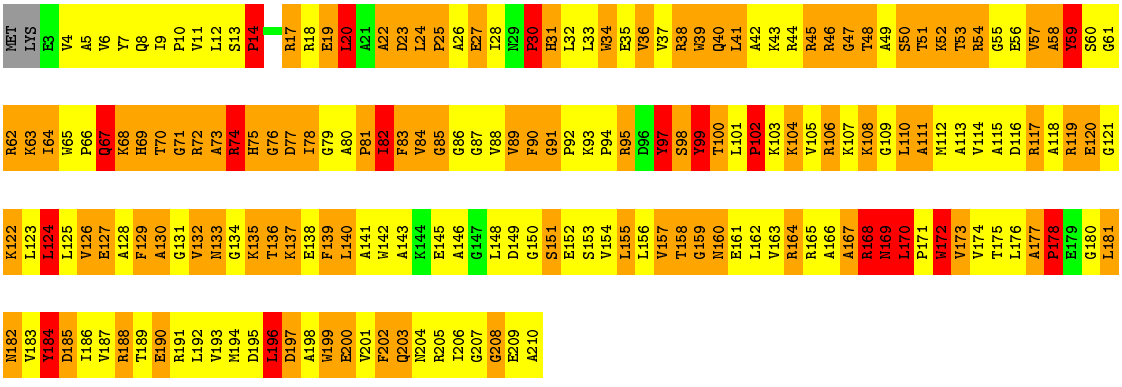
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE:



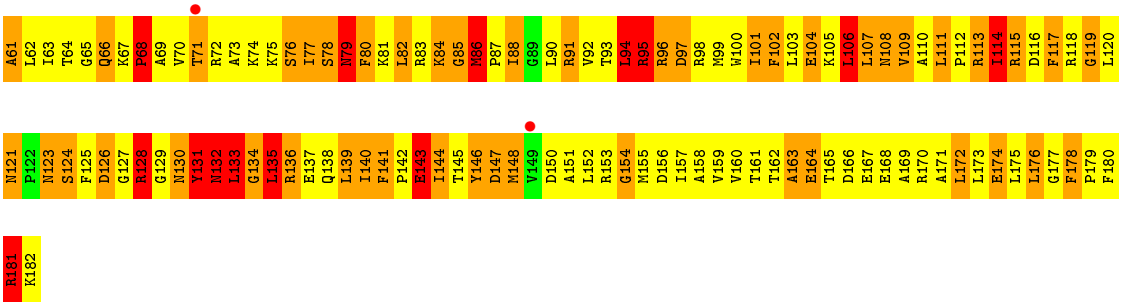
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain BF:



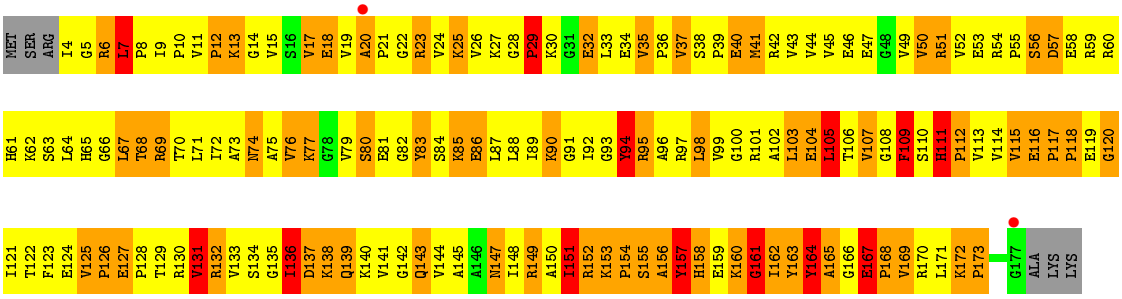
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG:



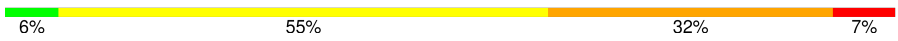
• Molecule 32: 50S RIBOSOMAL PROTEIN L6

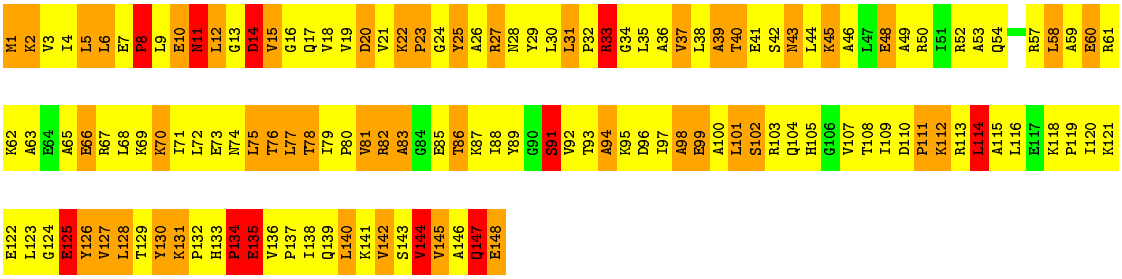
Chain BH:



• Molecule 33: 50S RIBOSOMAL PROTEIN L9

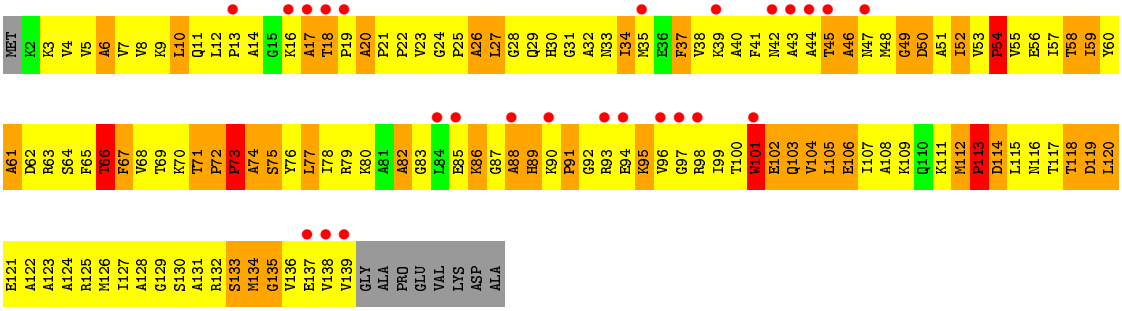
Chain BK:





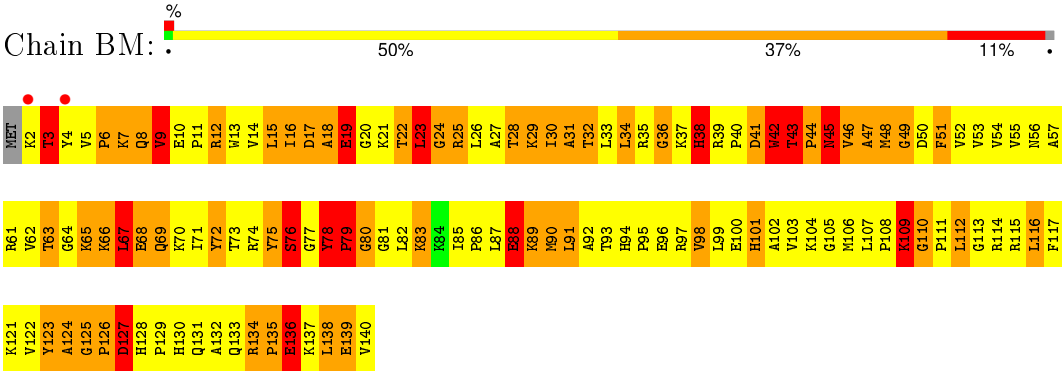
• Molecule 34: 50S RIBOSOMAL PROTEIN L11

Chain BL:



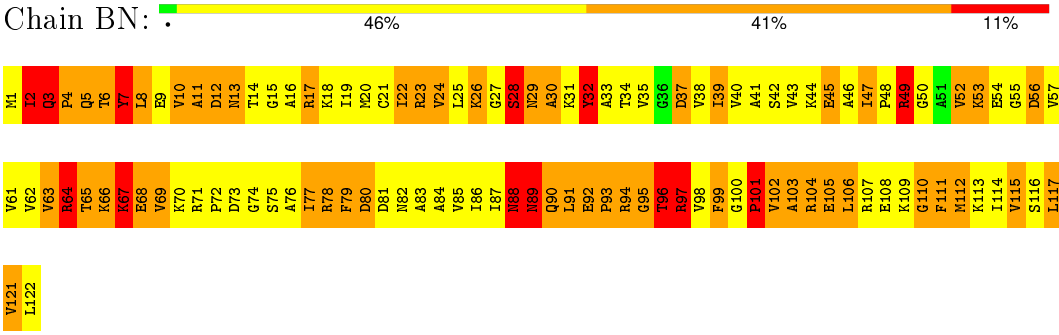
• Molecule 35: 50S RIBOSOMAL PROTEIN L13

Chain BM:



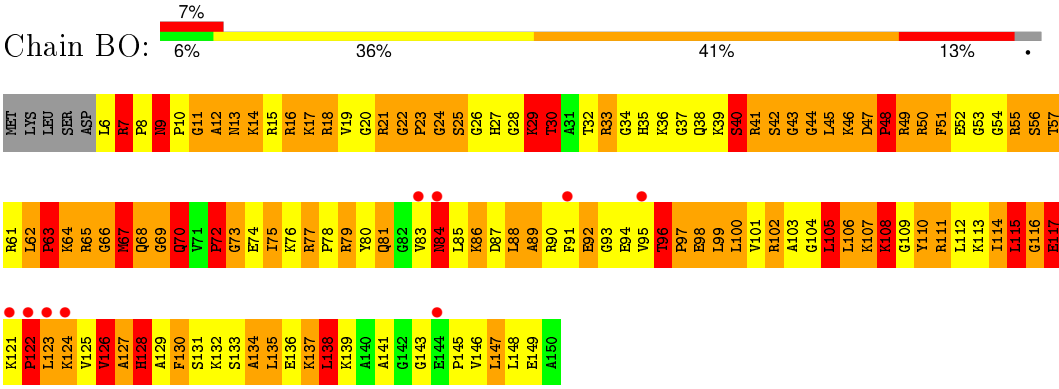
• Molecule 36: 50S RIBOSOMAL PROTEIN L14

Chain BN:



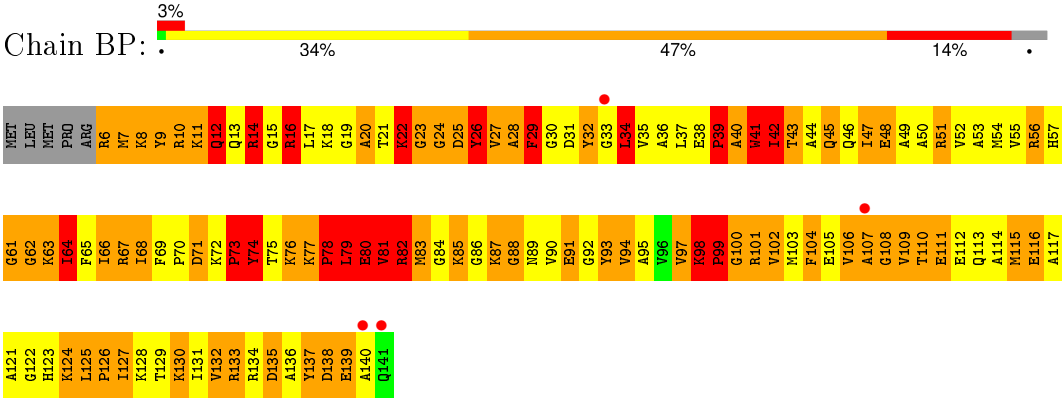
• Molecule 37: 50S RIBOSOMAL PROTEIN L15

Chain BO:



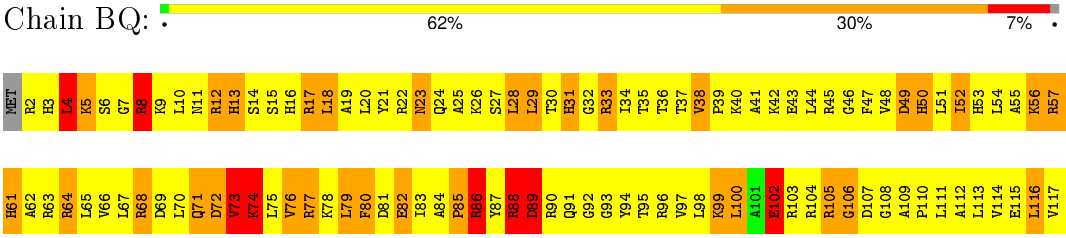
• Molecule 38: 50S RIBOSOMAL PROTEIN L16

Chain BP:



- Molecule 39: 50S RIBOSOMAL PROTEIN L17

Chain BQ:

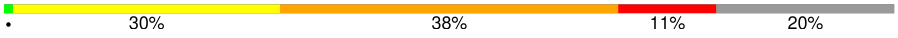


- Molecule 40: 50S RIBOSOMAL PROTEIN L18

Chain BR:

- Molecule 41: 50S RIBOSOMAL PROTEIN L19

Chain BS:



- Molecule 42: 50S RIBOSOMAL PROTEIN L20

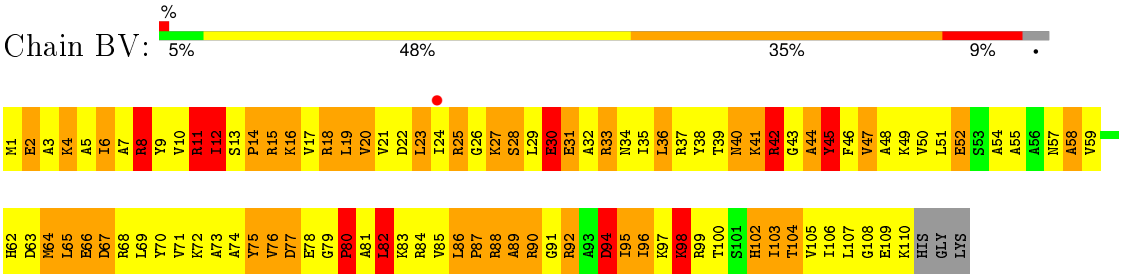
Chain BT:

- Molecule 43: 50S RIBOSOMAL PROTEIN L21

Chain BU:

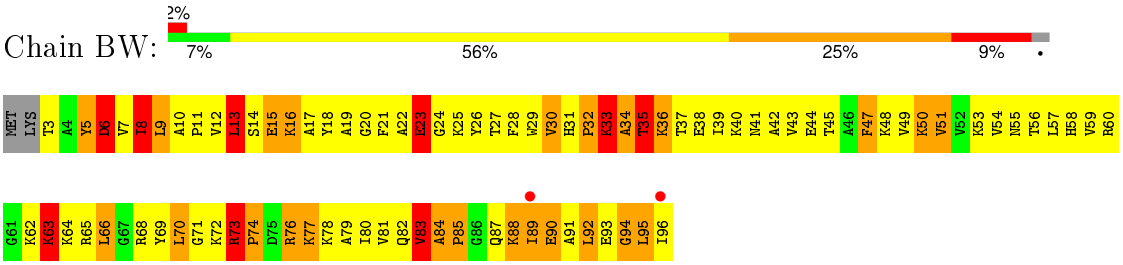
- Molecule 44: 50S RIBOSOMAL PROTEIN L22

Chain BV:



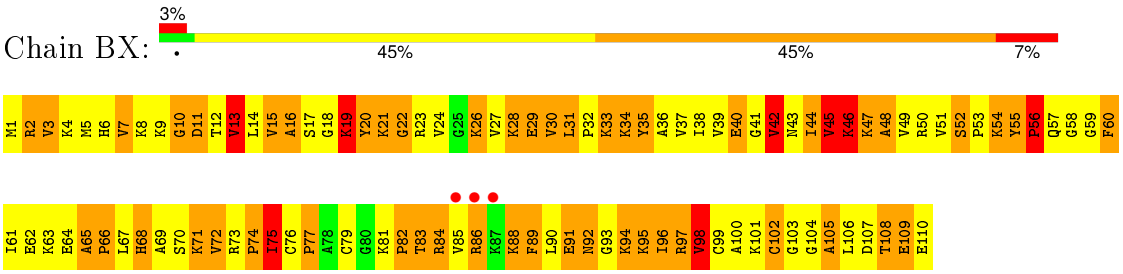
- Molecule 45: 50S RIBOSOMAL PROTEIN L23

Chain BW:



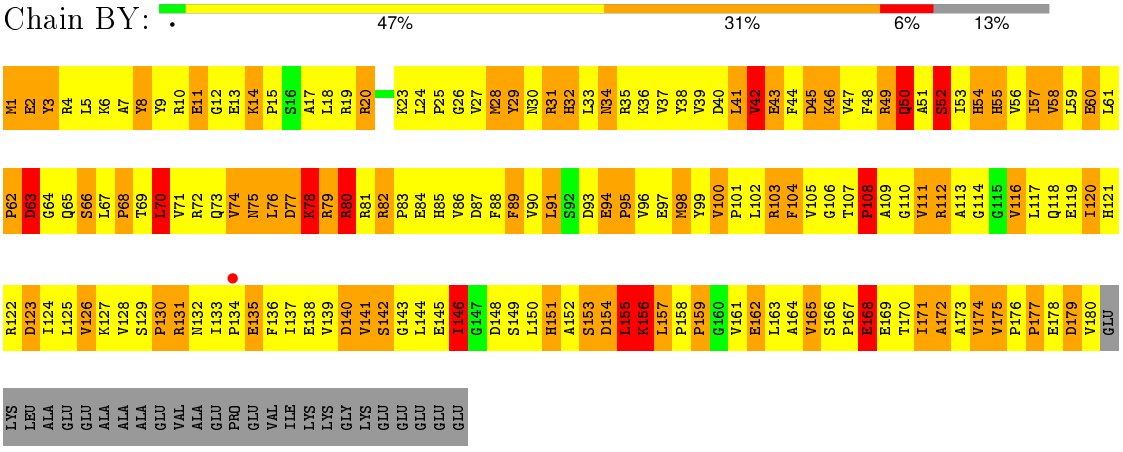
- Molecule 46: 50S RIBOSOMAL PROTEIN L24

Chain BX:



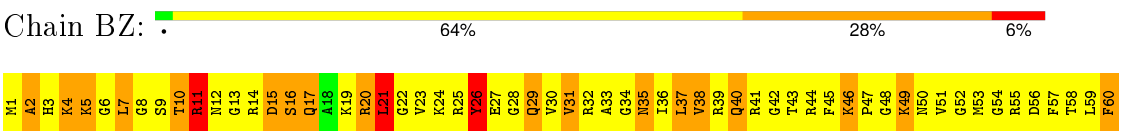
- Molecule 47: 50S RIBOSOMAL PROTEIN L25

Chain BY:



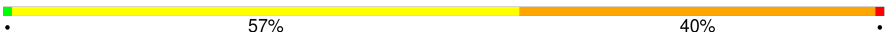
- Molecule 48: 50S RIBOSOMAL PROTEIN L27

Chain BZ:



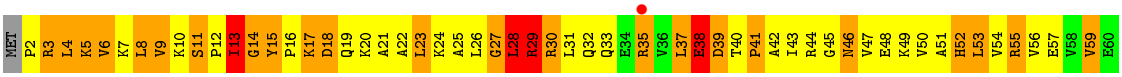
• Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain B1:



• Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain B2:

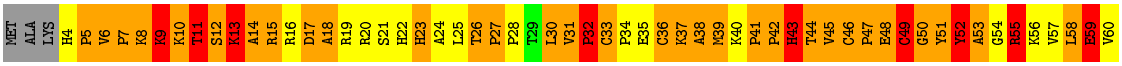


• Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain B3:

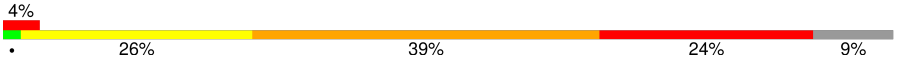
• Molecule 52: 50S RIBOSOMAL PROTEIN L32

Chain B4:



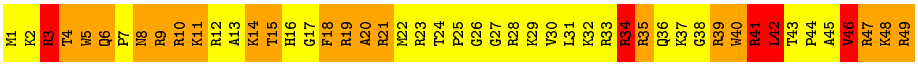
• Molecule 53: 50S RIBOSOMAL PROTEIN L33

Chain B5:



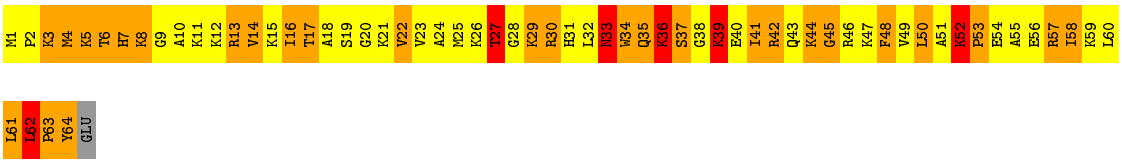
• Molecule 54: 50S RIBOSOMAL PROTEIN L34

Chain B6:



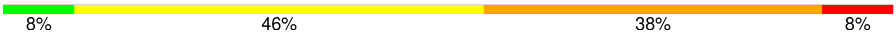
• Molecule 55: 50S RIBOSOMAL PROTEIN L35

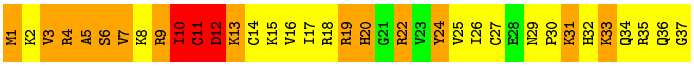
Chain B7:



- Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain B8:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 4.51 429.82 – 3.98	Depositor EDS
% Data completeness (in resolution range)	90.3 (300.00-4.51) 94.9 (429.82-3.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 4.02Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.298 , 0.345 0.300 , 0.346	Depositor DCC
R_{free} test set	14716 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	198.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 116.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Outliers	0 of 441813 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	149640	wwPDB-VP
Average B, all atoms (Å^2)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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	AA	0.93	38/36438 (0.1%)	1.05	172/56869 (0.3%)
2	AC	0.93	2/1814 (0.1%)	1.01	4/2825 (0.1%)
3	AD	1.47	34/1813 (1.9%)	1.27	21/2823 (0.7%)
4	A1	0.81	1/673 (0.1%)	1.07	3/1048 (0.3%)
5	AE	0.63	0/1935	1.01	4/2609 (0.2%)
6	AF	0.53	0/1636	0.93	4/2205 (0.2%)
7	AG	0.67	1/1733 (0.1%)	1.10	7/2318 (0.3%)
8	AH	0.70	0/1162	1.08	4/1564 (0.3%)
9	AI	0.69	0/856	1.03	3/1154 (0.3%)
10	AJ	0.54	0/1276	0.87	0/1709
11	AK	0.73	0/1136	1.08	3/1527 (0.2%)
12	AL	0.51	0/1029	0.84	1/1379 (0.1%)
13	AM	0.50	0/807	0.85	0/1085
14	AN	0.67	0/900	1.06	0/1213
15	AO	0.67	0/986	1.09	3/1320 (0.2%)
16	AP	0.51	0/1008	0.91	2/1347 (0.1%)
17	AQ	0.53	0/501	1.02	3/664 (0.5%)
18	AR	0.67	0/745	0.98	0/992
19	AS	0.72	0/716	1.04	4/963 (0.4%)
20	AT	0.67	0/870	1.05	2/1159 (0.2%)
21	AU	0.65	0/603	1.12	3/799 (0.4%)
22	AV	0.49	0/661	0.91	1/890 (0.1%)
23	AW	0.66	0/765	1.05	1/1007 (0.1%)
24	AX	0.47	0/212	0.82	0/277
25	BA	1.06	139/69685 (0.2%)	1.19	514/108786 (0.5%)
26	BB	0.80	2/2954 (0.1%)	1.00	4/4606 (0.1%)
27	BC	0.50	0/1775	0.89	2/2393 (0.1%)
28	BD	0.88	2/2174 (0.1%)	1.35	22/2927 (0.8%)
29	BE	0.87	0/1611	1.36	19/2171 (0.9%)
30	BF	0.74	0/1660	1.26	11/2247 (0.5%)
31	BG	0.60	0/1507	1.07	5/2027 (0.2%)
32	BH	0.64	0/1354	1.08	5/1831 (0.3%)
33	BK	0.68	0/1170	1.10	8/1581 (0.5%)
34	BL	0.50	0/1044	0.92	1/1415 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	BM	0.85	1/1140 (0.1%)	1.19	7/1537 (0.5%)
36	BN	1.07	4/942 (0.4%)	1.42	7/1268 (0.6%)
37	BO	0.75	0/1123	1.24	9/1493 (0.6%)
38	BP	0.86	1/1100 (0.1%)	1.23	9/1470 (0.6%)
39	BQ	0.70	0/974	1.07	2/1302 (0.2%)
40	BR	0.73	0/887	1.14	5/1180 (0.4%)
41	BS	0.98	0/990	1.52	16/1325 (1.2%)
42	BT	0.81	0/982	1.19	7/1306 (0.5%)
43	BU	0.94	1/790 (0.1%)	1.40	10/1057 (0.9%)
44	BV	0.73	0/886	1.21	7/1189 (0.6%)
45	BW	0.60	0/756	0.97	5/1015 (0.5%)
46	BX	0.61	0/857	1.10	3/1142 (0.3%)
47	BY	0.66	0/1467	1.11	5/1992 (0.3%)
48	BZ	0.67	0/679	1.02	1/902 (0.1%)
49	B1	0.60	0/569	0.89	1/751 (0.1%)
50	B2	0.71	1/474 (0.2%)	1.10	4/635 (0.6%)
51	B3	1.05	0/594	1.44	10/795 (1.3%)
52	B4	0.79	0/459	1.22	2/621 (0.3%)
53	B5	0.98	1/433 (0.2%)	1.49	6/576 (1.0%)
54	B6	0.84	1/438 (0.2%)	1.08	1/575 (0.2%)
55	B7	0.69	0/523	1.22	5/690 (0.7%)
56	B8	0.73	0/310	1.13	1/407 (0.2%)
All	All	0.94	229/162582 (0.1%)	1.13	959/242958 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	241
2	AC	0	9
3	AD	0	12
4	A1	0	5
7	AG	0	1
8	AH	0	1
11	AK	0	2
14	AN	0	1
15	AO	0	1
20	AT	0	1
24	AX	0	1
25	BA	0	610

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	BB	0	20
28	BD	0	1
30	BF	0	1
32	BH	0	3
36	BN	0	2
38	BP	0	3
41	BS	0	2
42	BT	0	1
43	BU	0	2
44	BV	0	1
51	B3	0	2
52	B4	0	1
53	B5	0	1
56	B8	0	1
All	All	0	926

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1203	G	O3'-P	-34.71	1.19	1.61
25	BA	1202	C	O3'-P	29.90	1.97	1.61
25	BA	2447	G	O3'-P	-21.30	1.35	1.61
25	BA	2601	C	O3'-P	19.66	1.84	1.61
25	BA	2756	U	O3'-P	19.18	1.84	1.61

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	412	A	O5'-P-OP2	-28.87	76.06	110.70
25	BA	1203	G	P-O3'-C3'	27.73	152.97	119.70
25	BA	2448	A	C5'-C4'-O4'	-27.33	76.31	109.10
30	BF	20	LEU	O-C-N	-25.54	81.83	122.70
1	AA	37	U	N3-C4-O4	-25.04	101.87	119.40

There are no chirality outliers.

5 of 926 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	16	A	Sidechain
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	24	U	Sidechain
1	AA	7	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	AA	32554	0	16429	6699	0
2	AC	1624	0	826	331	0
3	AD	1623	0	809	304	0
4	A1	596	0	296	65	0
5	AE	1900	0	1951	928	0
6	AF	1612	0	1677	661	0
7	AG	1703	0	1763	807	0
8	AH	1146	0	1207	482	0
9	AI	843	0	857	397	0
10	AJ	1257	0	1296	519	0
11	AK	1116	0	1177	666	0
12	AL	1010	0	1037	457	0
13	AM	794	0	840	327	0
14	AN	885	0	904	410	0
15	AO	970	0	1057	413	0
16	AP	997	0	1072	469	0
17	AQ	492	0	529	264	0
18	AR	734	0	771	353	0
19	AS	700	0	720	348	0
20	AT	857	0	930	385	0
21	AU	597	0	668	357	0
22	AV	647	0	673	241	0
23	AW	763	0	861	330	0
24	AX	208	0	221	87	0
25	BA	62218	0	31354	15682	0
26	BB	2641	0	1337	598	0
27	BC	1742	0	1796	761	0
28	BD	2124	0	2207	1434	0
29	BE	1578	0	1647	1120	0
30	BF	1625	0	1666	862	0
31	BG	1482	0	1546	838	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BH	1328	0	1408	664	0
33	BK	1155	0	1244	574	0
34	BL	1025	0	1074	414	0
35	BM	1113	0	1183	722	0
36	BN	932	0	994	703	0
37	BO	1106	0	1183	801	0
38	BP	1080	0	1127	691	0
39	BQ	960	0	1021	505	0
40	BR	877	0	938	472	0
41	BS	976	0	1033	699	0
42	BT	964	0	1022	709	0
43	BU	779	0	852	626	0
44	BV	876	0	941	423	0
45	BW	742	0	800	336	0
46	BX	844	0	930	493	0
47	BY	1435	0	1463	683	0
48	BZ	670	0	700	365	0
49	B1	567	0	621	303	0
50	B2	469	0	518	302	0
51	B3	581	0	577	375	0
52	B4	445	0	459	271	0
53	B5	426	0	452	306	0
54	B6	430	0	480	275	0
55	B7	515	0	587	415	0
56	B8	307	0	335	126	0
All	All	149640	0	102066	45475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 181.

The worst 5 of 45475 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)
25:BA:1204:A:C2	30:BF:188:ARG:HA	1.17	1.61
25:BA:2459:A:N3	25:BA:2460:U:H1'	1.22	1.46
25:BA:1204:A:C2	30:BF:188:ARG:CA	1.98	1.45
25:BA:2745:C:N4	25:BA:2756:U:C5	1.85	1.45
25:BA:1475:G:H1	25:BA:1477:A:N6	1.11	1.44

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	232/256 (91%)	112 (48%)	47 (20%)	73 (32%)	0	0
6	AF	204/239 (85%)	115 (56%)	43 (21%)	46 (22%)	0	1
7	AG	206/209 (99%)	103 (50%)	61 (30%)	42 (20%)	0	2
8	AH	148/162 (91%)	92 (62%)	34 (23%)	22 (15%)	0	5
9	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
10	AJ	153/156 (98%)	74 (48%)	40 (26%)	39 (26%)	0	1
11	AK	136/138 (99%)	71 (52%)	32 (24%)	33 (24%)	0	1
12	AL	125/128 (98%)	64 (51%)	33 (26%)	28 (22%)	0	1
13	AM	96/105 (91%)	55 (57%)	14 (15%)	27 (28%)	0	0
14	AN	117/129 (91%)	62 (53%)	30 (26%)	25 (21%)	0	2
15	AO	122/132 (92%)	62 (51%)	22 (18%)	38 (31%)	0	0
16	AP	123/126 (98%)	63 (51%)	36 (29%)	24 (20%)	0	3
17	AQ	58/61 (95%)	28 (48%)	14 (24%)	16 (28%)	0	0
18	AR	86/89 (97%)	40 (46%)	33 (38%)	13 (15%)	0	5
19	AS	81/88 (92%)	45 (56%)	21 (26%)	15 (18%)	0	3
20	AT	102/105 (97%)	63 (62%)	22 (22%)	17 (17%)	0	5
21	AU	71/88 (81%)	30 (42%)	18 (25%)	23 (32%)	0	0
22	AV	78/93 (84%)	32 (41%)	18 (23%)	28 (36%)	0	0
23	AW	97/106 (92%)	32 (33%)	36 (37%)	29 (30%)	0	0
24	AX	22/27 (82%)	9 (41%)	8 (36%)	5 (23%)	0	1
27	BC	226/229 (99%)	137 (61%)	52 (23%)	37 (16%)	0	5
28	BD	270/276 (98%)	129 (48%)	49 (18%)	92 (34%)	0	0
29	BE	204/206 (99%)	106 (52%)	39 (19%)	59 (29%)	0	0
30	BF	206/210 (98%)	100 (48%)	47 (23%)	59 (29%)	0	0
31	BG	180/182 (99%)	79 (44%)	42 (23%)	59 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	172/180 (96%)	89 (52%)	41 (24%)	42 (24%)	0	1
33	BK	146/148 (99%)	88 (60%)	32 (22%)	26 (18%)	0	3
34	BL	136/147 (92%)	66 (48%)	32 (24%)	38 (28%)	0	0
35	BM	137/140 (98%)	66 (48%)	31 (23%)	40 (29%)	0	0
36	BN	120/122 (98%)	63 (52%)	21 (18%)	36 (30%)	0	0
37	BO	143/150 (95%)	60 (42%)	31 (22%)	52 (36%)	0	0
38	BP	134/141 (95%)	51 (38%)	35 (26%)	48 (36%)	0	0
39	BQ	115/118 (98%)	64 (56%)	33 (29%)	18 (16%)	0	5
40	BR	108/112 (96%)	45 (42%)	30 (28%)	33 (31%)	0	0
41	BS	115/146 (79%)	53 (46%)	26 (23%)	36 (31%)	0	0
42	BT	115/118 (98%)	49 (43%)	39 (34%)	27 (24%)	0	1
43	BU	99/101 (98%)	51 (52%)	22 (22%)	26 (26%)	0	1
44	BV	108/113 (96%)	69 (64%)	15 (14%)	24 (22%)	0	1
45	BW	92/96 (96%)	59 (64%)	14 (15%)	19 (21%)	0	2
46	BX	108/110 (98%)	41 (38%)	27 (25%)	40 (37%)	0	0
47	BY	178/206 (86%)	93 (52%)	48 (27%)	37 (21%)	0	2
48	BZ	83/85 (98%)	50 (60%)	14 (17%)	19 (23%)	0	1
49	B1	65/67 (97%)	27 (42%)	26 (40%)	12 (18%)	0	3
50	B2	57/60 (95%)	32 (56%)	16 (28%)	9 (16%)	0	5
51	B3	69/71 (97%)	26 (38%)	19 (28%)	24 (35%)	0	0
52	B4	55/60 (92%)	16 (29%)	12 (22%)	27 (49%)	0	0
53	B5	47/54 (87%)	13 (28%)	7 (15%)	27 (57%)	0	0
54	B6	47/49 (96%)	16 (34%)	16 (34%)	15 (32%)	0	0
55	B7	62/65 (95%)	29 (47%)	11 (18%)	22 (36%)	0	0
56	B8	35/37 (95%)	20 (57%)	4 (11%)	11 (31%)	0	0
All	All	5988/6337 (94%)	2997 (50%)	1412 (24%)	1579 (26%)	0	1

5 of 1579 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	13	ALA
5	AE	15	VAL
5	AE	17	PHE

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Mol	Chain	Res	Type
5	AE	19	HIS
5	AE	20	GLU

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	AE	202/220 (92%)	135 (67%)	67 (33%)	0 2
6	AF	160/188 (85%)	123 (77%)	37 (23%)	1 8
7	AG	180/181 (99%)	127 (71%)	53 (29%)	0 4
8	AH	115/123 (94%)	75 (65%)	40 (35%)	0 2
9	AI	90/90 (100%)	64 (71%)	26 (29%)	0 4
10	AJ	126/127 (99%)	95 (75%)	31 (25%)	1 7
11	AK	119/119 (100%)	76 (64%)	43 (36%)	0 1
12	AL	98/99 (99%)	76 (78%)	22 (22%)	1 10
13	AM	88/92 (96%)	65 (74%)	23 (26%)	0 6
14	AN	90/99 (91%)	62 (69%)	28 (31%)	0 3
15	AO	104/109 (95%)	77 (74%)	27 (26%)	0 6
16	AP	100/101 (99%)	79 (79%)	21 (21%)	1 11
17	AQ	49/50 (98%)	37 (76%)	12 (24%)	1 7
18	AR	79/80 (99%)	56 (71%)	23 (29%)	0 4
19	AS	72/74 (97%)	48 (67%)	24 (33%)	0 2
20	AT	96/97 (99%)	71 (74%)	25 (26%)	0 6
21	AU	64/77 (83%)	41 (64%)	23 (36%)	0 1
22	AV	71/80 (89%)	57 (80%)	14 (20%)	1 13
23	AW	76/82 (93%)	56 (74%)	20 (26%)	0 6
24	AX	19/22 (86%)	13 (68%)	6 (32%)	0 3
27	BC	180/181 (99%)	151 (84%)	29 (16%)	3 22
28	BD	215/218 (99%)	151 (70%)	64 (30%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
30	BF	164/166 (99%)	104 (63%)	60 (37%)	0	1
31	BG	156/156 (100%)	112 (72%)	44 (28%)	0	4
32	BH	143/148 (97%)	97 (68%)	46 (32%)	0	3
33	BK	124/124 (100%)	87 (70%)	37 (30%)	0	3
34	BL	105/111 (95%)	85 (81%)	20 (19%)	2	14
35	BM	118/119 (99%)	80 (68%)	38 (32%)	0	3
36	BN	100/100 (100%)	65 (65%)	35 (35%)	0	2
37	BO	111/116 (96%)	64 (58%)	47 (42%)	0	0
38	BP	106/111 (96%)	55 (52%)	51 (48%)	0	0
39	BQ	100/101 (99%)	69 (69%)	31 (31%)	0	3
40	BR	87/88 (99%)	55 (63%)	32 (37%)	0	1
41	BS	105/127 (83%)	69 (66%)	36 (34%)	0	2
42	BT	93/94 (99%)	64 (69%)	29 (31%)	0	3
43	BU	82/82 (100%)	59 (72%)	23 (28%)	0	4
44	BV	90/92 (98%)	56 (62%)	34 (38%)	0	0
45	BW	76/78 (97%)	55 (72%)	21 (28%)	0	4
46	BX	91/91 (100%)	66 (72%)	25 (28%)	0	5
47	BY	159/179 (89%)	110 (69%)	49 (31%)	0	3
48	BZ	67/67 (100%)	52 (78%)	15 (22%)	1	10
49	B1	62/62 (100%)	46 (74%)	16 (26%)	0	6
50	B2	51/52 (98%)	34 (67%)	17 (33%)	0	2
51	B3	63/63 (100%)	42 (67%)	21 (33%)	0	2
52	B4	50/52 (96%)	30 (60%)	20 (40%)	0	0
53	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
54	B6	42/42 (100%)	30 (71%)	12 (29%)	0	4
55	B7	54/55 (98%)	40 (74%)	14 (26%)	0	6
56	B8	34/34 (100%)	25 (74%)	9 (26%)	0	5
All	All	5040/5237 (96%)	3520 (70%)	1520 (30%)	0	3

5 of 1520 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BE	101	ARG
32	BH	103	LEU
49	B1	45	ILE
29	BE	155	LYS
30	BF	175	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
22	AV	23	ASN
29	BE	129	HIS
51	B3	46	GLN
23	AW	45	GLN
28	BD	87	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	479 (31%)	151 (9%)
2	AC	75/76 (98%)	30 (40%)	7 (9%)
25	BA	2888/2916 (99%)	1241 (42%)	313 (10%)
26	BB	122/123 (99%)	46 (37%)	5 (4%)
3	AD	75/76 (98%)	27 (36%)	3 (4%)
4	A1	26/27 (96%)	11 (42%)	1 (3%)
All	All	4701/4740 (99%)	1834 (39%)	480 (10%)

5 of 1834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 480 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	562	U
25	BA	974(A)	C
25	BA	2610	C

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Mol	Chain	Res	Type
25	BA	616	A
25	BA	783	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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
25	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1202:C	O3'	1203:G	P	1.97
1	BA	1203:G	O3'	1204:A	P	1.19

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%)	-0.79	2 (0%) 95 95	188, 245, 349, 445	0
2	AC	76/76 (100%)	-0.95	0 100 100	213, 249, 283, 294	0
3	AD	76/76 (100%)	-0.82	0 100 100	301, 334, 358, 368	0
4	A1	27/27 (100%)	0.91	7 (25%) 1 2	225, 347, 415, 416	0
5	AE	234/256 (91%)	-0.23	10 (4%) 39 30	218, 248, 286, 307	0
6	AF	206/239 (86%)	0.29	14 (6%) 20 15	246, 269, 288, 296	0
7	AG	208/209 (99%)	-0.78	0 100 100	202, 233, 251, 265	0
8	AH	150/162 (92%)	-0.54	1 (0%) 89 84	202, 220, 245, 262	0
9	AI	101/101 (100%)	0.39	6 (5%) 26 19	219, 237, 254, 271	0
10	AJ	155/156 (99%)	0.19	8 (5%) 31 24	250, 273, 285, 301	0
11	AK	138/138 (100%)	-0.79	0 100 100	203, 222, 236, 246	0
12	AL	127/128 (99%)	-0.47	0 100 100	247, 317, 349, 353	0
13	AM	98/105 (93%)	0.36	12 (12%) 5 6	256, 296, 311, 317	0
14	AN	119/129 (92%)	-0.20	2 (1%) 73 64	214, 234, 252, 279	0
15	AO	124/132 (93%)	-0.26	0 100 100	189, 217, 243, 263	0
16	AP	125/126 (99%)	-0.66	0 100 100	253, 281, 302, 306	0
17	AQ	60/61 (98%)	-0.40	0 100 100	243, 273, 286, 290	0
18	AR	88/89 (98%)	-1.03	0 100 100	199, 222, 244, 251	0
19	AS	83/88 (94%)	-0.88	0 100 100	192, 212, 232, 267	0
20	AT	104/105 (99%)	-1.08	0 100 100	192, 218, 252, 296	0
21	AU	73/88 (82%)	-0.44	3 (4%) 41 32	192, 228, 255, 277	0
22	AV	80/93 (86%)	0.35	7 (8%) 12 10	251, 287, 306, 310	0
23	AW	99/106 (93%)	-0.93	0 100 100	200, 228, 250, 254	0
24	AX	24/27 (88%)	-1.05	0 100 100	268, 289, 303, 306	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	BA	2889/2916 (99%)	-0.78	3 (0%) 95 95	168, 241, 340, 398	0
26	BB	123/123 (100%)	-0.56	0 100 100	236, 293, 329, 343	0
27	BC	228/229 (99%)	1.07	58 (25%) 1 2	299, 326, 342, 347	0
28	BD	272/276 (98%)	-0.10	8 (2%) 55 44	184, 216, 235, 256	0
29	BE	206/206 (100%)	-0.59	3 (1%) 76 67	155, 205, 250, 276	0
30	BF	208/210 (99%)	-0.56	0 100 100	186, 255, 283, 288	0
31	BG	182/182 (100%)	-0.53	2 (1%) 82 76	247, 283, 306, 311	0
32	BH	174/180 (96%)	-0.37	2 (1%) 82 76	230, 260, 278, 284	0
33	BK	148/148 (100%)	-0.59	0 100 100	212, 241, 261, 265	0
34	BL	138/147 (93%)	0.69	25 (18%) 2 3	305, 358, 399, 403	0
35	BM	139/140 (99%)	-0.58	2 (1%) 78 69	187, 217, 245, 270	0
36	BN	122/122 (100%)	-0.65	0 100 100	172, 201, 228, 240	0
37	BO	145/150 (96%)	-0.16	10 (6%) 20 15	189, 271, 304, 346	0
38	BP	136/141 (96%)	-0.38	4 (2%) 55 44	199, 234, 257, 266	0
39	BQ	117/118 (99%)	-0.75	0 100 100	195, 214, 246, 256	0
40	BR	110/112 (98%)	-0.93	0 100 100	232, 266, 293, 300	0
41	BS	117/146 (80%)	-0.58	0 100 100	182, 205, 238, 244	0
42	BT	117/118 (99%)	-0.59	0 100 100	191, 221, 241, 250	0
43	BU	101/101 (100%)	-0.11	3 (2%) 54 42	190, 244, 272, 277	0
44	BV	110/113 (97%)	-0.40	1 (0%) 85 80	203, 226, 250, 260	0
45	BW	94/96 (97%)	-0.47	2 (2%) 67 57	237, 253, 304, 309	0
46	BX	110/110 (100%)	-0.28	3 (2%) 58 48	244, 282, 303, 312	0
47	BY	180/206 (87%)	-0.07	1 (0%) 90 86	235, 267, 281, 287	0
48	BZ	85/85 (100%)	-0.99	0 100 100	236, 259, 272, 289	0
49	B1	67/67 (100%)	-0.60	0 100 100	251, 264, 276, 281	0
50	B2	59/60 (98%)	-0.55	1 (1%) 73 64	208, 244, 261, 268	0
51	B3	71/71 (100%)	-0.93	0 100 100	212, 239, 259, 276	0
52	B4	57/60 (95%)	-0.59	0 100 100	200, 227, 276, 299	0
53	B5	49/54 (90%)	-0.34	2 (4%) 41 32	211, 247, 269, 277	0
54	B6	49/49 (100%)	-0.88	0 100 100	189, 228, 244, 250	0
55	B7	64/65 (98%)	-0.79	0 100 100	201, 220, 235, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	B8	37/37 (100%)	-1.10	0 100 100	212, 230, 240, 244	0
All	All	10794/11077 (97%)	-0.53	202 (1%) 70 61	155, 245, 336, 445	0

The worst 5 of 202 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BO	123	LEU	13.2
4	A1	1	G	10.6
27	BC	126	LYS	10.0
27	BC	125	SER	9.6
27	BC	121	GLY	8.9

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.