



# wwPDB X-ray Structure Validation Summary Report ⓘ

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-Briesse, 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
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

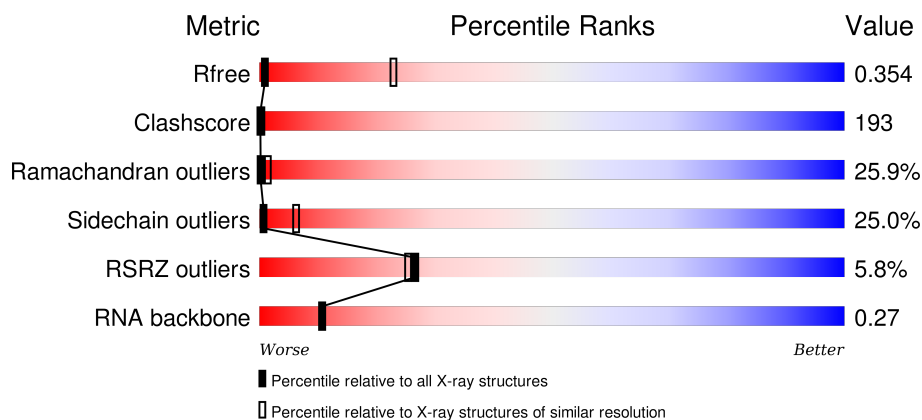
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	123	
2	AA	2915	
3	AC	228	
4	AD	178	


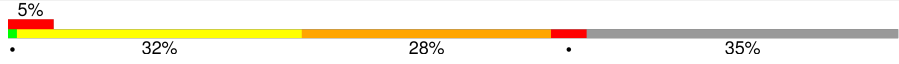


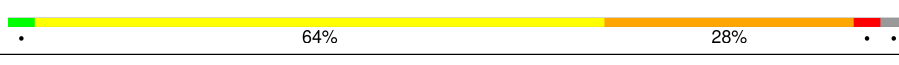
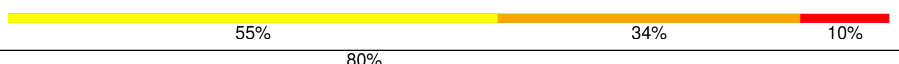





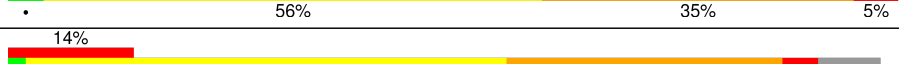
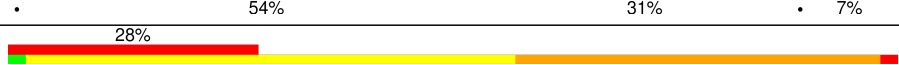
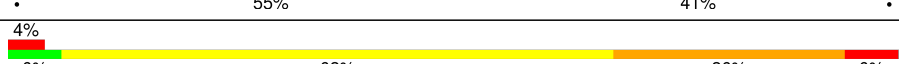

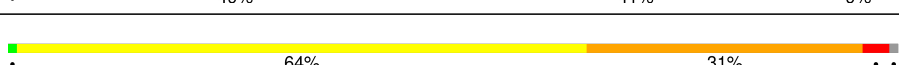
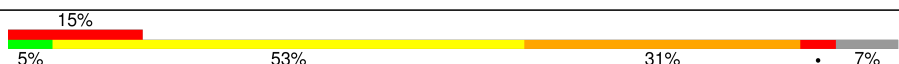
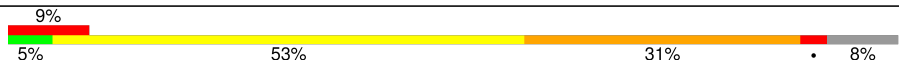
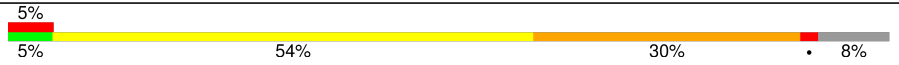


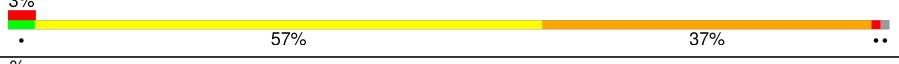

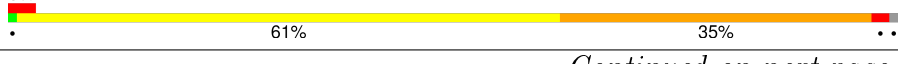

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Mol	Chain	Length	Quality of chain
5	AE	338	
6	AF	246	
7	AG	176	
8	AH	177	
9	AI	128	
9	AJ	128	
10	AK	149	
11	AL	141	
12	AM	145	
13	AN	122	
14	AO	164	
15	AP	138	
16	AQ	186	
17	AR	66	
18	AS	113	
19	AT	84	
20	AU	119	
21	AV	253	
22	AW	70	
23	AX	60	
24	A0	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	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>11%</div><div>49%</div><div>20%</div><div>10%</div><div>17%</div></div></div>
54	BV	93	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>6%</div><div>48%</div><div>28%</div><div>5%</div><div>14%</div></div></div>
55	BW	106	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>56%</div><div>32%</div><div>6%</div><div>7%</div></div></div>
56	BX	27	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>56%</div><div>30%</div><div></div><div>11%</div></div></div>

## 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
1	AB	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
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
2	AA	2872	Total	C	N	O	P	0	0	0
			61847	27526	11556	19893	2872			

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
3	AC	221	Total	C	N	O	S	0	0	0
			1687	1066	306	312	3			

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

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

- 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	S	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	S	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	S	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

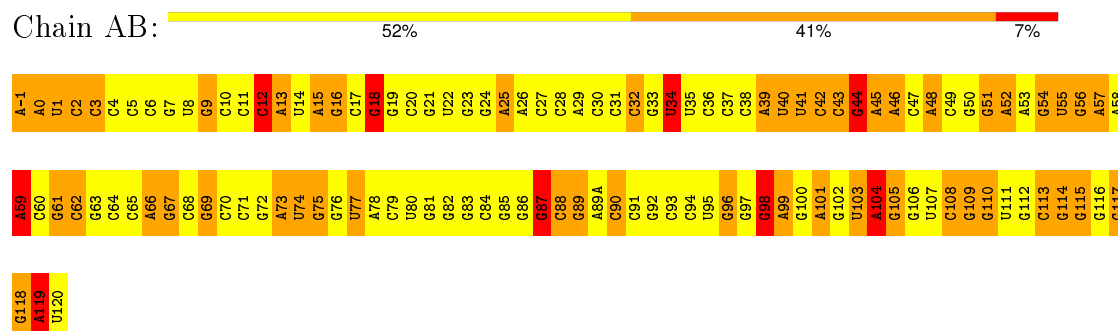
- Molecule 56 is a protein called 30S ribosomal protein Thx.

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

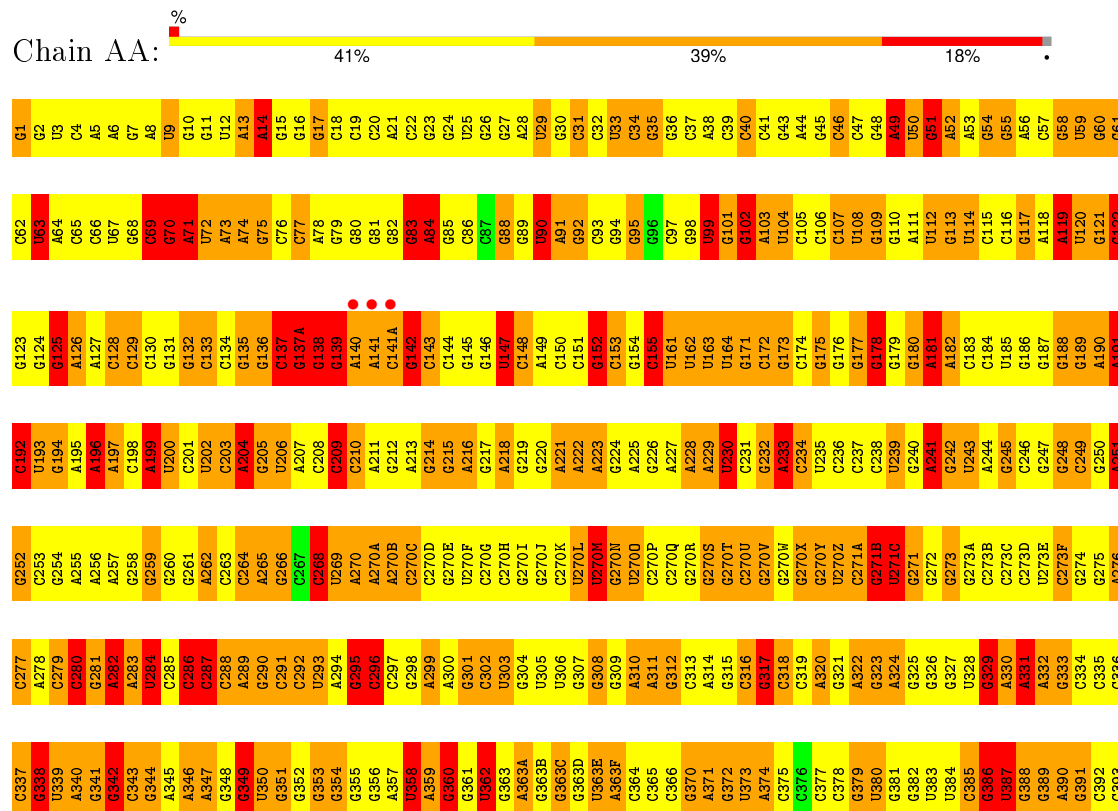
### 3 Residue-property plots

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

#### • Molecule 1: 5S ribosomal RNA



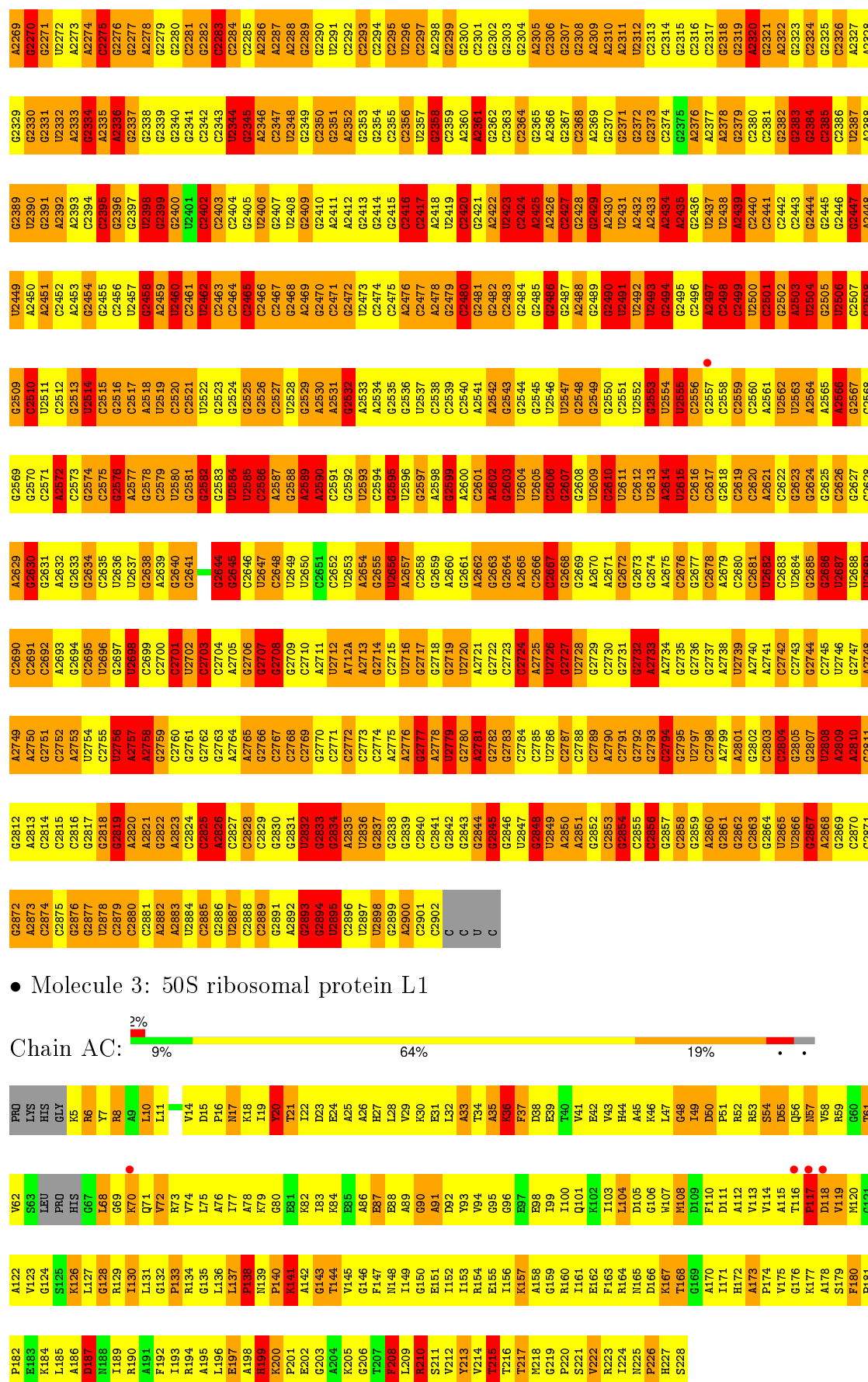
#### • Molecule 2: 23S ribosomal RNA



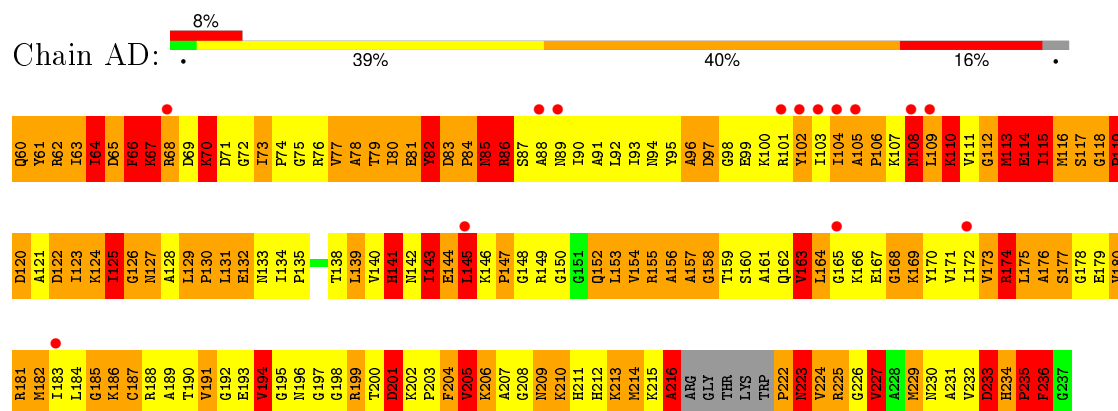
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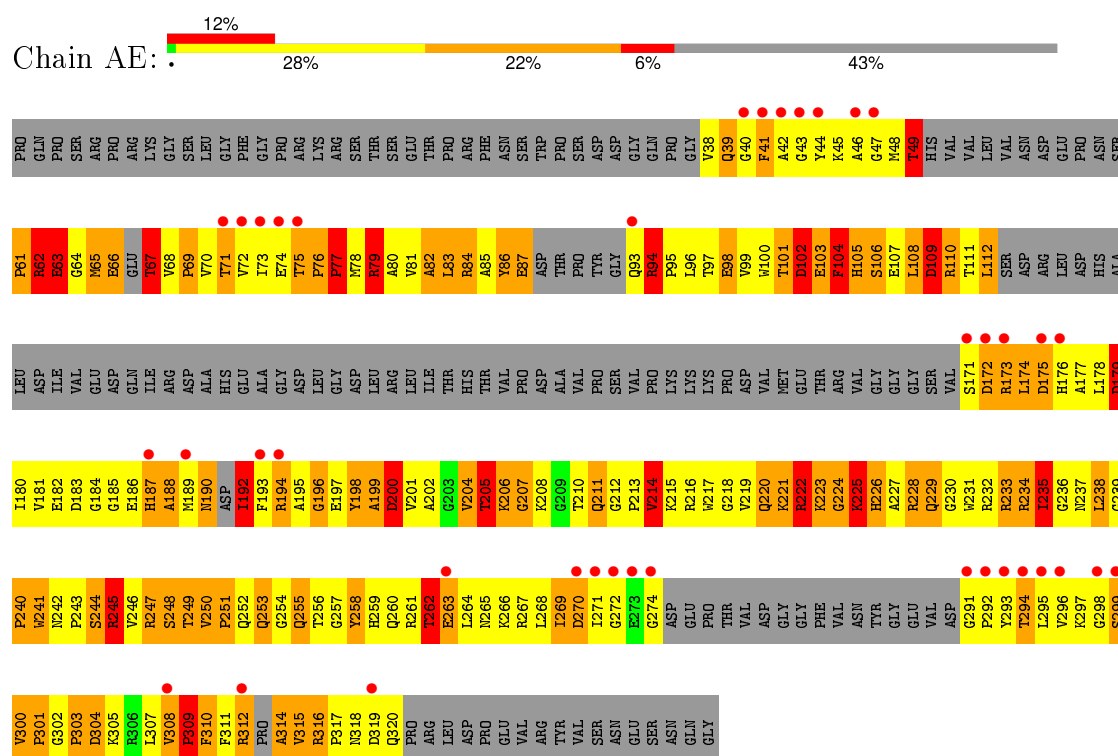
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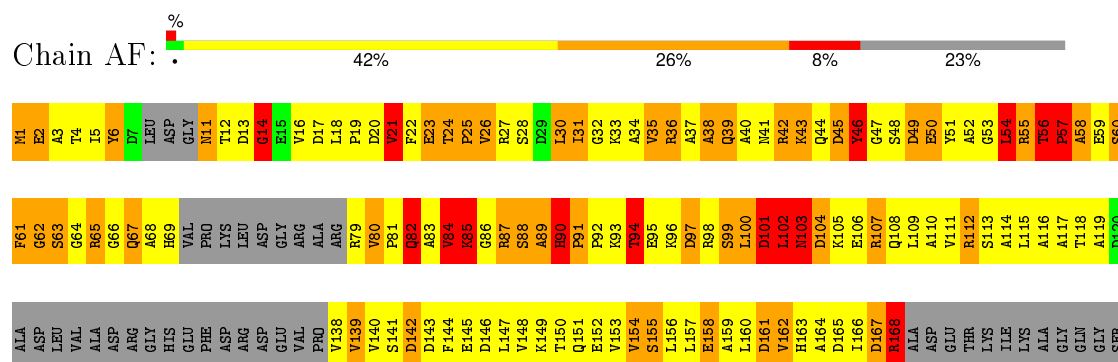
• Molecule 4: 50S ribosomal protein L2

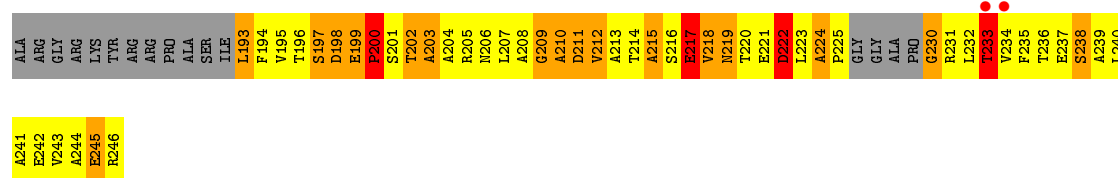


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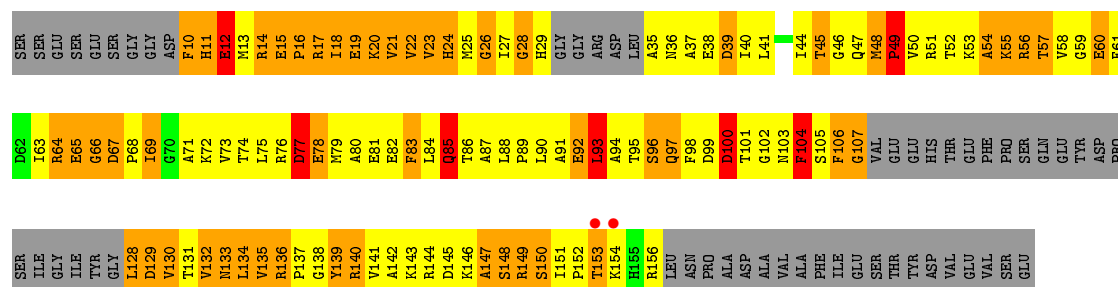


• Molecule 6: 50S ribosomal protein L4

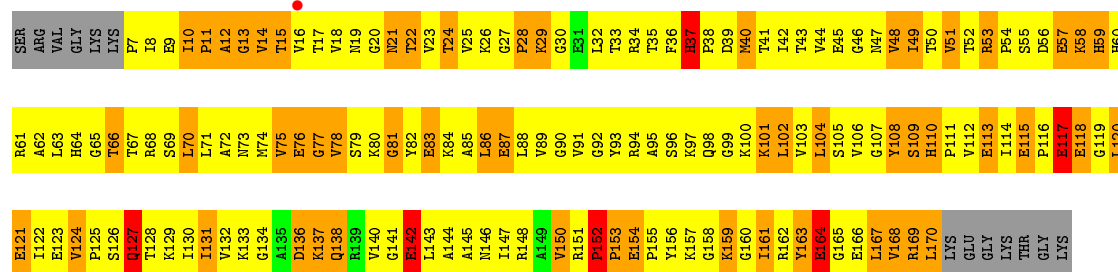




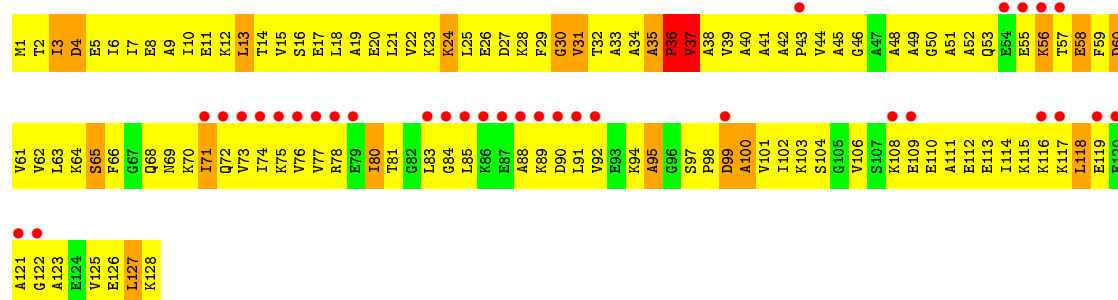
• Molecule 7: 50S ribosomal protein L5



• Molecule 8: 50S ribosomal protein L6

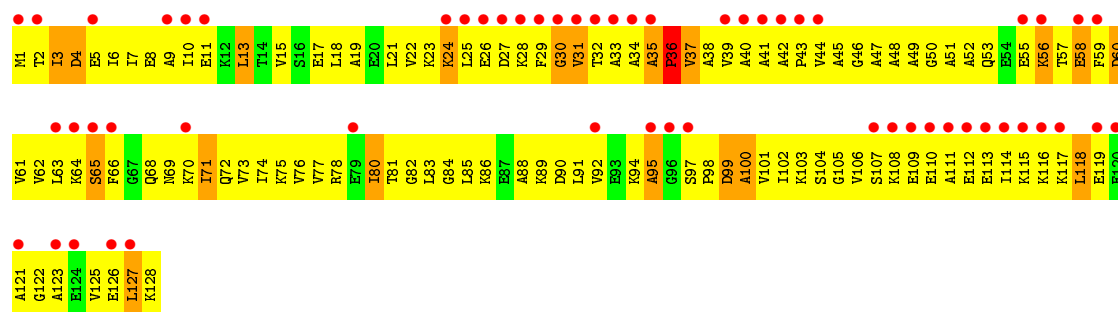


• Molecule 9: 50S ribosomal protein L7/L12



• Molecule 9: 50S ribosomal protein L7/L12





• Molecule 10: 50S ribosomal protein L9



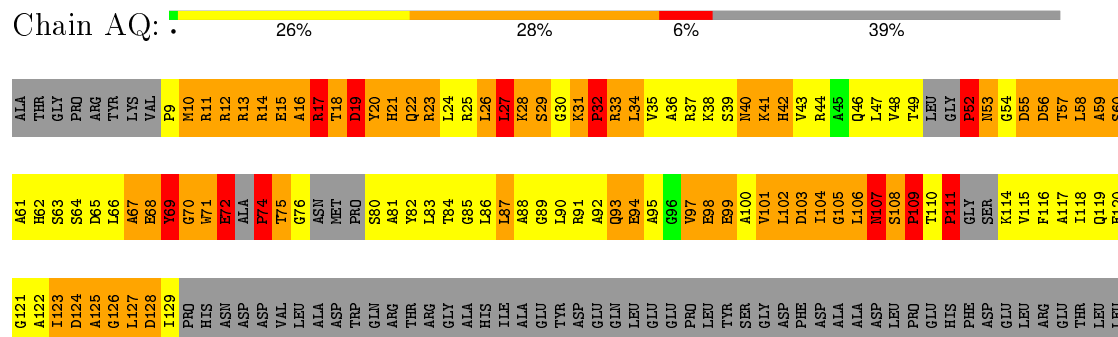
• Molecule 11: 50S ribosomal protein L11



• Molecule 12: 50S ribosomal protein L13



• Molecule 13: 50S ribosomal protein L14



ASP  
GLY  
ASP  
ILE  
GLU  
LEU

• Molecule 17: 50S ribosomal protein L19

Chain AR: 15% 35% 20% 24% 21%

PRO ARG THR R4 E5 A5 C6 D7 Y8 C9 G9 G10 T11 D12 D13 E14 P15 G16 T17 T18 G18 T19 T20 F21 R22 R23 K24 D25 G26 A27 T28 T29 T30 H30 R31 F32 G33 S33 S34 K35 R36 R37 R38 N39 A40 D41 L42 L43 GLY R44 E45 A46 R47 N48 L49 E50 E51 D52 D53 T54 A55 R56 GLY GLU ALA GLY

GLU  
ALA  
GLU  
ASP  
GLU  
ALA

• Molecule 18: 50S ribosomal protein L22

Chain AS: 3% 61% 24% 6%

MET E2 K3 K4 A5 I6 A7 R8 Y9 V10 R11 V12 I13 S13 A14 P15 R16 K15 R17 V18 R18 R19 V20 V21 D22 L23 R24 R25 G26 A27 R28 S28 L29 A30 R31 E32 A33 R34 N35 I36 R37 R38 Y39 T39 N40 R41 R42 R43 G43 A44 A45 Y46 F47 V47 G48 A49 E50 V50 L51 E52 S53 A54 A55 A56 N57 A58 V59 N60

N61 H62 H63 MET K65 E66 D67 R68 R69 V70 Y71 W72 K73 A74 A75 V76 V77 E78 G79 P80 P81 K82 K83 R84 V85 L86 R87 R88 A89 R90 G91 R92 A93 A94 I95 I96 R97 R98 R99 T100 T101 S101 H102 R103 I104 T104 V105 I106 G108 E109 K110 HIS GLY LYS

• Molecule 19: 50S ribosomal protein L23

Chain AT: 5% 52% 25% 13% 10%

S1 R2 D3 V4 I5 K6 H7 R8 H9 V10 T11 E12 R13 K14 A15 M15 M16 R17 D18 M18 D19 F20 GLN R21 R22 R23 L24 Q25 F26 A27 V28 D29 R30 R31 A32 A33 S33 K34 G35 Y36 R37 V37 A38 D39 A40 V41 E42 E43 Q44 Y45 D46 T47 T48 V49 E50 Q51 V52 N53 T54 Q55 N56 T57 P58 D59 G60

E61 K62 K63 A64 V65 V66 R67 L68 S69 D70 E71 D72 D73 A74 A75 E76 A77 A78 S79 ARG ILE VAL PHE

• Molecule 20: 50S ribosomal protein L24

Chain AU: 8% 61% 24% 7% 8%

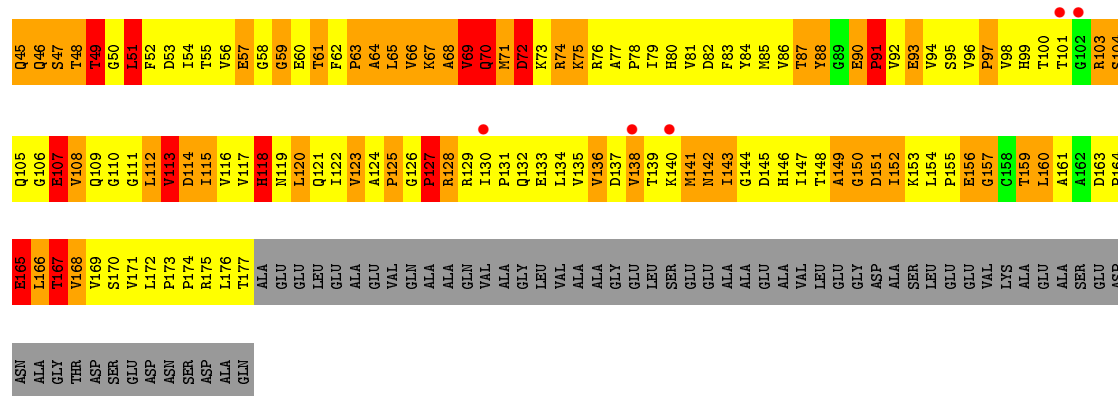
S1 R2 Q3 P4 D5 K6 Q7 R8 R9 S10 S11 Q11 R12 R13 R14 A15 P15 L16 H17 E18 R19 R20 R21 Q22 V23 R24 A25 T26 T27 S28 A29 D30 R31 R32 R33 E34 Y35 G36 GLN ARG ASN V40 V41 V42 V43 A44 A45 G45 D46 T47 T48 E49 V50 L51 R52 G53 D54 F55 Q56 A57 E58 D59 G60

E61 V62 I63 N64 V65 D66 L67 L68 D69 K69 A70 V71 I72 H73 V74 E75 D76 D77 T78 L79 E80 R81 T82 D83 G84 E85 E86 V87 P88 R89 P90 P91 L91 D92 T93 E94 N95 Y96 R97 V98 T99 D100 L101 D102 L103 E104 D105 E106 K107 R108 E109 A110 R111 L112 E113 SER GLU ASP ASP SER

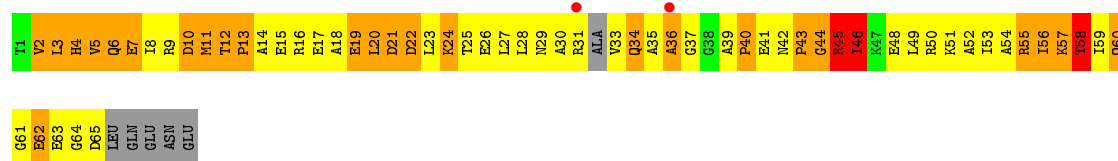
• Molecule 21: 50S general stress protein CTC (L25)

Chain AV: 3% 35% 24% 9% 30%

MET ALA THR THR GLN THR ALA LYS SER GLN ASP THR M1 E2 I3 T4 A5 K6 K7 P7 R8 T9 F10 K11 Q12 K13 L14 D15 E16 S17 M18 I19 A20 A21 V22 A23 Y24 N25 R26 E27 R28 N29 V30 S31 F32 A33 I34 D35 R36 R37 A38 F39 D40 R41 A42 F43 R44



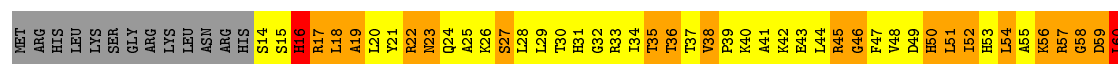
• Molecule 22: 50S ribosomal protein L29



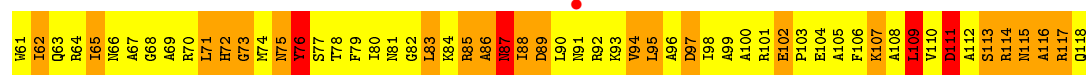
• Molecule 23: 50S ribosomal protein L30



• Molecule 24: 50S ribosomal protein L17

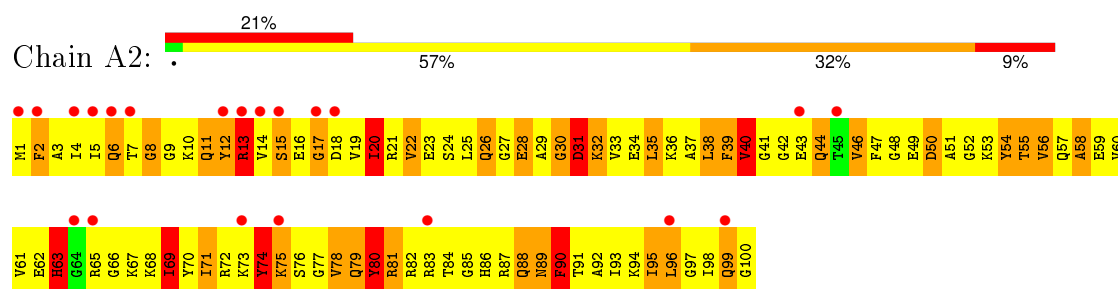


• Molecule 25: 50S ribosomal protein L20

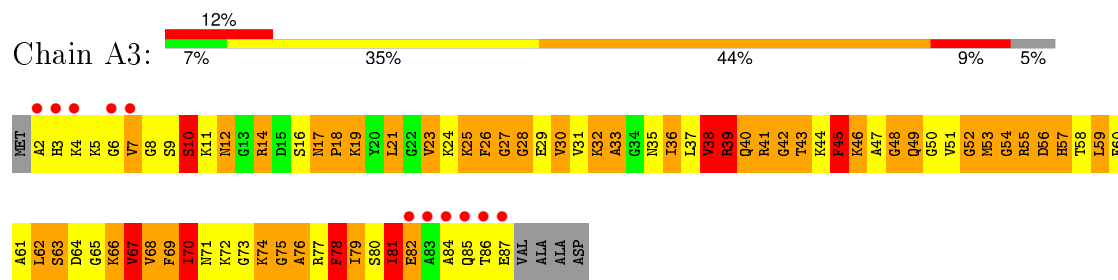


• Molecule 26: 50S ribosomal protein L21

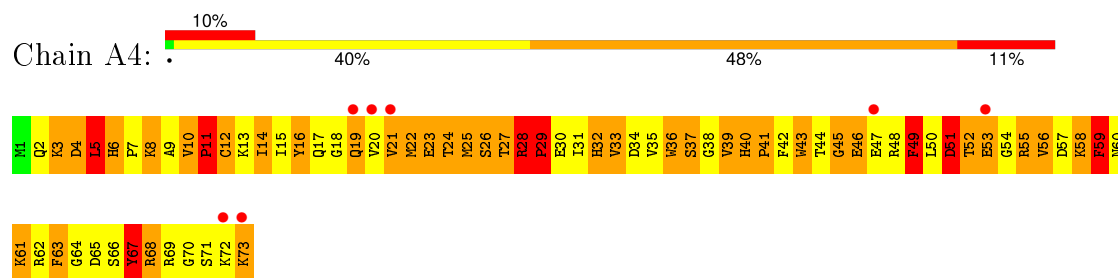




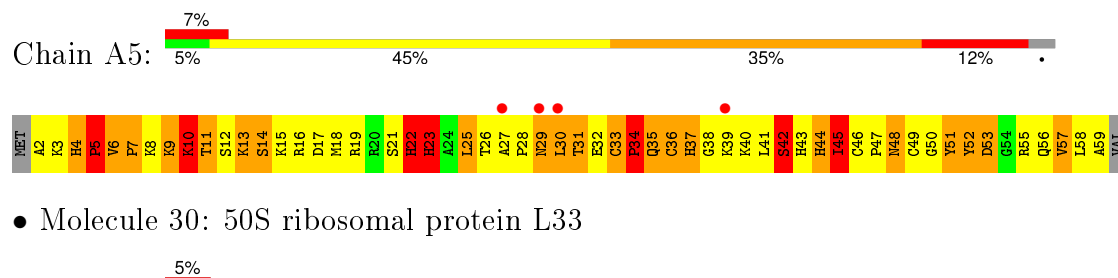
• Molecule 27: 50S ribosomal protein L27



• Molecule 28: 50S ribosomal protein L31



• Molecule 29: 50S ribosomal protein L32

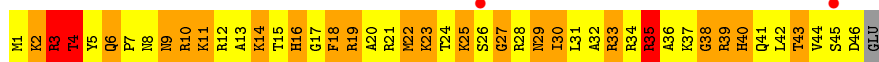


• Molecule 30: 50S ribosomal protein L33

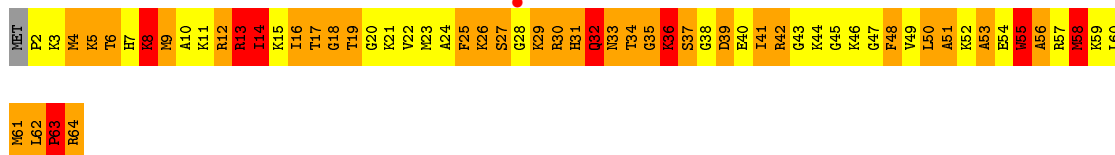


• Molecule 31: 50S ribosomal protein L34

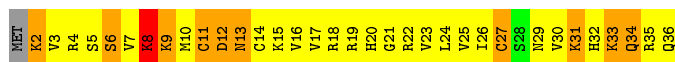




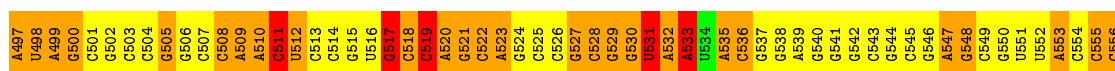
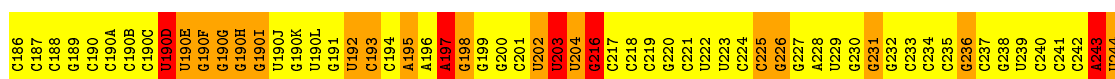
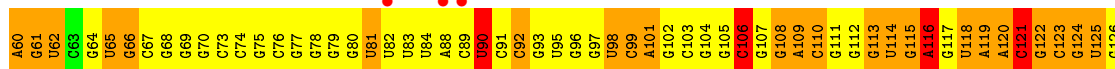
• Molecule 32: 50S ribosomal protein L35



• Molecule 33: 50S ribosomal protein L36



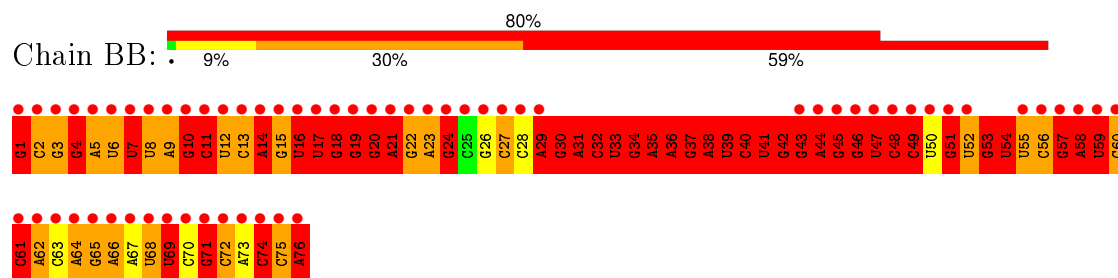
• Molecule 34: 16S rRNA



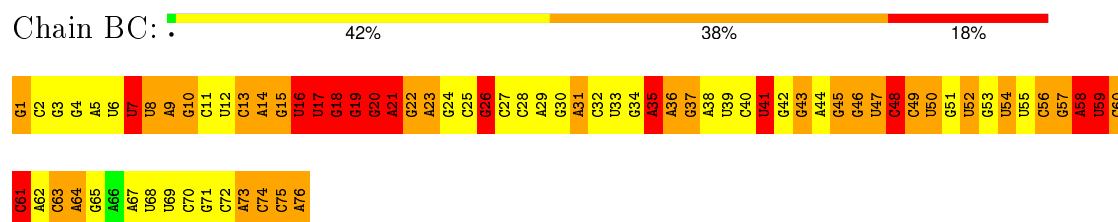
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G1464	C1399	G1220	U1189	G1099	C1039	C984	C924	A864	G798	C738	U678	C618	G558
C1465	C1400	G1221	U1190	G1100	U1040	C985	G925	A865	G799	C739	C679	U619	A559
C1466	C1341	G1222	C1161	A1101	A1041	A986	G926	A866	G800	U740	C680	C620	U560
C1467	C1342	G1223	C1162	C1102	G1042	C987	G927	G867	U801	G741	C681	A621	U561
A1468	C1343	G1224	C1163	C1103	C1043	G988	G928	G868	A802	G742	C682	C562	C562
G1469	C1344	G1225	G1164	G1104	A1044	C989	G929	G869	G803	U743	C683	G623	A863
C1404	U1345	A1225	G1165	A1105	C1045	C990	C930	G870	U804	C744	A684	C624	C564
G1405	A1286	C1226	C1166	G1106	A1046	U991	C931	U871	C805	C745	G685	G625	U565
G1470	A1287	A1227	C1167	C1107	G1047	U992	C932	A872	C806	U746	G686	U626	G566
U1406	C1288	G1228	A1168	G1108	G1048	G993	G933	A873	A807	C747	A687	G627	G567
A1408	A1289	A1229	G1169	C1109	U1049	A994	C934	G874	C808	C748	G688	G628	G568
C1409	G1290	C1230	G1170	A1110	C1050	C995	A935	C875	G809	C749	C689	G629	C569
G1410	U1291	G1231	G1171	A1111	C1051	A996	C936	G876	C810	G750	G690	G630	G570
C1411	U1292	U1232	C1172	A1112	U1052	U997	A937	C877	G691	U751	G691	G631	U571
C1412	G1293	G1233	G1173	C1113	G1053	G998	A938	G878	C812	G752	G692	A632	A572
C1413	G1294	C1234	G1174	C1114	C1054	C999	G939	C879	U813	A753	G693	G633	A573
C1414	G1295	U1235	A1175	C1115	A1055	U1000	C940	C880	A814	C754	A694	C634	A574
G1415	C1296	A1236	G1176	C1116	U1056	A1001	G941	G881	A815	G755	A695	G635	G575
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G1417	C1298	A1238	G1178	G1118	G1058	G1003	G943	C883	C822	U757	G697	G637	G577
A1418	A1299	A1239	A1179	C1119	C1059	G3A	G944	U884	G818	G758	G698	G638	C578
C1419	A1360	U1240	A1180	C1120	C1060	A1004	G945	G885	A819	A759	C699	G639	C579
U1485	G1361	G1241	G1181	G1121	G1061	A1005	A946	G886	U820	G760	G700	U640	U580
G1486	C361A	C1242	G1182	U1122	U1062	C1006	G947	G887	G821	G761	C701	U641	G581
G1487	U1302	C1243	A1183	U1123	G1063	G1007	G948	C888	C822	C762	A702	A642	U582
G1488	G1303	C1244	G1184	A1123	C1063	C1008	G949	A889	G823	G763	G703	C643	A583
G1489	G1305	A1245	G1185	G1124	U1064	G1009	U950	G890	C824	C764	A704	G644	G584
C1424	A1306	C1246	U1186	U1125	U1065	G1010	G951	U891	G825	G765	U705	C645	G585
C1426	C1366	U1247	G1187	U1126	C1066	G1011	U952	A892	G826	A766	A706	U646	C586
A1492	C1367	A1248	A1188	G1127	A1067	G1012	G953	C893	U827	A767	C707	C647	C587
A1493	G1368	C1249	C1189	C1128	G1068	G1013	G954	C894	A828	A768	C708	A648	G588
C1429	C1369	A1250	G1190	C1129	C1069	A1014	U955	G895	G829	G769	G709	G649	C589
U1495	G1370	A1251	A1191	U1130	U1070	A1015	U956	C896	G830	C770	G710	C650	U590
C1496	C1371	C1252	C1192	C1131	G1071	A1016	U957	C897	U831	G771	G711	C651	U591
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U1498	G1373	C1254	U1194	G1133	U1073	C1018	A959	C899	U833	G773	G713	A653	G593
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G1495	A1375	A1256	U1196	U1135	C1075	U1020	U961	A901	U835	G775	A715	A655	G595
U1496	U1376	U1257	G1197	U1136	C1076	G1021	C962	G902	G836	G776	A716	C656	C596
C1437	A1377	G1258	G1198	C1137	U1077	U1022	G963	G903	G837	A777	C717	G657	G597
G1440	C1378	C1259	U1199	G1138	U1078	G1023	A964	C904	G838	G778	G718	G658	U598
U1441	C1379	A1261	A1201	C1139	G1079	G1024	A965	U905	U839	C779	C719	U659	C599
G1442	C1380	C1262	G1202	C1141	G1081	U1025	G966	G906	C840	A780	C720	G660	C600
G1443	C1381	C1263	C1203	G1142	G1082	G1026	C967	A907	U841	A781	G721	G661	C601
C1444	C1382	C1264	A1204	G1143	U1083	C1027	A968	A908	C948	A782	A722	G662	A602
C1508	C1383	G1265	U1205	G1144	G1084	C1028	A969	A909	C949	C783	U723	A663	U603
C1509	C1384	G1266	G1206	C1145	U1085	C1029	C970	C910	U850	C784	G724	G664	G604
U1510	G1385	C1326	G1207	A1146	U1086	C1030	G971	U911	G851	G785	G725	A665	U605
G1448	C1386	C1267	G1208	C1147	G1087	G30A	C972	C912	G852	G786	C726	G666	G606
U1512	G1387	A1268	C1209	U1148	G1088	C30B	G973	A913	G853	A787	G727	G667	A607
A1513	C1388	A1269	C1210	U1149	G1089	G30C	A974	A914	G854	A788	A728	G668	A608
C1514	U1390	C1270	C1211	C1149	U1090	A30D	A975	A915	G855	U789	A729	U669	A609
C1515	G1391	G1271	U1211	U1150	U1091	G1031	G976	G916	C956	A790	G730	G670	G610
G1516	A1332	G1272	U1212	A1151	U1092	G1032	G977	G917	C957	G791	G731	U671	A611
G1517	C1333	G1273	A1213	A1152	A1093	G1033	A978	A918	G858	A792	C732	U672	C612
A1518	U1393	G1274	C1214	C1153	A1094	G1034	C979	A919	A859	U793	A733	G673	C613
G1459	A1394	A1275	G1215	G1154	G1094	G1035	C980	U921	A860	A794	G734	A674	A614
G1520	C1395	G1276	G1216	G1155	U1095	A1036	U981	U922	G861	C795	C735	G675	C615
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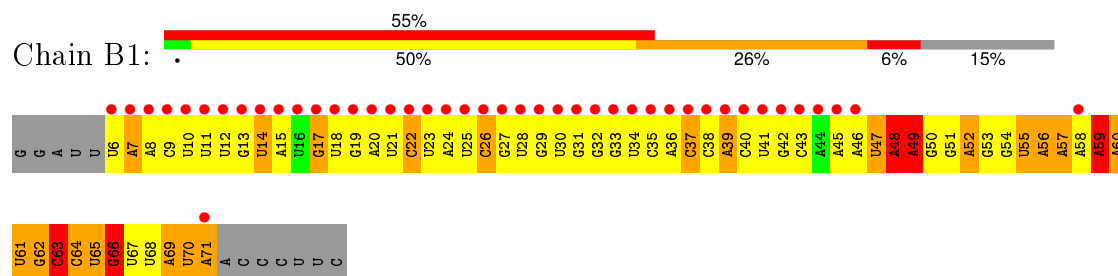
• Molecule 35: tRNA Phe (unmodified bases)



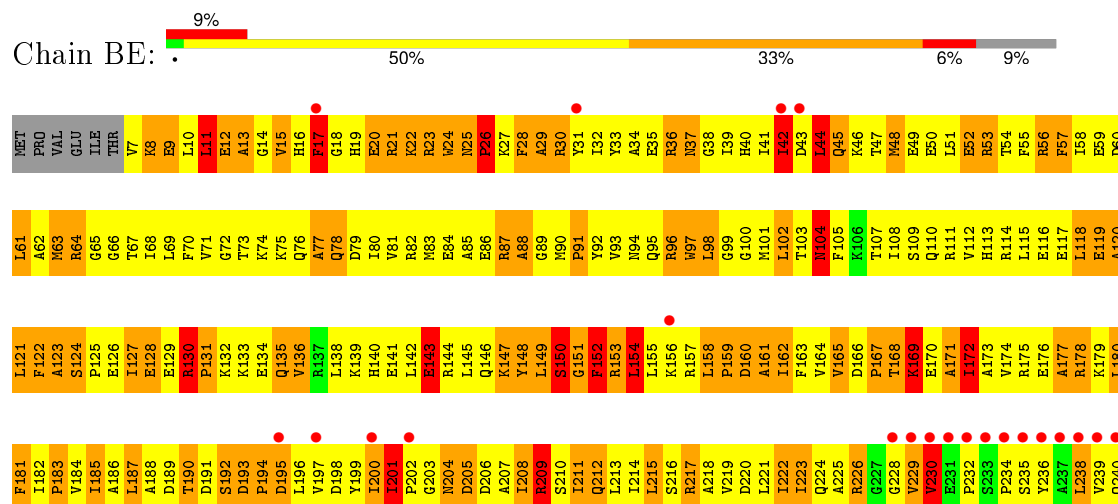
• Molecule 35: tRNA Phe (unmodified bases)



• Molecule 36: thrS mRNA operator

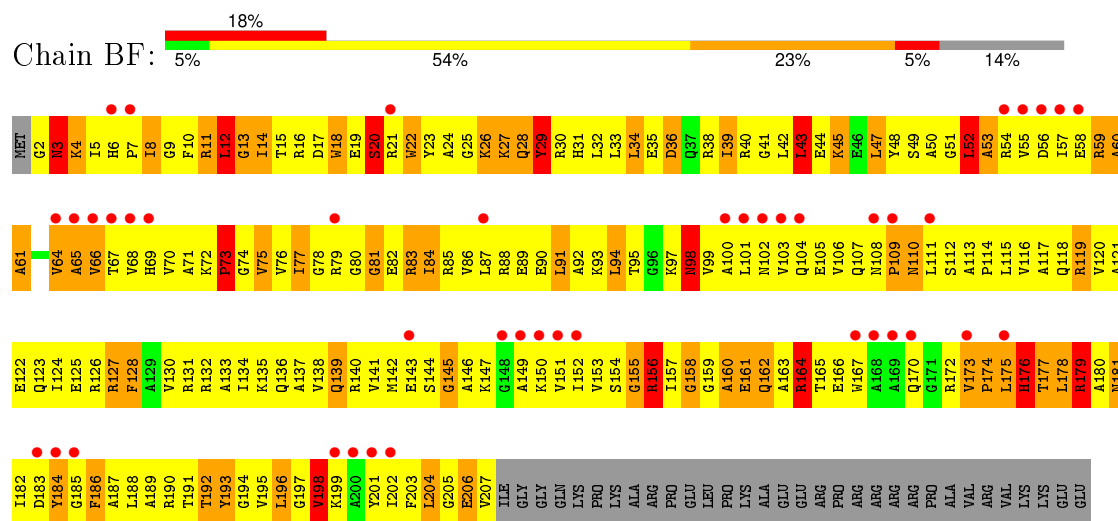


• Molecule 37: 30S ribosomal protein S2

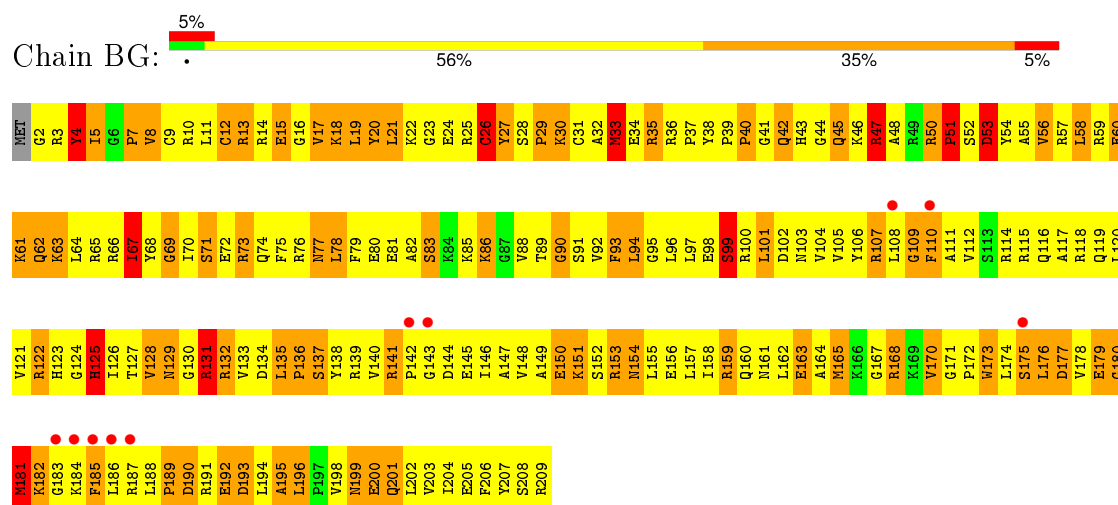


GLU  
ALA  
GLU  
ALA  
THR  
GLU  
THR  
PRO  
GLU  
GLU  
GLU  
SER  
GLU  
VAL  
GLU  
ALA

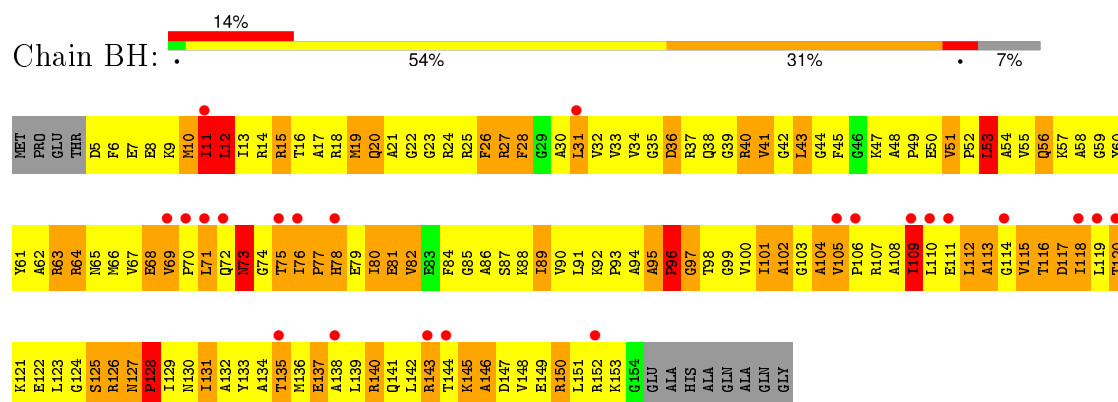
• Molecule 38: 30S ribosomal protein S3



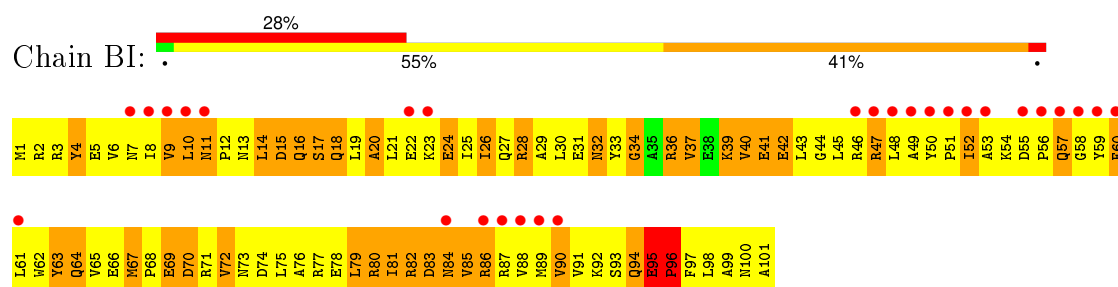
• Molecule 39: 30S ribosomal protein S4



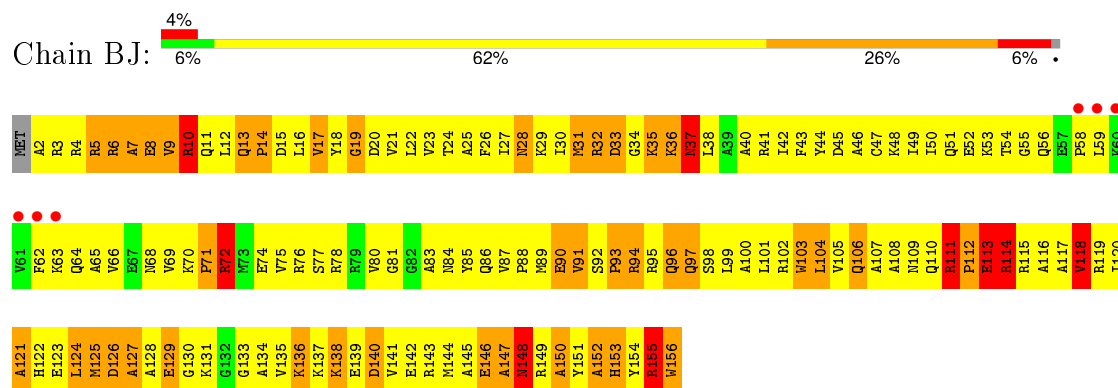
• Molecule 40: 30S ribosomal protein S5



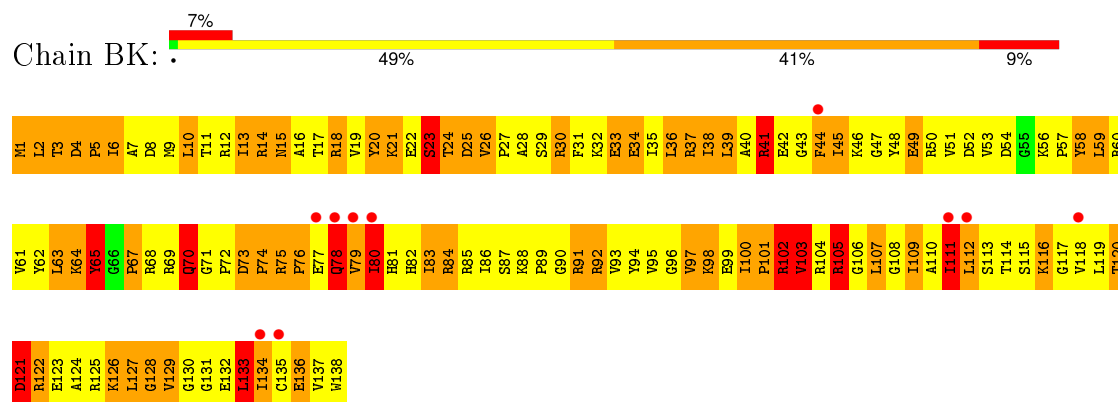
• Molecule 41: 30S ribosomal protein S6



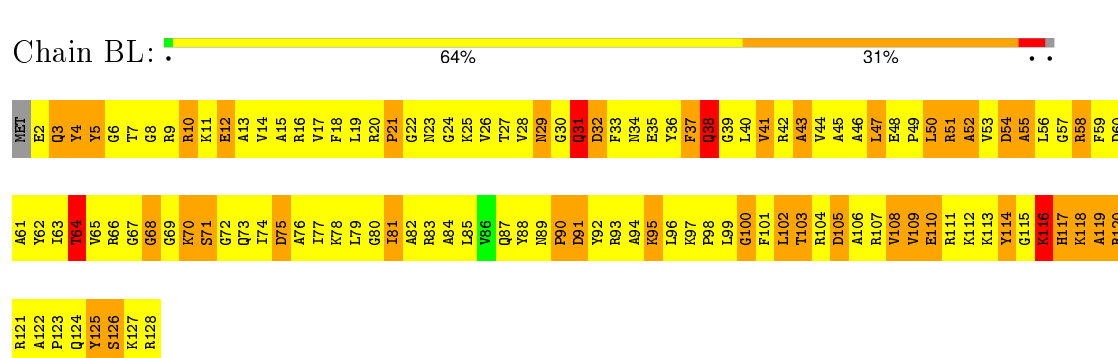
- Molecule 42: 30S ribosomal protein S7



- Molecule 43: 30S ribosomal protein S8

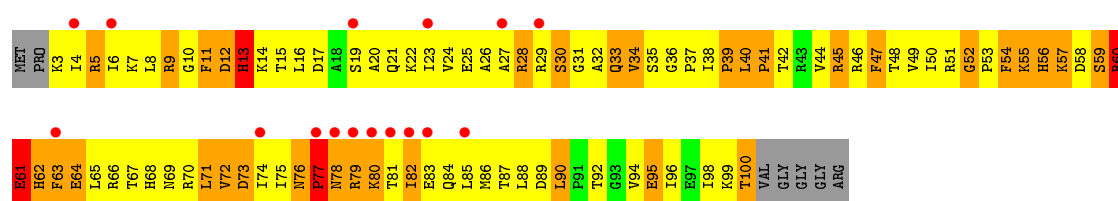


- Molecule 44: 30S ribosomal protein S9



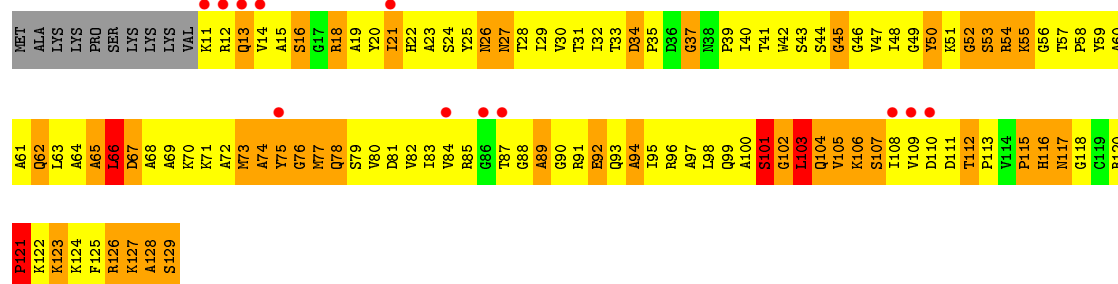
- Molecule 45: 30S ribosomal protein S10

Chain BM: 



• Molecule 46: 30S ribosomal protein S11

Chain BN: 



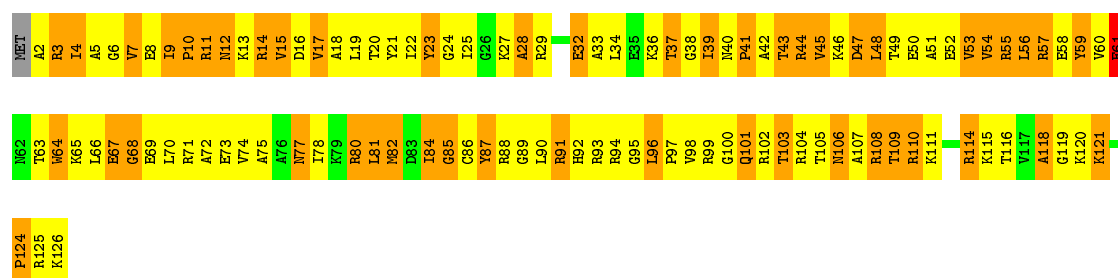
• Molecule 47: 30S ribosomal protein S12

Chain BO: 

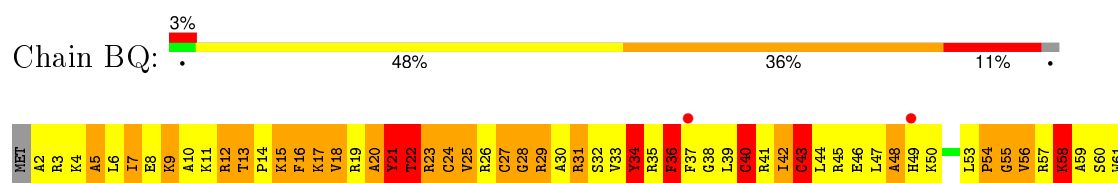


• Molecule 48: 30S ribosomal protein S13

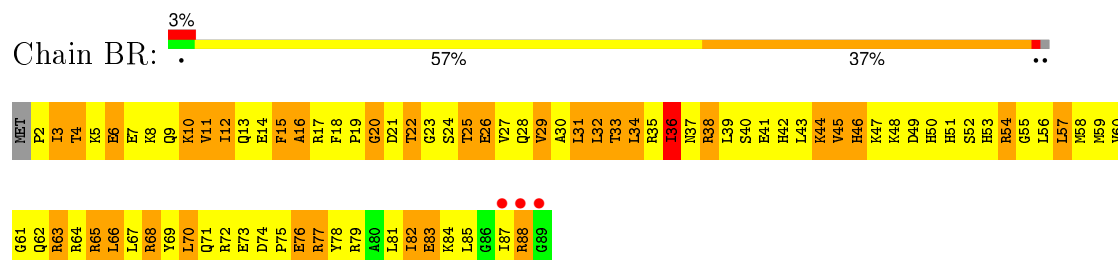
Chain BP: 



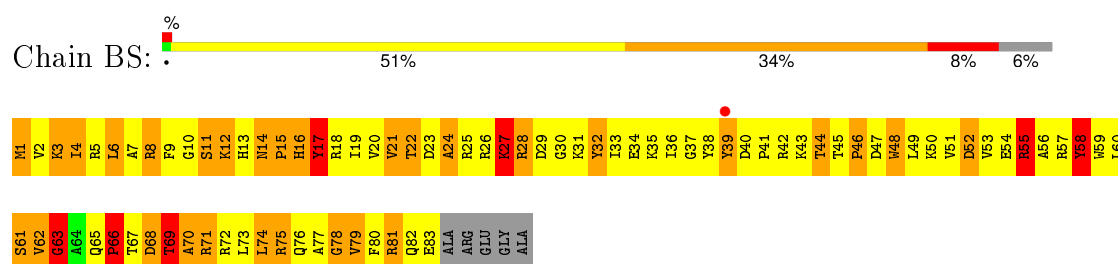
• Molecule 49: 30S ribosomal protein S14



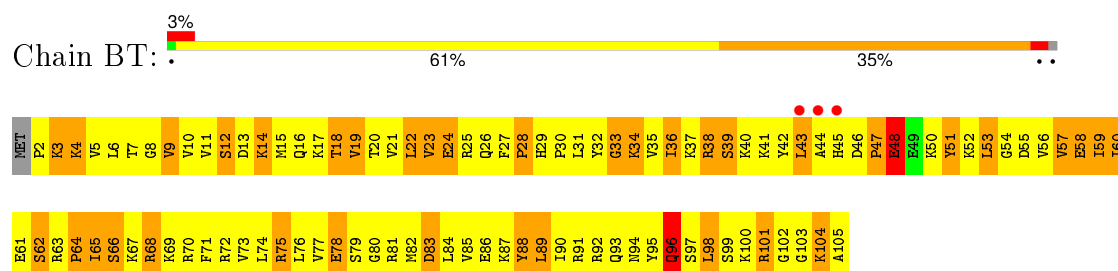
• Molecule 50: 30S ribosomal protein S15



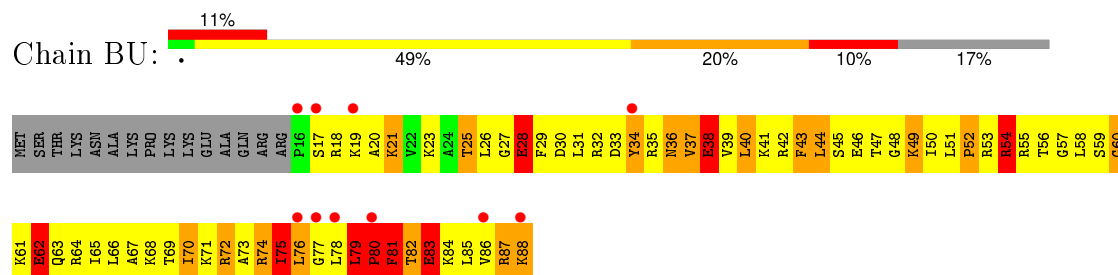
• Molecule 51: 30S ribosomal protein S16



• Molecule 52: 30S ribosomal protein S17



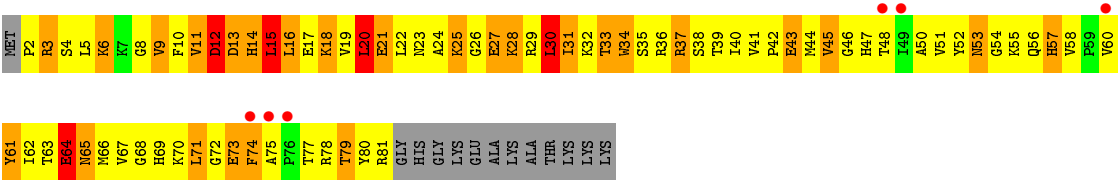
• Molecule 53: 30S ribosomal protein S18



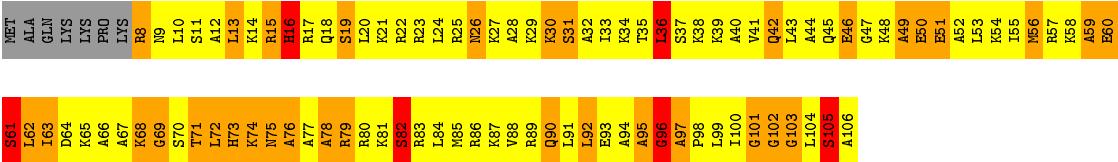
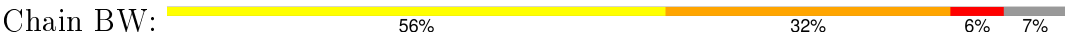
• Molecule 54: 30S ribosomal protein S19







● Molecule 55: 30S ribosomal protein S20



● Molecule 56: 30S ribosomal protein Thx



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	206.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.11 , 178.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	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 <sup>2</sup> )	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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

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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(°)	Ideal(°)
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

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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	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 <sup>2</sup> )	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 <sup>2</sup> )	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.