



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:34 pm GMT

PDB ID : 4V75  
EMDB ID: : EMD-1721  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in classic post-translocation state (post1)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 12.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

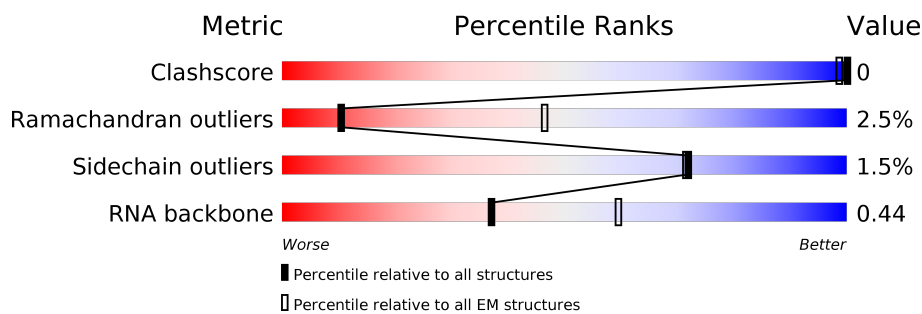
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AB	220	97% .
2	AC	208	91% 8%
3	AD	206	89% 11%
4	AE	152	89% 11%
5	AF	101	87% 13%
6	AG	152	88% 11% .
7	AH	130	94% 5% .
8	AI	128	85% 15%









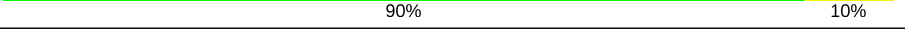

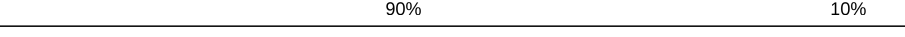
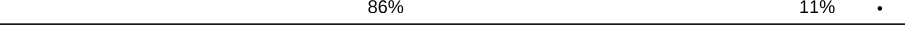

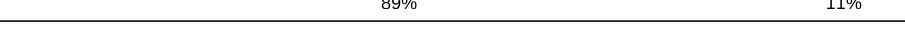




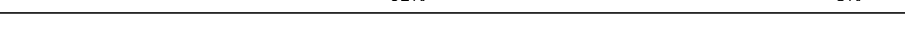
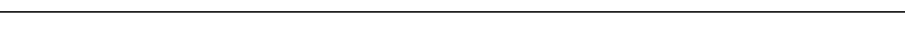

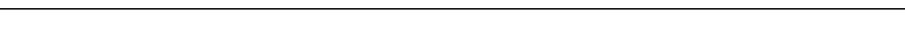
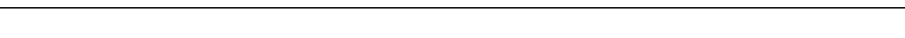
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Mol	Chain	Length	Quality of chain
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	177	
30	BH	149	
31	BI	142	
32	BJ	142	
33	BK	123	

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Mol	Chain	Length	Quality of chain
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	ACETYLATION	UNP P0A7V0
AB	226	NH2	-	AMIDATION	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	AMIDATION	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	ACETYLATION	UNP P0A7W1
AE	159	NH2	-	AMIDATION	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	AMIDATION	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	ACETYLATION	UNP P02359
AG	152	NH2	-	AMIDATION	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	ACETYLATION	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	ACETYLATION	UNP P0A7R5
AJ	103	NH2	-	AMIDATION	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	ACETYLATION	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	AMIDATION	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	AMIDATION	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	ACETYLATION	UNP P0AG63
AQ	83	NH2	-	AMIDATION	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AR	57	Total	C	N	O	0	1
			459	290	87	82		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	ACETYLATION	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	AMIDATION	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	ACETYLATION	UNP P0A7U3
AS	81	NH2	-	AMIDATION	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	ACETYLATION	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	ACETYLATION	UNP P68679
AU	54	NH2	-	AMIDATION	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	AMIDATION	UNP P60422

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	AMIDATION	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	AMIDATION	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	AMIDATION	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	AMIDATION	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	ACETYLATION	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	ACETYLATION	UNP P0A7M2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	ACETYLATION	UNP P0A7N9
B1	53	NH2	-	AMIDATION	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

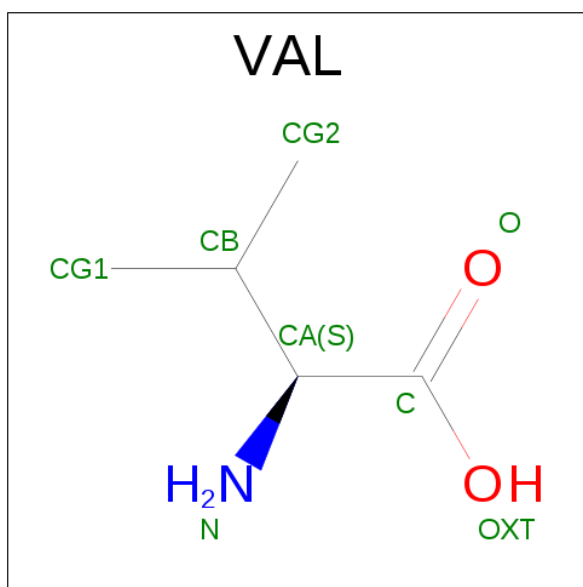
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

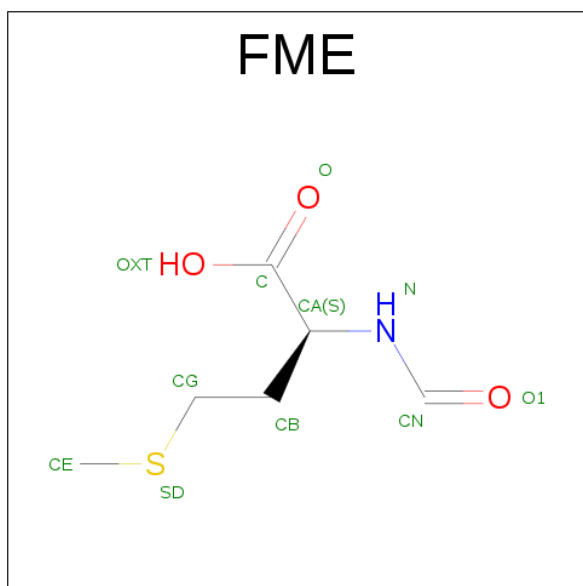
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



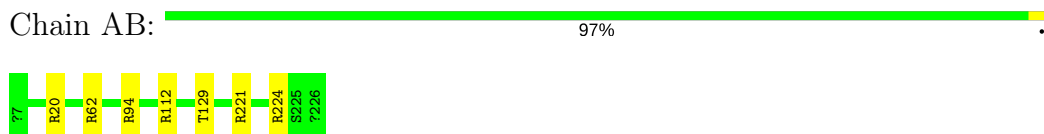
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



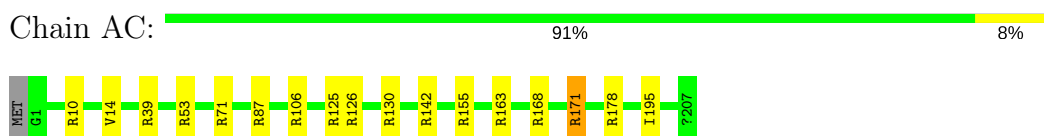
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

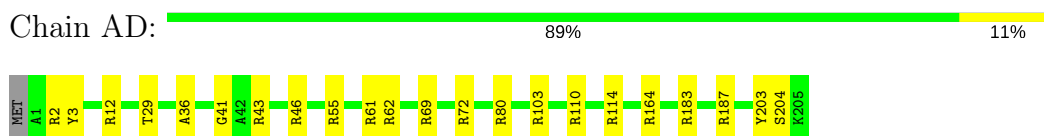
- Molecule 1: 30S ribosomal protein S2



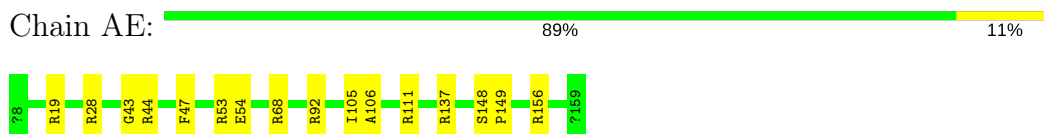
- Molecule 2: 30S ribosomal protein S3



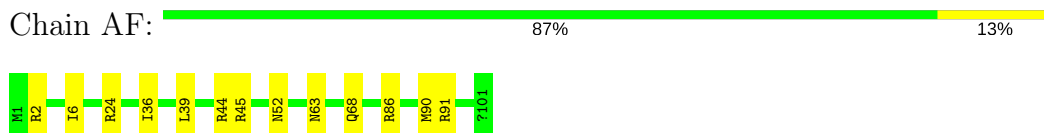
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





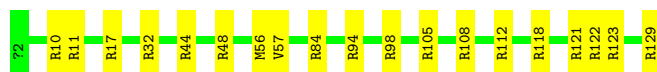
- Molecule 7: 30S ribosomal protein S8

Chain AH: 94% 5%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 85% 15%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 87% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 91% 9%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 89% 10%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%

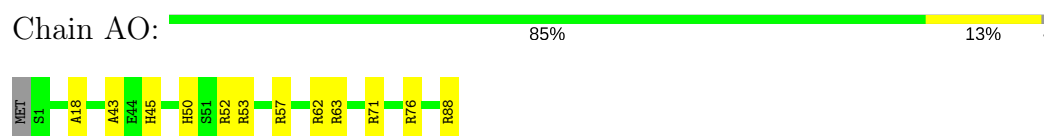


- Molecule 13: 30S ribosomal protein S14

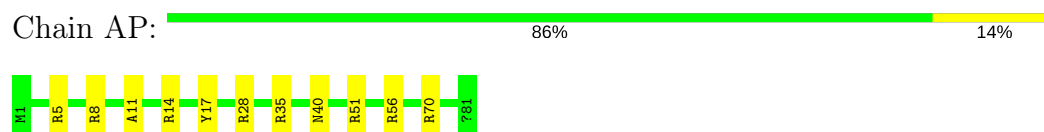
Chain AN: 84% 13%



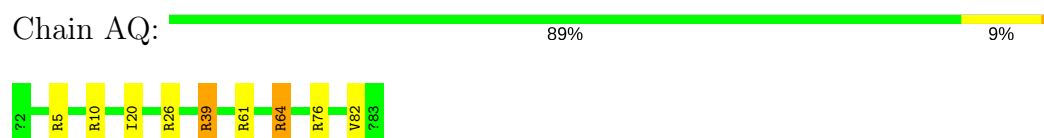
- Molecule 14: 30S ribosomal protein S15



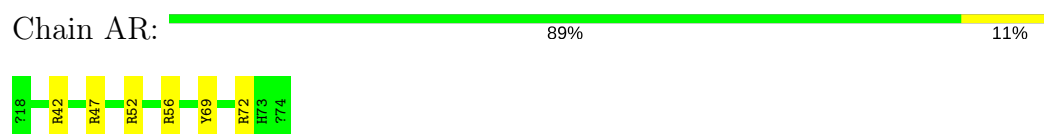
- Molecule 15: 30S ribosomal protein S16



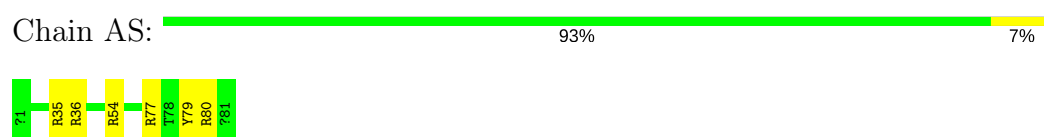
- Molecule 16: 30S ribosomal protein S17



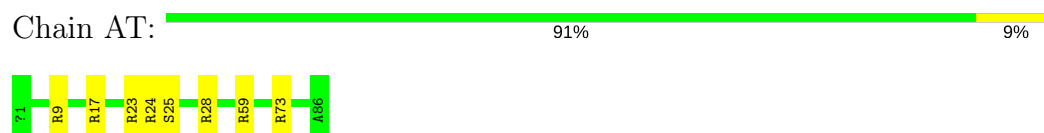
- Molecule 17: 30S ribosomal protein S18



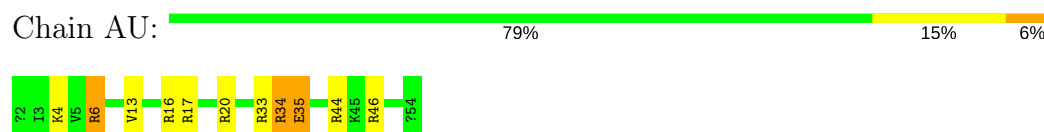
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



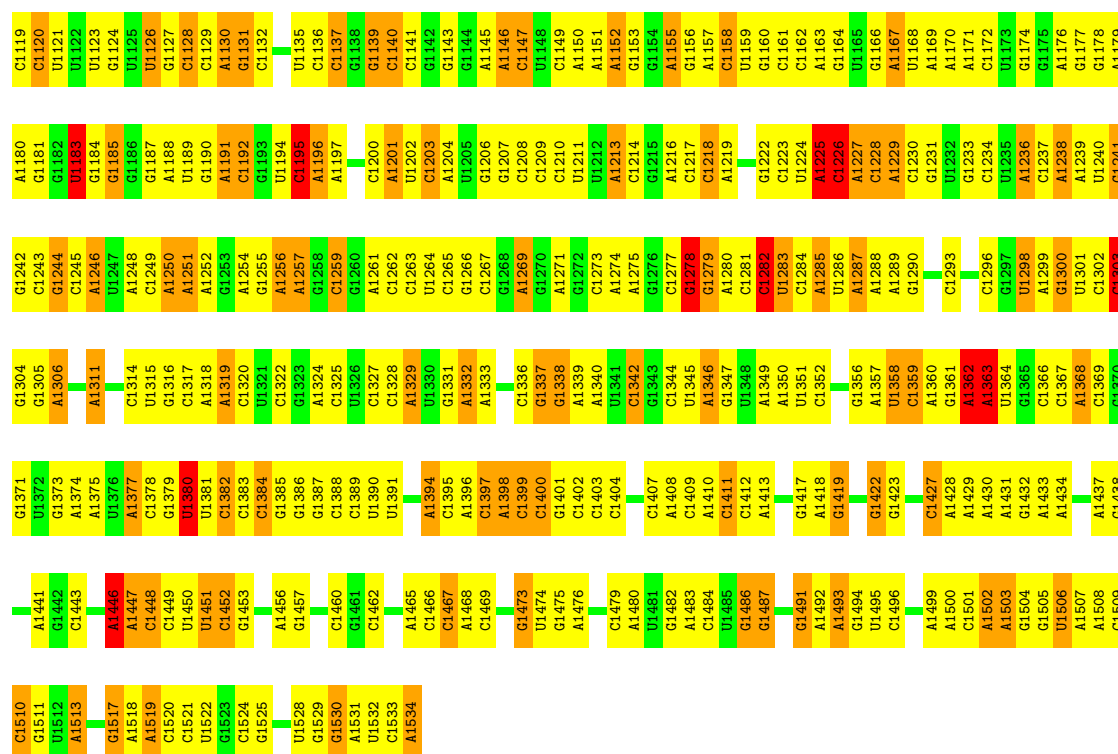
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA



C1051	C984	A923	C856	A790	U723	U852	G585	G521	A459	C332	C269	C136	C67	A
U1052	C985	C924	C857	A791	G724	U853	C586	C522	U898	U333	A270	A205	G68	A
G1053	U985	G925	C858	G792	G725	G854	U589	G523	G399	C334	C271	C206	G69	A
C1054	G987	G926	C859	U793	G726	G855	U590	G524	C400	C335	C272	C207	U70	U
A1055		G927	A860	U794	G727	G856	G592	C525	G401	A336	A273	U208	A71	G
U1056		G928	C861	C795	G728	U857	U593	C526	G402	G337	A274	U209	A72	G
	U991	C930	C862	C796	G729	C858	U594	G527	G403	A338	G275	C210	A73	A
C1059	U992	C931	U863	C797	G730	U859	A595	G528	G404	C339	G276	G211	A74	A
	U993	C932	C864	C798	G731	C860	A596	G529	U405	U340	G277	G212	A75	A
U1062	A994	C933	A865		G732	G861	A597		G406	C341	G278	U150	G76	U
C1063	A995	G934	C866	U801	C735	U862	C599	A532	U407	C342	G279	G213	U13	U
G1064	A996	C935	C867	A802	C736	G863	A600	U534	G408	U343	C280	C215	U14	U
U1065	U997	C936	C868	C803	C737	G864	G601	A535		C344	A282	U216	G15	G
C1066	C998	A937	C869	U804	C738	G865	A602	A536		C345	A283	C217	A16	A
A1067	C999	G938	A872	U805	C739	G866	G603	C537	A411	G346	U283	U218	A81	U
G1068	A1000	C939	C873	C806	U740	G867		G538	A412	G347	C284	U219	G82	C
C1069	C1001	G940	A874	C807	G741	U868	U605	G539	A413	G348	G285	G220	C83	A
U1070	A1004	G941	C875	C808	G742	G869	G606	G540	G414	A349	C286	G221	U84	U
C1071	A1005	G942	U876	C809	G743	A873	A607	G541	G415	G350	U287	C222	U85	G
G1072		G943	C877	C810	G744	A874	A608	G542	C417	C351	A288	A223	G88	C
U1073		G944	C878	C811	G745	A875	U610		C418	C352	G289	U224	C87	C
	U1010	G945	A879	C812	G746	A876	C611	C545	C419	C353	C290	C225	U88	U
G1077	C1011	A946	C880	U813	G747	A877	C612	A546	U420	G354	U291	G226	U89	C
U1078	A1012	G947	C881	A814	G748	A878	C613	A547	C421	C355	G292	G227	C90	A
G1079	G1013	G948	C882	A815	G749	C879	C614	G548	G422	A356	G293	A228	U91	U
A1080	A1014	A949	C883	A816	C750	C880	C615	C549	G423	C357	U294	U229	A167	A
U1081	G1015	U950	C884	C817	G751	A881	C616	A553	G424	U358	C295	G230	C95	C
A1082	A1016	G951	U885	C818	U752	A882	U619	A554	U425		U296		U96	G
G1083	U1017	U952	C886	C819	G753	A883	C620	A555	A426	G361	C297	C233	U97	G
C1084	G1018	G953	C887	A820	G754	C884	A621	U556		C362	C298	C234	A98	A
U1085	A1019	U954	C888	U821	C755	C885	A622	C556	U429	A363	G299	C235	C99	A
U1086	G1020	U955	A889	U822	G756	A890	C623	C557	A430	A364	A300	A236	G100	C
G1087	A1021	U956	C890	U823	C757	A891	C624	C558	A431	U365	G301	G237	A101	C
	U1022	U957	U891	C823	U758	A892	U625	A559	A432	A366	G302	A238	C106	G
A1092	G1024	A958	C892	G824	C759	A893	G626	A560	A433	U367	A303	G240	G38	C
C1093	U1025	U960	C893	A825	A759	U894	G627	U561	U434	U368		G241	G107	G
U1095	G1026	U961	C894	C826		G895	G628	U562	A435	C370	A306	G242	C40	C
C1096	C1027	C962	C895	U827	G765	C896	A629	A563	C436	A371	C307	A243	A109	C
C1097	C1028	G963	C896	U828	A766	G897	A630	C564	U437	C372	A308	U244	G110	C
C1098	U1029	C964	C897	G829	U767	A898	C631	U565	U438	C373	A309	U245	G111	C
G1099	U1030	U965	A900	A830	A768	C899	U632	G566	C440	A374	C310	A246	G112	C
C1100	G1031	G966	A901	G832	G769	U900	C633	G567	A441		C311	G247	G113	C
A1101	U1032	C967	G902	G833	C770	A704	C634	G568	G442	C379	C312	C248	U114	C
C1102		A968				A705	A635	C569	C443	G380	A313	U249	G115	C
C1103	A1035	A969	A906	G838	G773	U707	U636	G570	G444	C381	C314	A250	A116	C
G1104	A1036	C970	A907	C839	G774	C708	C637	U571	G445	C382	A315	G251	A119	A
A1105	C1037	G971	A908	C840	G775	U709	U638	A572	G446	A383	A189	U252	C52	C
G1106	C1038	G972	A909	C841	G776	G710	G639	A573	U508	G384	A190	G191	U121	C
C1107	U1039	G973	C910	U842	A777	G711	A640	G574	A448	C385	G192	G255	C54	C
G1108	U1040	A974	U911	U843	G778	A712	U641	G575	G449	C386	C322	G256	U123	C
C1109	G1041	A975	C912	G844	C779		A642	C576	G450		U323	U256	C124	C
A1110	A1042	G976	A913	A845	A780	A715	C643	C577	G324	A389	C194	A252	C58	C
G1111	G1043	A977	A914	G846	A781	A716	C513	G578	A452	U390	A195	A253	A129	C
C1112	A1044	A978	A915	G847	A782	U717	C514	A579	G326	G391	A196	G197	A60	C
C1113	U1045	C979	U916	C848	C783	A718	U516	G454	C327	C392	A197	C264	A131	C
C1114	A1046	C980	G917	A784	A784	C719	G517	G455	C328	A393	G198	G265	C132	C
		U981	A918	G852	G720	A649	C582	A456	A329	G394	C329	G266	U133	C
A1117	U1049	U982	A919	C853	G721	C721	A583	C518	A330	C395	C330	C267	G64	C
U1118	G1050	A983	U920		G722		C584	A520	U458	C396	G331	U268	A66	C



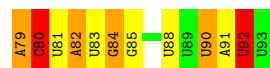
### • Molecule 22: fMet-Val-tRNA-Val

Chain A1: 28% 55% 12% 5%



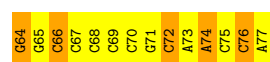
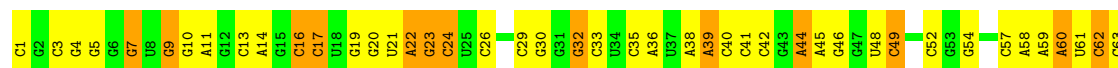
### • Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 27% 33% 27% 13%

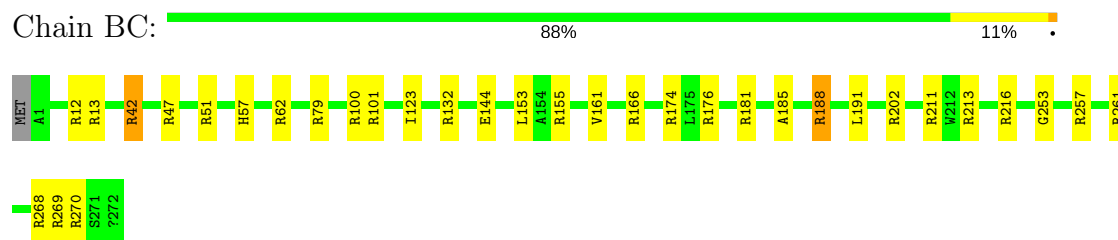


### • Molecule 24: tRNA-fMet

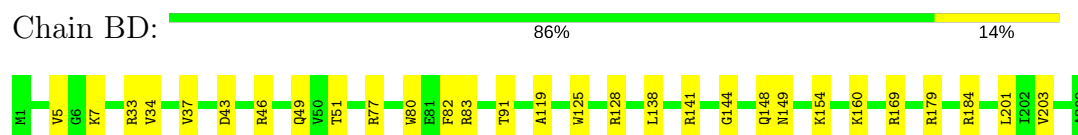
Chain A3: 25% 52% 23%



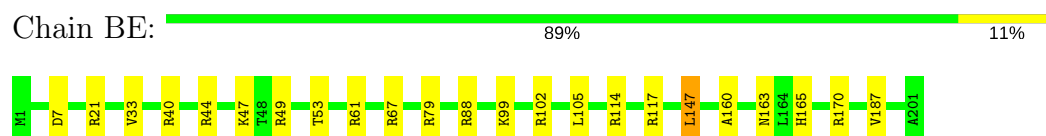
### • Molecule 25: 50S ribosomal protein L2



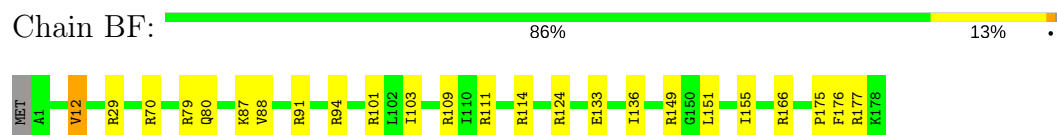
- Molecule 26: 50S ribosomal protein L3



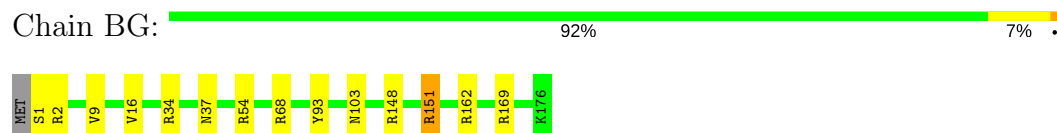
- Molecule 27: 50S ribosomal protein L4



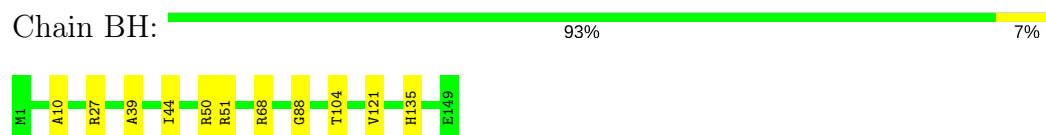
- Molecule 28: 50S ribosomal protein L5



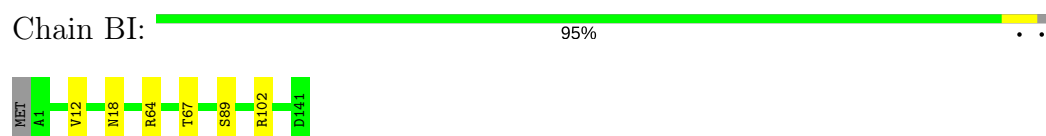
- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  92% 8%




- Molecule 33: 50S ribosomal protein L14

Chain BK:  88% 11%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  82% 17%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  88% 12%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  85% 15%




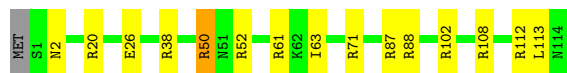
- Molecule 37: 50S ribosomal protein L18

Chain BO:  89% 10%




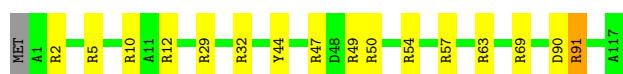
- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  86% 13%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 90% 10%



- Molecule 41: 50S ribosomal protein L22

Chain BS: 93% 7%



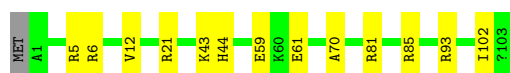
- Molecule 42: 50S ribosomal protein L23

Chain BT: 90% 10%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 87% 13%



- Molecule 44: 50S ribosomal protein L25

Chain BV: 90% 10%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 11%



- Molecule 46: 50S ribosomal protein L28

Chain BX: 82% 14%






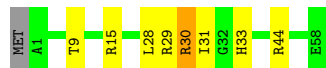
- Molecule 47: 50S ribosomal protein L29

Chain BY:  89% 11%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  85% 12% . .




- Molecule 49: 50S ribosomal protein L32

Chain B0:  84% 14% .



- Molecule 50: 50S ribosomal protein L33

Chain B1:  85% 15%



- Molecule 51: 50S ribosomal protein L34

Chain B2:  80% 20%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  91% 8% .



- Molecule 53: 50S ribosomal protein L36

Chain B4:  84% 16%

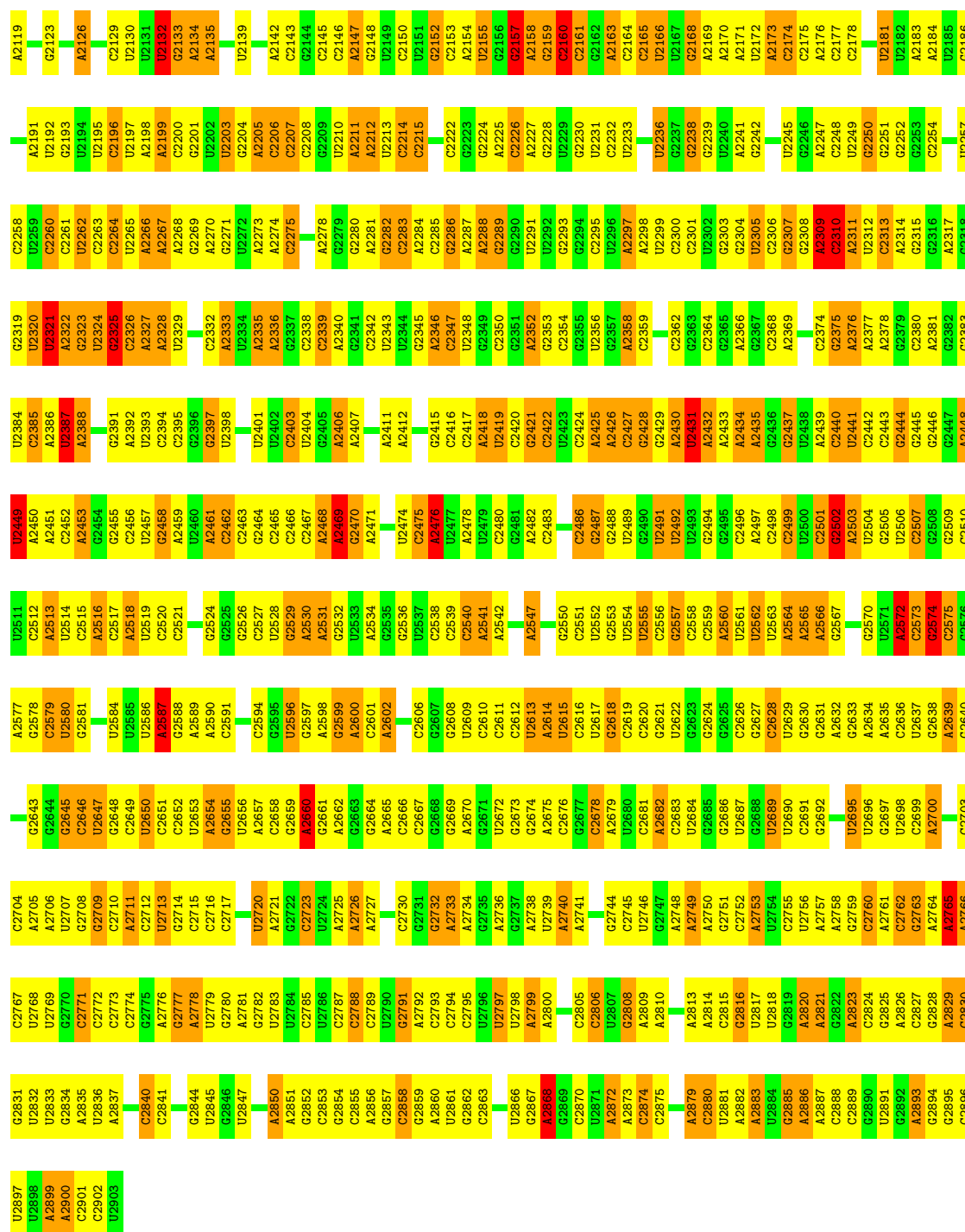


- Molecule 54: 23S ribosomal RNA

Chain BA:  23% 52% 21% .

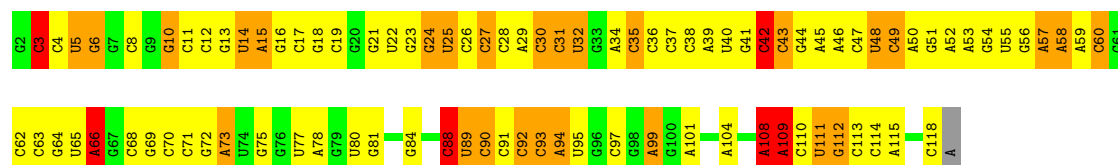
G1034	A972	C908	G841	G776	U710	A643	U580	A514	U451	G386	A320	G132	C69	G1
U1035	A973	A909	A844	G780	A715	A644	C581	A515	C452	U387	U321	U133	G70	G2
G1036	A974	A910	A845	A781	A716	C645	A582	C316	A453	G388	A322	G134	A71	U4
G1037	A975	A911	U846	C782	A717	G647	G583	C517	A454	G389	C323		U72	U5
A1038	A976	C912	U847	A783	C717		C584	G518	C455	U390	A324	U138	A73	A6
A1040	A977	U913	U848	A784	C718	C650	G585	G519	C456	A391		U139	A74	A7
	A980	C915	C849	G785	C719		A586	G520	A457	U392	G327	C140	A75	G7
C1043	A981	G916	A849	A786	U720	U853	C587	U521	C458	C393	U328	C141	C8	C3
C1044	A982	U850	U850	C786	A721	U854	U588	A522	U459	A203	G329	G142	C76	G9
C1045	A983	C851	C851	C787	A722	A654	U589	C523	C460	A204	A330	C143	G77	G8
A1046	A984	A918	U852	A788	C723	A655	A590	G524	C461	U206	C331	A144	U78	A10
A1047	C985	U919	C853	A789	U724	U857	U591	U525	C462	C267	A332	C145	C79	C11
C1048	C986	A920	C854	U790	G725	G657	A592	A526	G463	C268	G333	C146	U12	U12
A1048	C987	C921		C791	G726	U858		C527	U464	C269	C334	C147	A83	A13
C1049	A988	C922	G858	A792	A727	U859	C595	A528	U465	C270	C335		A84	A14
A1050	A989	G923	C859	A793	G728	C660	U596	A529	A402	G271	C336	U148	G85	G15
G1051	A990	G924	U860	C789	A729	A661	G597	G530	A403	A272	C337	A149	G86	C16
C1052	C991	A925	A861	C795	A730	G662	U598	G531	U404	G273		C151	U87	A19
C1053	C992	G926	G862	C796	C731	G663	A599	A532	A405	C274	A340	C152	A89	C20
A1054	C993	A927	A863		C732	G664	G600	G533	U406		C341	U153	U90	A21
G1055	C994	A928	G864	A800	G733	U865	C601	A538	C474	G407	A342	U154	A91	C22
G1056	C995		C865	G801	A734	A666	A603	G539	C475	G411	C343	U155	U92	U25
A1057	A996	U931	A866	A802	A735	U667	A602	A541	C476	A412	A344	A156	G93	
U1058	C997	A932	C867	U803	C736	A668	A603	C540	C477	C413	A345	C157	A94	A28
G1059	C998	A933	U868	A804	C737	A670	U607	C542	A478	C414	A347	U158	A95	U29
U1060	U999	U934	G869	G805	G738	A671	U608	G543	C479	A415	A348	A160	C97	U30
U1061	A1000	C935	U870	C806	A739	C672	A609	G544	A480	U416	U349	A161	C98	C31
G1062	A1001	A936	U871	U807	C740	C673	C610	U545	G481	C417	G350	U162	U99	C32
C1063	G1002	C937	U872	G808	U741	G674	C611	U546	A482	C418	C351	C163	U100	C33
G1064	G1003		C873	G809	A742	G675	C612	A547	A483	U419	A352	C164	A101	U34
U1065	U1004	A941		U810	A743	A676	G613	G548	C484	C420	C353	A165	U102	
U1066	C1005	G942	C876	U811	U744	A677	A613	G549	C485	C421	A354	U166	A103	C37
A1067	C1006	A943	A877	C812	G745	A678	U615	C550	C486	A422		U167	A104	A38
G1068	C1007	C944	A878	U813	U746	C679	A616	U554	C487	A423	C357	U170	C105	G39
A1069	A1008	A945		C814	U747	C680	G617	U555	C488	G232	A231	U171	C41	U40
A1070	A1009	C946	G883	C815	G748			G556	C489	A233	A233	A172	A42	A44
G1071	A1010	A947	C884	C816	A749	U683	G620	A557	C490	U427	U360	A173	G43	
C1072	G1011	C948	C885	C817	A750	G684	A621	C557	C491	A428	A362	A174	A111	
A1073			A886	G818	A751	U685	G622	U558	A492	A429	G363	A175	G108	
G1074	C1013	C951	U887	A819	A752	A686	C623	G559	C493	A430	C364	U176	G109	
C1075	U1014	G952	C888	A820	A753	U686	C624	C560	C494	U431	U365	G175	U112	
C1076	U1015	G953	C889	A821	U754	C687	C624	G561	G495	A432	C366	A176	U113	
A1077	G1016	G954	C890	G822	U755	U688	G625	U562	C496	U433	G367	G177	U114	
U1078	G1017	U955	C891	C823	A756	A689	A626	G563	A497	C434	A368	G178	G48	
C1079	U1018	G956	A892	U824	G757	G900	A627	U564		U435	U369	C240	C115	A49
U1080	U1019	C957	C893	A825	C758	C891	G628	C564		C436	U370	A241	C116	A52
U1081	A1020	U958	U894	U826	G759	C892	G629	C565	G500	G242	G180	G179	G117	A53
U1082	A1021	A959	U895	U827	G760	A693	G630	U566	A501	U243	A371	A181	G54	G54
U1083	G1022	A960	A896	U828	A761	U694	A631	U567	A502	G308	G372	A182	A119	G55
A1084	U1023	C961	C897	A829	U762		A632	U568	A503	G245	C183	U120	A56	A56
A1085	G1024	C962	C898		G763	C698	A633		A504	C246	C184	G121	C57	
U1086	G1025	U963	A899	U832	A764	A699	C634	U571	A505	G247		G187	G60	C60
G1087	G1026	C964	A900	A833	C765		C635	A572	U506	G248	G312		A125	C61
A1088	A1027	C965	C901	G834	U766	U702	G636	A573	A507	C249	G313	A190	U62	U62
A1089	A1028	G966	C902	C835	U767	U703	A637	A574	A508	G250	G314	A191	A127	A63
A1090	A1029	U967	C903	G836		G704	G638	A575	C509	G251	G315	A192	A64	A64
G1091	C1030	C968	G904	C837	C772	A705	U639	U576	C510	G252		C192	C128	
C1092	G1031	U969	A905	C838	U773	A706	U641	G577	U511	C253	C316	U193	C65	C65
G1093	U1032	G970	U906	U839	G774	A707	U642	G578	U512	G254	C317	C130	C56	
U1094	U1033	G971	G907	C840	G775	U709	U644	G579	A513	A450	G319	A195	A131	



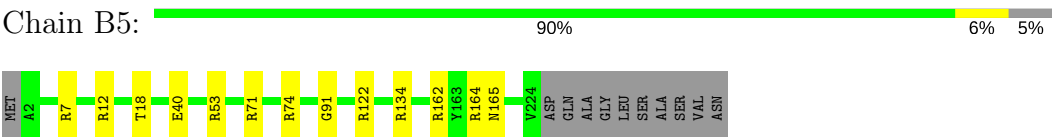



# • Molecule 55: 5S ribosomal RNA

Chain BB: 21% 50% 23% 5% •



● Molecule 56: 50S ribosomal protein L1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13207	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, FME, ACE, H2U, CM0, 6MZ, NH2, 4SU, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AB	0.70	0/1736	0.99	6/2340 (0.3%)
10	AK	0.74	0/894	1.23	11/1207 (0.9%)
11	AL	0.74	0/969	1.22	13/1300 (1.0%)
12	AM	0.76	0/884	1.30	14/1181 (1.2%)
13	AN	0.78	0/817	1.25	11/1088 (1.0%)
14	AO	0.72	0/722	1.19	8/964 (0.8%)
15	AP	0.77	0/648	1.19	8/870 (0.9%)
16	AQ	0.70	0/658	1.14	7/883 (0.8%)
17	AR	0.81	0/463	1.22	5/623 (0.8%)
18	AS	0.74	0/653	1.08	5/879 (0.6%)
19	AT	0.69	0/672	1.12	8/890 (0.9%)
2	AC	0.73	0/1651	1.13	16/2225 (0.7%)
20	AU	0.83	0/431	1.51	9/572 (1.6%)
21	AA	1.53	0/36759	2.21	1951/57346 (3.4%)
22	A1	1.55	0/1668	2.23	94/2595 (3.6%)
23	A2	1.46	1/343 (0.3%)	2.24	14/531 (2.6%)
24	A3	1.52	0/1722	2.20	88/2685 (3.3%)
25	BC	0.74	0/2121	1.26	28/2852 (1.0%)
26	BD	0.69	0/1586	1.17	11/2134 (0.5%)
27	BE	0.67	0/1571	1.18	13/2113 (0.6%)
28	BF	0.75	0/1444	1.24	15/1937 (0.8%)
29	BG	0.69	0/1343	1.17	10/1816 (0.6%)
3	AD	0.75	0/1665	1.16	16/2227 (0.7%)
30	BH	0.65	0/1122	1.07	4/1515 (0.3%)
31	BI	0.66	0/1046	1.00	2/1410 (0.1%)
32	BJ	0.71	0/1152	1.14	8/1551 (0.5%)
33	BK	0.70	0/947	1.28	11/1268 (0.9%)
34	BL	0.73	0/1054	1.32	13/1403 (0.9%)
35	BM	0.74	0/1093	1.15	10/1460 (0.7%)
36	BN	0.77	0/973	1.27	14/1301 (1.1%)
37	BO	0.73	0/902	1.28	12/1209 (1.0%)
38	BP	0.76	0/929	1.28	12/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.78	0/960	1.32	14/1278 (1.1%)
4	AE	0.69	0/1119	1.12	11/1506 (0.7%)
40	BR	0.73	0/829	1.16	8/1107 (0.7%)
41	BS	0.64	0/864	1.18	8/1156 (0.7%)
42	BT	0.64	0/744	1.21	7/994 (0.7%)
43	BU	0.69	0/787	1.17	7/1051 (0.7%)
44	BV	0.70	0/766	1.20	8/1025 (0.8%)
45	BW	0.73	0/604	1.28	9/799 (1.1%)
46	BX	0.76	0/635	1.31	10/848 (1.2%)
47	BY	0.67	0/510	1.24	6/677 (0.9%)
48	BZ	0.71	0/453	1.22	5/605 (0.8%)
49	B0	0.74	0/450	1.31	8/599 (1.3%)
5	AF	0.72	0/835	1.09	6/1128 (0.5%)
50	B1	0.74	0/417	1.16	3/556 (0.5%)
51	B2	0.81	0/380	1.48	8/498 (1.6%)
52	B3	0.72	0/513	1.18	4/676 (0.6%)
53	B4	0.67	0/303	1.29	4/397 (1.0%)
54	BA	1.41	1/69796 (0.0%)	2.21	4036/108888 (3.7%)
55	BB	1.41	0/2800	2.17	154/4367 (3.5%)
56	B5	0.64	0/1673	1.10	11/2255 (0.5%)
6	AG	0.74	0/1188	1.23	15/1593 (0.9%)
7	AH	0.70	0/989	1.00	5/1326 (0.4%)
8	AI	0.79	0/1035	1.28	19/1377 (1.4%)
9	AJ	0.71	0/797	1.18	10/1079 (0.9%)
All	All	1.28	2/160085 (0.0%)	1.99	6823/239402 (2.9%)

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
21	AA	0	350
22	A1	0	14
23	A2	0	5
24	A3	0	16
25	BC	0	1
3	AD	0	2
38	BP	0	1
4	AE	0	1
54	BA	0	663
55	BB	0	31
All	All	0	1084



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	80	C	C4-N4	-5.22	1.29	1.33
54	BA	1314	C	C4-N4	-5.09	1.29	1.33

The worst 5 of 6823 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2740	A	O4'-C1'-N9	13.91	119.33	108.20
54	BA	1610	A	O4'-C1'-N9	13.75	119.20	108.20
54	BA	1584	U	O4'-C1'-N1	12.72	118.38	108.20
54	BA	280	U	O4'-C1'-N1	12.43	118.14	108.20
54	BA	1854	A	N1-C6-N6	-12.29	111.23	118.60

There are no chirality outliers.

5 of 1084 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	14	U	Sidechain
21	AA	6	G	Sidechain
3	AD	3	TYR	Sidechain
3	AD	36	ALA	Peptide
4	AE	148	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	1	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	1	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	4	0
22	A1	1627	0	832	1	0
23	A2	309	0	156	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B4	302	0	343	0	0
54	BA	62317	0	31339	3	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99657	11	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 0.

The worst 5 of 11 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)
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
21:AA:730:G:C5	21:AA:731:G:H1'	2.48	0.48
6:AG:148:LYS:HE3	10:AK:60:PHE:CZ	2.48	0.47
26:BD:125:TRP:CE3	26:BD:160:LYS:HE3	2.48	0.47
29:BG:1:SER:HA	54:BA:2749:A:OP1	2.18	0.43

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 PDB entries followed by that with respect to all EM entries.

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
1	AB	218/220 (99%)	202 (93%)	15 (7%)	1 (0%)	32 74
2	AC	205/208 (99%)	190 (93%)	12 (6%)	3 (2%)	12 53
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	9 46
4	AE	150/152 (99%)	135 (90%)	11 (7%)	4 (3%)	6 40
5	AF	99/101 (98%)	90 (91%)	4 (4%)	5 (5%)	2 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AG	150/152 (99%)	130 (87%)	18 (12%)	2 (1%)	14	56
7	AH	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	22	67
8	AI	126/128 (98%)	114 (90%)	11 (9%)	1 (1%)	22	67
9	AJ	98/100 (98%)	92 (94%)	3 (3%)	3 (3%)	5	37
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	20	63
11	AL	121/124 (98%)	108 (89%)	11 (9%)	2 (2%)	11	50
12	AM	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	10	49
13	AN	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	9	46
14	AO	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	4	34
15	AP	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	4	32
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	6	41
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	10	49
18	AS	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	14	56
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	36 (71%)	12 (24%)	3 (6%)	2	23
25	BC	270/273 (99%)	241 (89%)	22 (8%)	7 (3%)	6	40
26	BD	207/209 (99%)	172 (83%)	20 (10%)	15 (7%)	1	19
27	BE	199/201 (99%)	179 (90%)	17 (8%)	3 (2%)	12	53
28	BF	176/179 (98%)	142 (81%)	25 (14%)	9 (5%)	2	26
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	11	50
30	BH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	4	35
31	BI	139/142 (98%)	128 (92%)	9 (6%)	2 (1%)	13	54
32	BJ	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	13	54
33	BK	121/123 (98%)	102 (84%)	15 (12%)	4 (3%)	4	35
34	BL	141/144 (98%)	111 (79%)	19 (14%)	11 (8%)	1	18
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	44
36	BN	119/121 (98%)	108 (91%)	9 (8%)	2 (2%)	11	50
37	BO	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	6	40
39	BQ	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	6	40
40	BR	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	9	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BS	108/110 (98%)	95 (88%)	13 (12%)	0	100	100
42	BT	92/94 (98%)	77 (84%)	12 (13%)	3 (3%)	4	35
43	BU	101/104 (97%)	83 (82%)	12 (12%)	6 (6%)	2	23
44	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	17	60
45	BW	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	2	26
46	BX	75/79 (95%)	66 (88%)	8 (11%)	1 (1%)	14	56
47	BY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	11	51
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	25
49	B0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
50	B1	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	17
51	B2	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	7	43
52	B3	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	B4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	25
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	32	74
All	All	5876/6008 (98%)	5234 (89%)	497 (8%)	145 (2%)	10	41

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AH	105	THR
9	AJ	74	VAL
12	AM	65	GLU
14	AO	45	HIS
16	AQ	39	ARG

### 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 PDB entries followed by that with respect to all EM entries.

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	
1	AB	180/180 (100%)	180 (100%)	0	100	100
2	AC	170/171 (99%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	112 (99%)	1 (1%)	82	91
5	AF	87/87 (100%)	85 (98%)	2 (2%)	56	79
6	AG	123/123 (100%)	121 (98%)	2 (2%)	68	85
7	AH	104/105 (99%)	103 (99%)	1 (1%)	80	90
8	AI	105/105 (100%)	104 (99%)	1 (1%)	80	90
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	101 (98%)	2 (2%)	62	82
12	AM	91/92 (99%)	90 (99%)	1 (1%)	78	89
13	AN	83/84 (99%)	78 (94%)	5 (6%)	22	55
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	50	74
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	64 (98%)	1 (2%)	70	85
20	AU	44/44 (100%)	42 (96%)	2 (4%)	32	63
25	BC	216/217 (100%)	214 (99%)	2 (1%)	82	91
26	BD	164/164 (100%)	162 (99%)	2 (1%)	75	88
27	BE	165/165 (100%)	156 (94%)	9 (6%)	25	58
28	BF	149/150 (99%)	146 (98%)	3 (2%)	60	82
29	BG	137/138 (99%)	135 (98%)	2 (2%)	70	85
30	BH	114/114 (100%)	112 (98%)	2 (2%)	64	84
31	BI	109/110 (99%)	107 (98%)	2 (2%)	64	84
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	66	84
33	BK	103/103 (100%)	102 (99%)	1 (1%)	80	90
34	BL	102/103 (99%)	100 (98%)	2 (2%)	60	82
35	BM	109/109 (100%)	106 (97%)	3 (3%)	49	74
36	BN	100/100 (100%)	98 (98%)	2 (2%)	60	82
37	BO	86/87 (99%)	85 (99%)	1 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BP	99/100 (99%)	98 (99%)	1 (1%)	80	90
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	83 (99%)	1 (1%)	75	88
41	BS	93/93 (100%)	92 (99%)	1 (1%)	78	89
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	54	78
44	BV	78/78 (100%)	76 (97%)	2 (3%)	51	75
45	BW	59/59 (100%)	57 (97%)	2 (3%)	42	69
46	BX	67/68 (98%)	64 (96%)	3 (4%)	32	63
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	59	80
49	B0	47/48 (98%)	46 (98%)	1 (2%)	59	80
50	B1	45/45 (100%)	44 (98%)	1 (2%)	57	79
51	B2	38/38 (100%)	37 (97%)	1 (3%)	51	75
52	B3	51/52 (98%)	50 (98%)	1 (2%)	60	82
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	66	84
All	All	4842/4870 (99%)	4769 (98%)	73 (2%)	72	85

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	BF	12	VAL
31	BI	67	THR
50	B1	39	ASP
29	BG	103	ASN
32	BJ	43	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
10	AK	23	HIS
34	BL	35	HIS
44	BV	88	HIS
49	B0	40	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	251 (16%)	0
22	A1	73/76 (96%)	10 (13%)	0
23	A2	14/15 (93%)	8 (57%)	0
24	A3	76/77 (98%)	13 (17%)	0
54	BA	2902/2903 (99%)	462 (15%)	0
55	BB	116/118 (98%)	18 (15%)	0
All	All	4710/4722 (99%)	762 (16%)	0

5 of 762 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	CM0	A1	34	22,23	16,26,27	1.78	3 (18%)	14,37,40	3.36	2 (14%)
22	6MZ	A1	37	22	18,25,26	1.02	0	16,36,39	1.71	2 (12%)
22	7MG	A1	46	22	20,26,27	2.26	4 (20%)	22,39,42	1.89	2 (9%)
22	5MU	A1	54	22	14,22,23	1.27	2 (14%)	16,32,35	4.07	2 (12%)
22	PSU	A1	55	22	16,21,22	1.15	1 (6%)	20,30,33	5.31	7 (35%)
22	4SU	A1	7	22	14,21,22	1.12	0	15,30,33	2.69	2 (13%)
24	H2U	A3	21	24	17,21,22	1.40	2 (11%)	21,30,33	1.54	4 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	OMC	A3	33	24	15,22,23	1.14	0	19,31,34	0.73	0
24	5MU	A3	55	24	14,22,23	1.09	2 (14%)	16,32,35	4.10	2 (12%)
24	PSU	A3	56	24	16,21,22	1.23	2 (12%)	20,30,33	5.48	8 (40%)
24	4SU	A3	8	24	14,21,22	1.31	3 (21%)	15,30,33	2.68	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22,23	-	0/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/3/25/26	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/3/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.32	1.33	1.45
22	A1	34	CM0	O5-C5	-5.59	1.26	1.37
24	A3	21	H2U	C4-N3	-3.39	1.32	1.37
24	A3	21	H2U	C2-N3	-3.24	1.32	1.38
22	A1	46	7MG	C8-N7	-2.94	1.30	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	N1-C2-N3	-15.68	117.12	128.40
24	A3	56	PSU	N1-C2-N3	-15.55	117.22	128.40
24	A3	56	PSU	C5-C4-N3	-12.93	114.82	125.43
22	A1	55	PSU	C5-C4-N3	-11.98	115.61	125.43
24	A3	55	5MU	C5-C4-N3	-9.99	114.23	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0
22	A1	55	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	6,6,7	1.22	1 (16%)	6,7,9	1.77	1 (16%)
58	FME	BA	3001	57	9,9,10	1.69	1 (11%)	7,9,11	1.48	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/5/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A1	101	VAL	CA-C	2.62	1.53	1.50
58	BA	3001	FME	CA-C	4.66	1.56	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.90	118.39	125.15
57	A1	101	VAL	C-CA-N	3.96	117.84	109.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.