



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:54 PM BST

PDB ID : 4V72
EMDB ID: : EMD-1719
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet complex in hybrid pre-translocation state (pre4)
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 : 13.00 Å(reported)
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

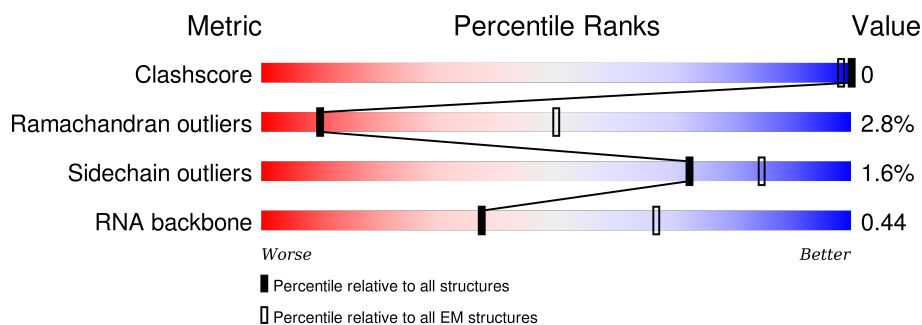
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 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.












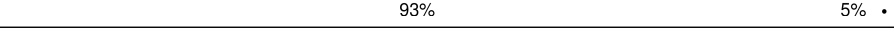

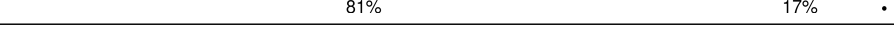
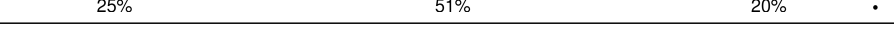


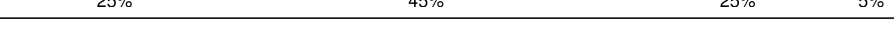



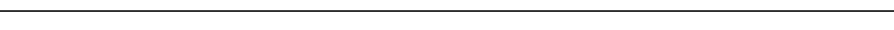

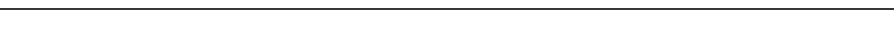
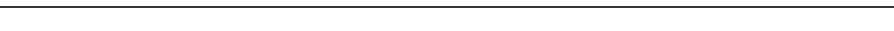


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 ≥ 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	92% 8%
2	AC	208	87% 13%
3	AD	206	87% 13%
4	AE	152	90% 10%
5	AF	101	82% 18%
6	AG	152	86% 13% .
7	AH	130	92% 6% ..
8	AI	128	82% 17% .

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Mol	Chain	Length	Quality of chain
9	AJ	100	 88% 10% .
10	AK	118	 90% 9% .
11	AL	124	 89% 10% .
12	AM	115	 83% 15% ..
13	AN	101	 88% 10% ..
14	AO	89	 88% 11% .
15	AP	81	 88% 12%
16	AQ	82	 89% 10% .
17	AR	57	 89% 11%
18	AS	81	 93% 5% .
19	AT	86	 91% 9%
20	AU	53	 81% 17% .
21	AA	1533	 25% 51% 20% .
22	A1	76	 33% 47% 16% .
23	A2	15	 27% 27% 33% 13%
24	A3	77	 25% 45% 25% 5%
25	BC	273	 87% 12%
26	BD	209	 91% 8%
27	BE	201	 90% 10%
28	BF	179	 88% 11% ..
29	BG	177	 90% 10% .
30	BH	149	 95% 5%
31	BI	142	 96% . .
32	BJ	142	 90% 9% .
33	BK	123	 85% 13% .

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Mol	Chain	Length	Quality of chain
34	BL	144	85% 14% ..
35	BM	136	87% 13% .
36	BN	121	89% 11% .
37	BO	117	85% 13% ..
38	BP	115	84% 14% ..
39	BQ	118	84% 14% ..
40	BR	103	94% 5% .
41	BS	110	90% 9% .
42	BT	94	94% 6% .
43	BU	104	88% 9% ..
44	BV	94	95% 5% .
45	BW	80	86% 13% .
46	BX	79	86% 11% .
47	BY	63	90% 10% .
48	BZ	59	83% 15% .
49	B0	57	88% 11% .
50	B1	52	92% 8% .
51	B2	46	78% 20% .
52	B3	65	83% 14% ..
53	B4	38	89% 11% .
54	BA	2903	22% 51% 22% .
55	BB	118	21% 54% 20% ..
56	B5	234	90% 5% 5% .

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*P*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		

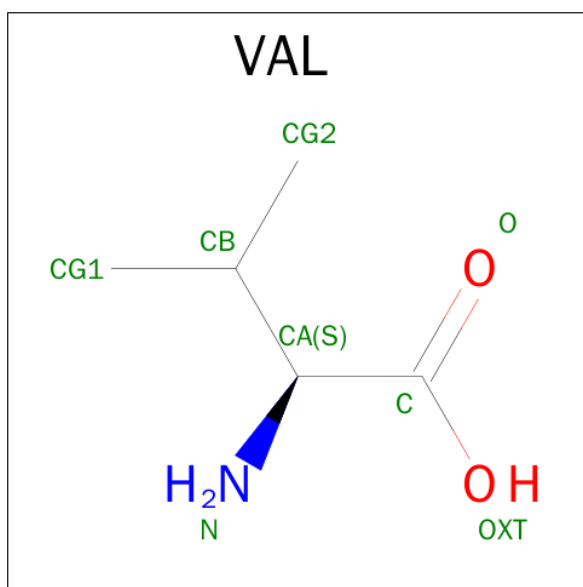
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

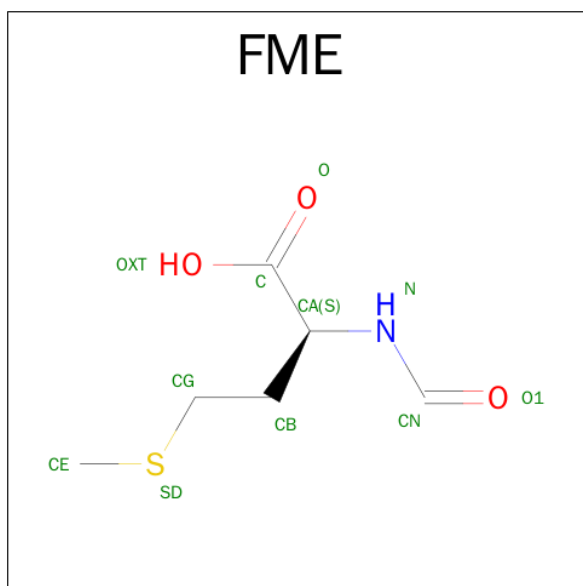
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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: $C_6H_{11}NO_3S$).

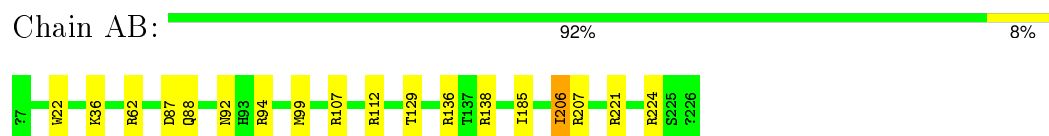


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

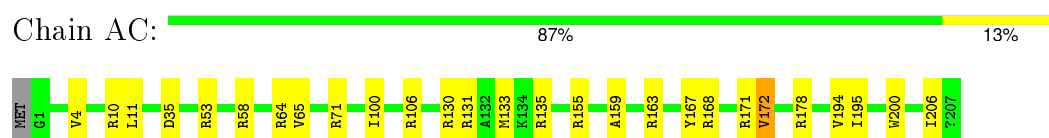
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

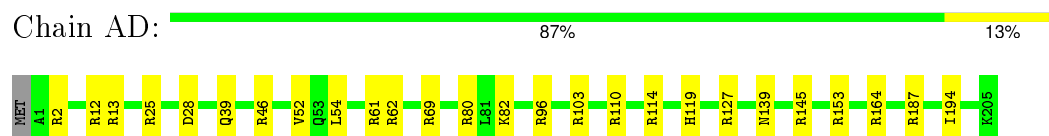
- Molecule 1: 30S ribosomal protein S2



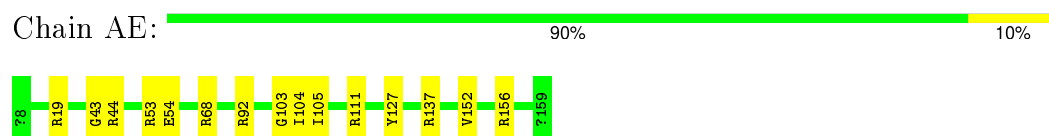
- Molecule 2: 30S ribosomal protein S3



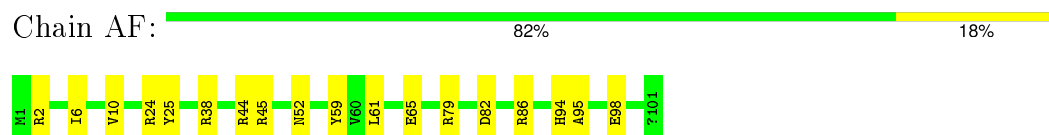
- Molecule 3: 30S ribosomal protein S4



- 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: 92% 6% ..



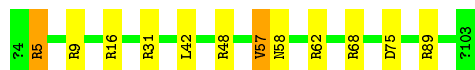
- Molecule 8: 30S ribosomal protein S9

Chain AI: 82% 17% .



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 88% 10% .



- Molecule 10: 30S ribosomal protein S11

Chain AK: 90% 9% .



- Molecule 11: 30S ribosomal protein S12

Chain AL: 89% 10% .



- Molecule 12: 30S ribosomal protein S13

Chain AM: 83% 15% ..




- Molecule 13: 30S ribosomal protein S14

Chain AN: 88% 10% ..



- Molecule 14: 30S ribosomal protein S15

Chain AO:  88% 11%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  88% 12%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  89% 10%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 11%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  93% 5%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  91% 9%



- Molecule 20: 30S ribosomal protein S21

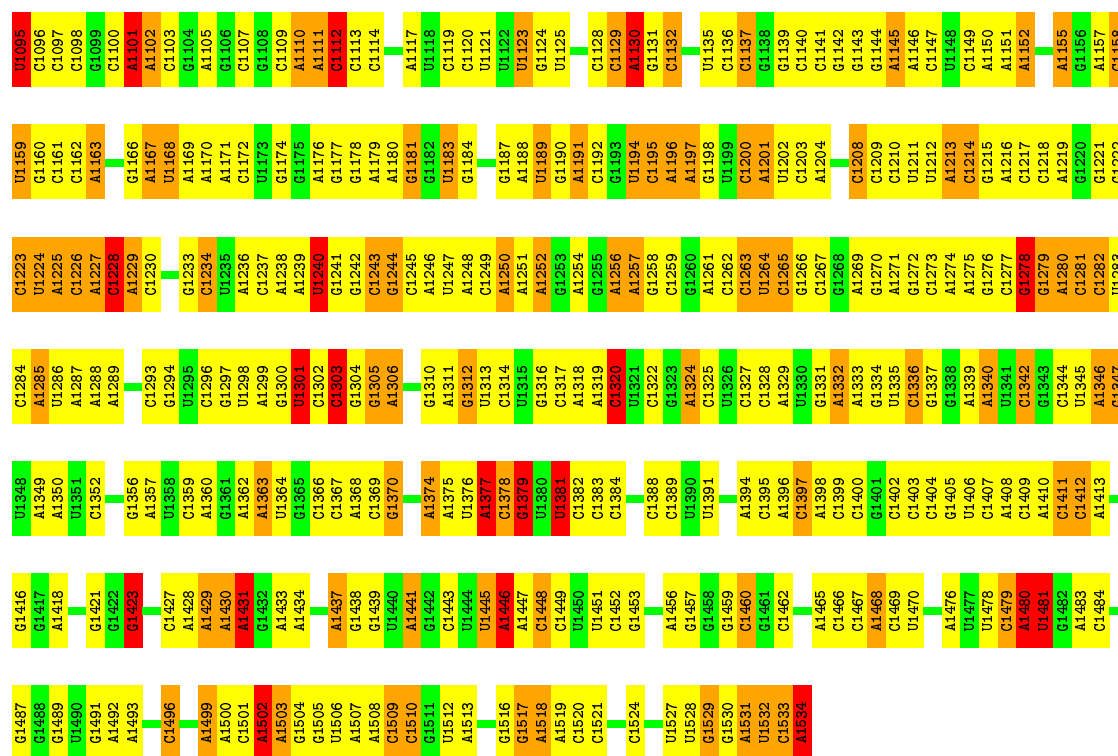
Chain AU:  81% 17%



- Molecule 21: 16S ribosomal RNA

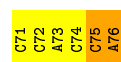
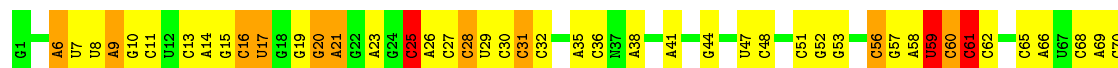
Chain AA:  25% 51% 20%

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U1029	C967	A907	U843	G778	G714	C947	C578	C514	G450	C385	A320	G257	C193	A130	G64	A
U1030	A968	A908	C844	C779	A715	C948	A579		A452	C386	A321	G258	C194	A131	A65	U
C1031	A969	A909	A845	A780	A716	A648	C580	G517		U387	C322	G259	A195	C132	A66	
G1032	C970	C910	C846	A781	U717	A649	G581	C519		G388	U323	G260	A196	C135	C67	G6
G1033	G971	U911	G847	A782	A718	G650	C582	C519		A389	G324	U261	A197	C135	G68	A7
G1034	C972	C912	C848	G783	C719	C851	A583	A520		U390	A325	A262	C198	C136	A68	A8
A1035	G973	A913	G849	G784	G720	U852	G584	G521		U391	G326	A263	A199	U137	G69	G9
A1036	A974	A914		G785	G721	U853	C585	C522		C392	A327	G264	G203	A139	A71	G11
C1037	G975	A915	C852	G786	G722	A655	C586	A523		G394	C328	G265	G204		A72	
G1038	G976	U916	C853	G787	U723	G656	U589	G524		C395	A329	G266	G205		C73	
G1039	A977	G917	U854	A790	G724	U857	U590	C525		C396	G330	G267	A206		A74	
U1040	A978	A918	U855	G791	G725	C858	U591	G526		A397	C331	U268	C206		G75	
G1041	C979	A919	C856	G792	C726	U859	G592	G527		U398		C269	C207		G76	
A1042	C980	U920	C857	A792	G727	U859	G592	C528		A466	A327	A270	U208		A77	
G1043	U981	U921	U858	U793	A728	C660		G529		U467	G332	C271	U209		A78	
A1044	U982	G922	C859	A794		A663	A595	U531		C401	G337	U273	G211		G79	
C1045	A983	A923	A860	C795	C732	G664	A596	U531		G402	A338	A274	G212		A80	
A1046	C984	C924	C861	C796	G733	A665	G597	A532		C403	U340	G275	G213		A81	
G1047	C985	G925	C862	C797	U734	A666	U598	A533		G404	C339	G276	G214		G82	
U1048	U986	U798	U863	U799	G735	G666	C599	U534		U405	U341	C277	C215		G83	
U1049	G987	G927	A864	G799	C735	G667	A600	A535		G406	C342	G278	U216		G86	
G1050	G988	G928	A865	G800	C736	G670	G601	C536		U407	U343	A279	U217		C87	
C1051	U989	G929	C866	U801	C737		A602			C408	A344	C280	U218		G88	
U1052	C990	C930	G867	A802	C738	A873		A539		U409	C345	G281	U219		G89	
G1053	U991	C931	C868		C739	G874	U605	G540		U409	C346	A282	U220		A28	
C1054	U992	G932		C805	U740	A875	G606	G541		G410	G347	U283	G221		U91	
A1055	G993	G933	U871	C806	G741	A876	A607	U479		A411	U348	G284	C222		U92	
U1056	A994	C934	A872	A807	G742	A608	U479	C481		A412	G348	C285	G223		G94	
	C995	A935	A873	C808	A743	C679	A609	A482		G413	A349	C286	G224		G95	
C1059	A996	C936		G809	C744	C680	U610	C545		A414	C352	U287	G225		U96	
U1060	U997	A937	C876	C810	G745	A881	C611	A546		U415	C353	A288	G226		G97	
G1061	C998	A938	G877	C811	A746	G885	C612	A547		G416	A354	G289	G227		A98	
U1062	C999	G939	A878	G812	G747	U886	C613	G548		U417	G355	C290	G228		C99	
C1063	A1000	C940	C879	U813	A748	U887	C614	C549		C418	C356	C291	G229		G100	
G1064	C1001	G941	C880	A814	A749	A887	C488	C550		C419	A356	U291	U230		A101	
U1065	G1002	G942	G881	A815	C750	G888	C489	U551		U420					G38	
C1066	G1003	U943	C882	A816	U751	C889	C490	U552		U421	G359		G232		C39	
A1067	A1004	G944	C883	C817	G752	G890	G491	C422		C422		U296	G233		G41	
G1068	U1005	G945	U884	G818	A753	G891	C492	G423		G423	G362	U297	C234		G105	
C1069	G1006	A946	C885	A819	C754	U892	A493	G424		G425	A363	A298	C235		G107	
U1070	U1007	G947	C886	U820	G755	G893	G500				A364	G299	A236		G108	
C1071	U1008	C948	G887	G821	C756	A694	C501				U365	A300	G237		A109	
	U1009	A949	C888	U822	U757	A695	A496				A366	G301	A238		G45	
U1075	U1010	U950	A889	C823	C758	A696	G497	A450			U367	G302	U239		C47	
	C1011	G951	C890	G824	A759	U897	A498	A431			U368	A303	G240		G111	
U1078	A1012	U952	U891	A825	G760	G898	A499	A432			G369	U304	G241		G112	
G1079	G1013	G953	C892	C826	G761	C699	C500	A433			C370	G305	G242		G113	
A1080	A1014	G954	C893	U827	U762	G700	U434				A371	A306	G243		U114	
A1081	G1015	U955	C894	U828	G763	U701	A435	A436			C372	C307	A244		G115	
A1082	A1016	U956	G895	G829	C764	A702	C437	C503			A374	C308	U245		A116	
		U957	C896	G830	G765	G703	U438	C504			A374	C309	U246		A182	
U1083		A958	C897	A831	A766	A704	U439	G505				G310	G247		C183	
G1084	G1020	A959	C898	G832	A767	A705	G506	U439			G377	C311	G248		A119	
U1085	A1021	U960	C899	A768	U636	A706	U507	C440			C378	U249	C249		A120	
	A1022	U961	A900	C637	U637	U508	U508	A441			C379	A312	G122		G57	
U1090	U1091	C862	A901	U837	C708	C708	A509	G442			G380	C313	A250		G123	
A1092	G1026	G963	G902	C839	G711		A510	C443			C381	A315	G252		U124	
A1093	G1027	U965	G903	C840	G712		C576	U512			A382	C316	A253		G61	
G1094				C841							A383		G254		U62	



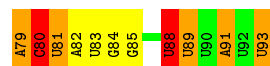
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 33% 47% 16%



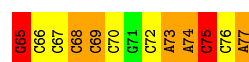
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 27% 27% 33% 13%

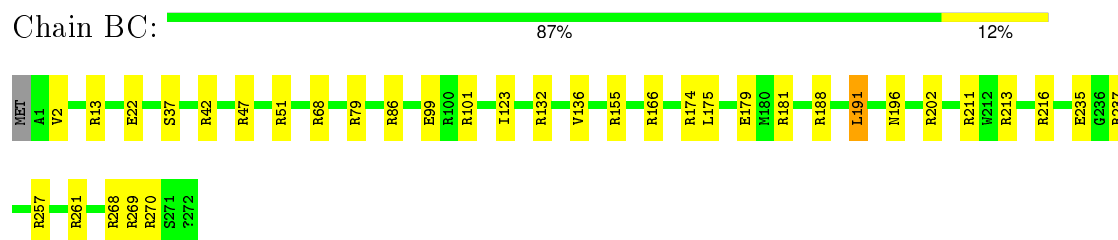


• Molecule 24: tRNA-fMet

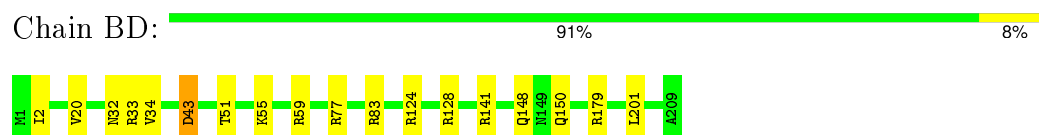
Chain A3: 25% 45% 25% 5%



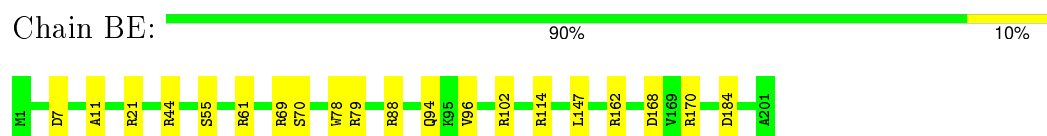
• Molecule 25: 50S ribosomal protein L2



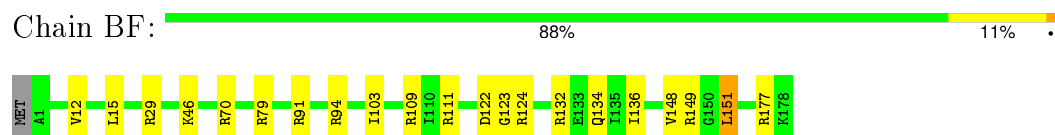
- Molecule 26: 50S ribosomal protein L3



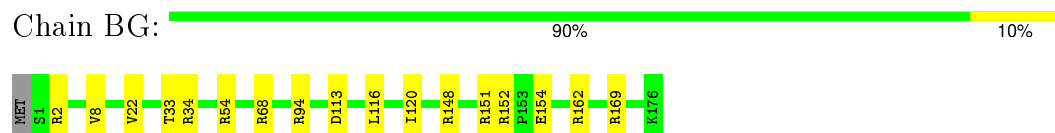
- Molecule 27: 50S ribosomal protein L4



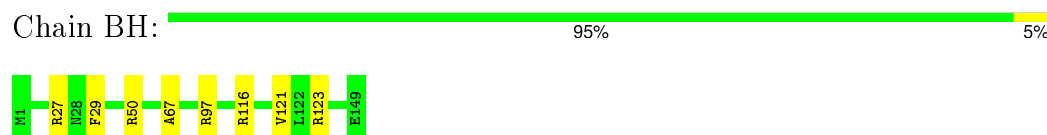
- Molecule 28: 50S ribosomal protein L5



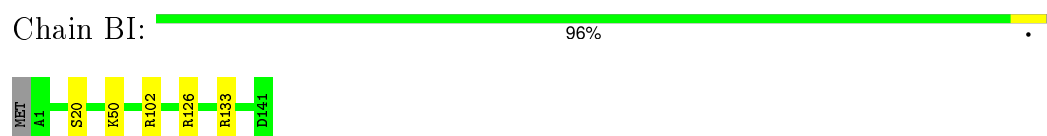
- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11




- Molecule 32: 50S ribosomal protein L13

Chain BJ:  90% 9% .




- Molecule 33: 50S ribosomal protein L14

Chain BK:  85% 13% .




- Molecule 34: 50S ribosomal protein L15

Chain BL:  85% 14% ..



- Molecule 35: 50S ribosomal protein L16

Chain BM:  87% 13% .




- Molecule 36: 50S ribosomal protein L17

Chain BN:  89% 11%




- Molecule 37: 50S ribosomal protein L18

Chain BO:  85% 13% ..




- Molecule 38: 50S ribosomal protein L19

Chain BP:  84% 14% ..



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  84% 14% ..



- Molecule 40: 50S ribosomal protein L21

Chain BR: 94% 5% .



- Molecule 41: 50S ribosomal protein L22

Chain BS: 90% 9% .



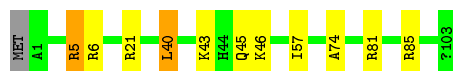
- Molecule 42: 50S ribosomal protein L23

Chain BT: 94% 6%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 88% 9% ..



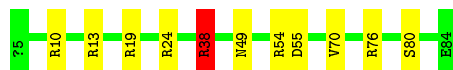
- Molecule 44: 50S ribosomal protein L25

Chain BV: 95% 5%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 13% .

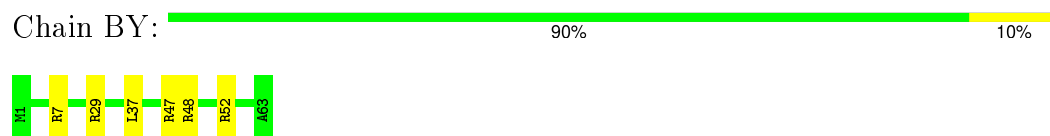


- Molecule 46: 50S ribosomal protein L28

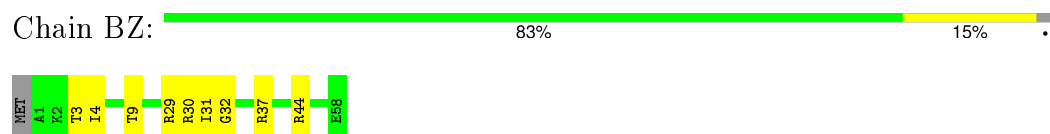
Chain BX: 86% 11% .



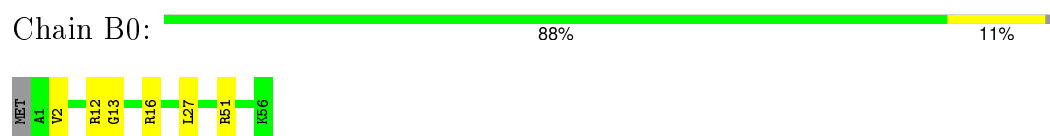
- Molecule 47: 50S ribosomal protein L29



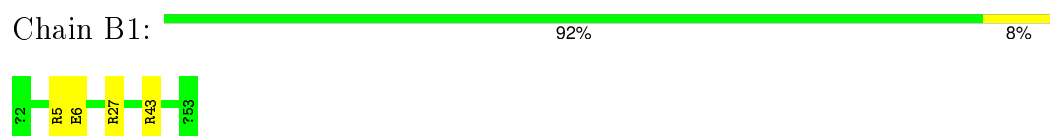
- Molecule 48: 50S ribosomal protein L30



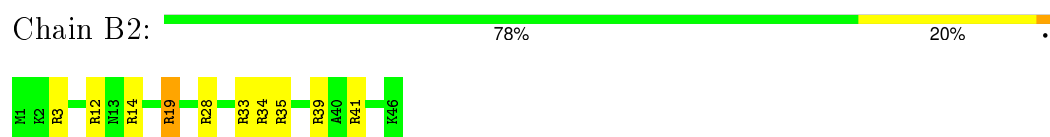
- Molecule 49: 50S ribosomal protein L32



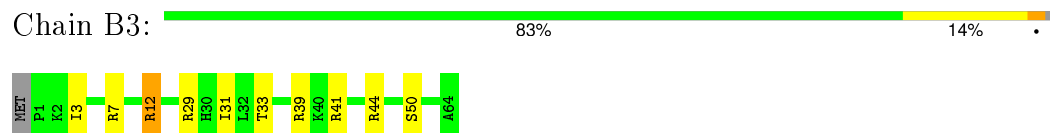
- Molecule 50: 50S ribosomal protein L33



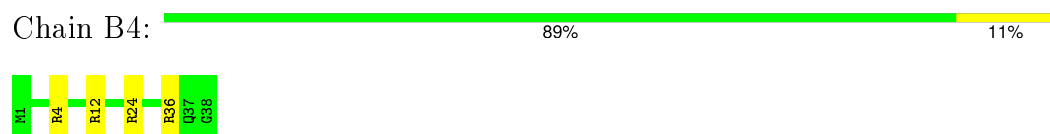
- Molecule 51: 50S ribosomal protein L34



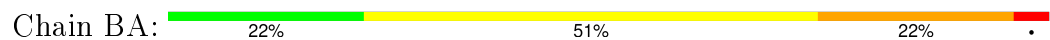
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36

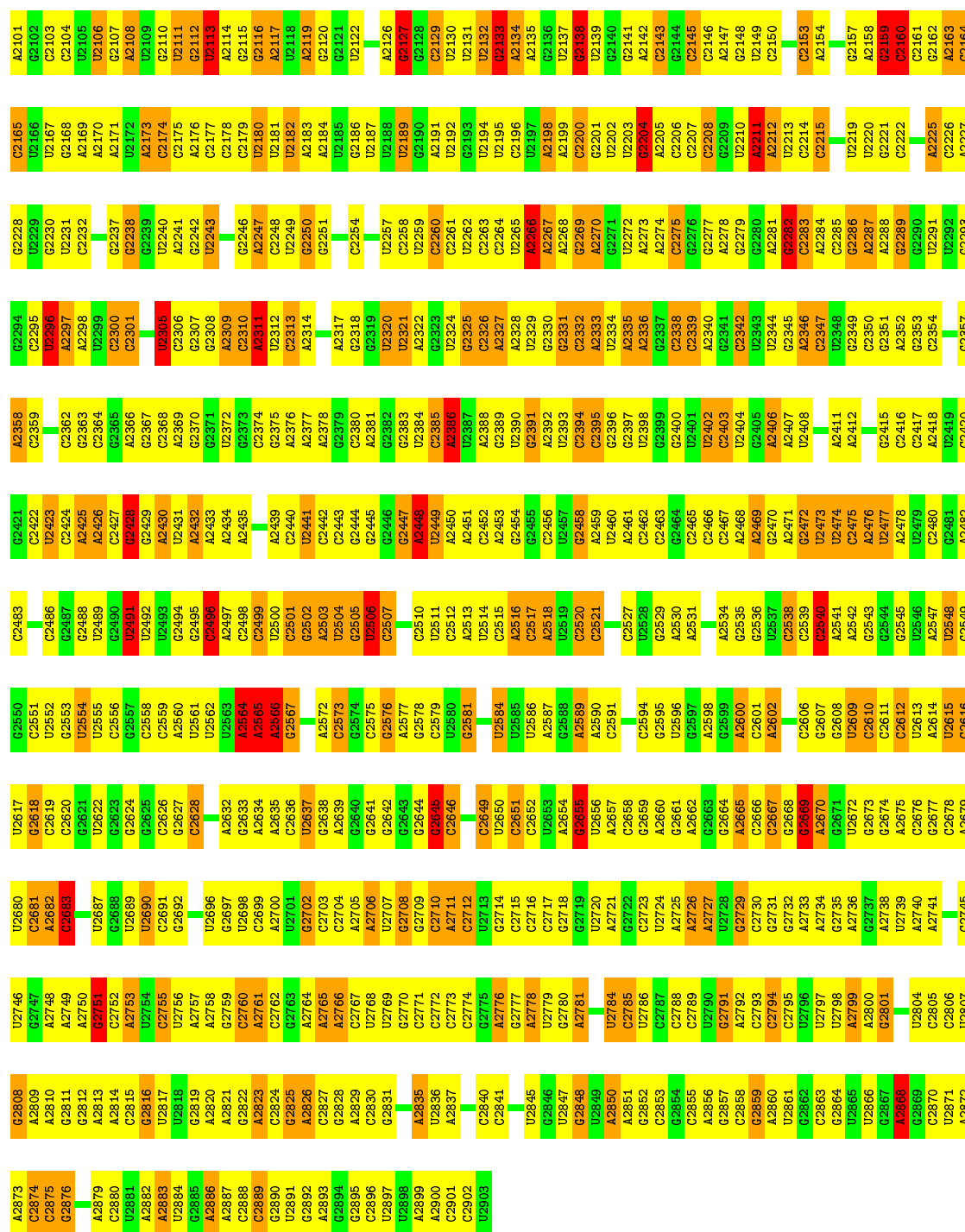


- Molecule 54: 23S ribosomal RNA

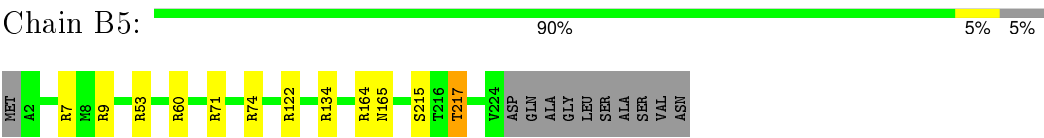


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G962	G963	C964	C965	G968	G969	U970	G971	A972	A973	G974	A975	G976	G977	A978	A979	A980	A981	C982	A983	A984	C985	C986	C987	A988	A989	A990	A991	A992	C993	C994	C995	A996	C997	C998	U999	A1000	A1001	C1005	C1006	C1007	A1008	A1009	A1010	G1011	U1012	C1013	A1014	U1015	U1016	A1017	U1018	U1019	A1020	A1021	U1022	A1023	G1024
A889	A900	C901	C902	C903	G904	A905	U906	C907	C908	A909	A910	A911	C912	U913	C914	C915	C916	A917	A918	A919	A920	C921	C922	C923	C924	A925	G926	A927	A928	U929	C930	U931	U932	U933	A934	C935	A936	C937	A941	G942	A943	C944	A945	C946	A947	C948	G949	G950	C951	G954	U955	C956	A957	C958	U959	A960	C961
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G1087	U1148	G1219	U1344	G1478	A1544	C1606	A1668	G1731	C1793	U1855	A1918	A1978	G2038
A1088	G1149	G1220	C1345	G1479	A1545	C1607	A1669	C1732	A1794	U1856	A1919	U1979	U2039
A1089	C1150	G1221	G1346	U1480	G1546	A1608	U1671	G1733	C1795	G1857	C1920	G1980	A2042
A1090	A1151	U1282	A1347	U1481	C1547	A1609	G1672	G1734	U1796	A1858	G1921	A1981	C2043
C1091	C1152	G1283	C1348	U1415	A1548	A1610	A1673	A1735	G1797	U1859	G1922	G1982	C2044
C1092	G1153	G1223	C1349	U1416	A1549	C1611	G1674	G1736	U1798	G1860	G1923	G1983	G2045
C1093	G1154	U1224	C1350	G1417	C1550	C1612	G1675	G1738	G1799	G1861	C1924	G1984	C2046
U1094	A1155	G1225	C1351	A1418	A1551	G1613	C1676	A1739	C1800	G1862	G1925	C1985	G2047
A1095	A1156	A1226	U1352	U1419	A1552	A1614	U1676	G1740	A1801	G1863	U1926	C1986	C2048
A1096	G1157	G1227	A1353	A1420	A1553	C1615	A1677	C1741	A1802	U1864	A1927	A1987	C2049
U1097	C1158	G1228	A1354	U1490	A1554	A1616	U1678	U1742	A1803	U1865	A1928	G1988	C2050
A1098	U1159	C1229	G1355	C1492	G1555	C1617	A1679	G1743	C1804	A1866	G1929	G1989	A2051
G1099	G1160	A1230	C1356	C1493	C1556	A1618	U1680	A1744	A1805	G1867	G1930	C1990	A2052
C1100	C1161	G1231	C1357	G1425	C1557	G1619	G1681	A1745	C1806	C1868	U1931	U1991	G2053
U1101	G1162	U1233	G1358	A1426	C1558	G1620	U1682	A1746	G1807	C1869	U1932	G1992	A2054
C1102	C1164	U1234	A1359	A1496	U1559	U1621	G1683	U1747	A1808	C1870	C1933	U1993	C2055
A1103	A1165	G1235	G1360	U1497	G1560	G1622	G1684	C1748	A1809	A1871	C1934	C1994	C2056
C1104	G1166	G1236	G1361	U1498	C1561	G1623	G1685	A1749	A1810	A1872	G1935	U1995	C2057
U1105	C1167	A1237	C1362	C1499	U1562	U1624	C1686	G1750	G1813	G1873	G1936	C1996	A2058
G1106	G1168	G1238	C1363	A1502	U1563	G1625	A1689	U1751	G1814	C1874	C1937	C1997	A2059
U1107	A1169	G1239	G1364	A1503	C1564	A1626	G1695	C1752	G1815	G1875	A1938	A1998	A2060
U1108	C1170	U1240	A1365	A1504	C1565	G1627	A1690	G1753	C1816	A1876	U1939	C1999	A2061
C1109	G1171	A1241	A1366	A1505	A1566	G1628	C1691	A1754	G1817	A1877	U1940	C2000	C2062
G1110	C1172	U1242	A1367	A1506	G1567	U1629	U1692	A1755	G1818	G1878	C1941	C2001	C2063
A1111	U1173	C1243	G1368	U1507	G1568	A1630	U1693	G1756	U1819	C1879	C1942	C2002	C2064
G1112	U1174	A1244	G1369	C1507	A1569	G1631	C1694	A1757	A1819	U1880	U1943	A2003	C2065
U1113	A1175	G1245	G1370	A1508	C1570	A1632	G1695	U1758	G1820	C1881	G2004	G2004	C2066
C1114	U1176	A1246	G1371	A1509	A1571	G1633	G1696	A1759	A1821	U1882	U1945	A2005	G2067
G1115	G1177	U1247	U1372	G1510	A1572	A1634	G1697	C1760	C1822	U1883	U1946	C2006	C2068
U1116	C1177	A1248	A1373	G1511	G1573	A1635	U1698	C1761	G1823	G1884	C1947	U2007	A2070
C1117	C1178	U1249	G1376	G1512	C1574	U1636	G1699	A1762	G1824	A1885	G1948	C2008	A2071
U1118	U1183	G1250	C1377	A1515	C1575	A1637	A1700	G1763	U1825	U1886	G1949	A2009	C2072
C1119	U1184	U1251	U1377	G1445	U1576	U1638	A1701	C1764	G1826	C1887	G1950	G2010	C2073
G1120	G1185	G1252	A1378	C1446	C1577	C1639	G1702	U1765	U1827	U1888	A1951	U2011	U2074
U1121	G1186	A1253	U1379	G1447	G1450	A1640	G1703	G1766	G1828	A1889	A1952	A2012	U2075
G1122	C1123	A1254	C1315	G1451	C1452	A1641	C1704	U1769	A1829	A1890	G1954	A2013	U2076
U1123	A1189	U1255	C1319	G1452	U1520	G1642	A1705	U1770	C1830	G1891	U1955	A2014	A2077
G1124	G1125	G1256	G1383	A1463	G1521	G1643	C1706	G1770	G1831	C1892	U1956	A2015	C2078
U1125	A1194	C1257	A1384	C1454	U1522	C1644	G1707	C1771	C1832	C1893	U1957	U2016	U2079
A1126	C1195	U1258	A1385	G1455	U1523	G1645	C1708	A1772	C1833	C1894	C1957	U2017	A2080
U1127	C1196	G1259	C1386	G1456	G1524	U1584	U1709	A1773	U1834	C1895	C1958	A2018	U2081
G1128	G1197	A1260	A1387	A1525	C1585	U1647	G1710	C1774	G1835	G1907	G1959	A2019	A2082
U1129	U1198	C1261	G1388	U1526	A1586	U1648	A1711	U1775	C1836	A1899	A1960	C2020	G2083
G1132	U1199	A1262	G1389	G1527	C1459	U1649	U1712	G1776	C1837	A1900	C1961	C2021	C2084
U1133	C1200	U1263	U1390	A1528	U1460	A1650	A1713	U1777	C1838	A1901	C1962	C2022	C2085
A1134	U1201	A1264	U1391	G1529	C1461	G1651	G1714	U1778	G1839	C1902	U1963	C2023	U2086
C1135	A1204	A1265	C1462	G1530	C1462	A1652	G1715	U1779	G1840	G1905	G1964	G2024	G2087
G1136	A1205	G1266	A1392	C1531	A1593	G1653	U1716	A1780	U1841	C1906	C1965	C2025	A2088
U1137	G1206	U1267	U1393	G1532	U1594	A1654	A1717	U1781	G1842	G1907	A1966	U2026	C2089
G1138	C1207	A1268	A1395	C1533	C1595	A1655	G1718	U1782	C1843	C1908	C1967	G2027	A2090
C1139	C1208	A1269	U1396	U1534	A1596	C1656	U1719	A1783	C1844	C1909	G1968	U2028	C2091
U1140	C1209	G1270	U1397	A1535	A1597	U1657	G1720	A1784	G1845	G1909	A1969	G2029	U2092
C1141	U1209	G1271	C1398	C1536	U1598	C1658	G1721	A1785	A1847	G1910	U1970	G2030	C2093
U1141	G1210	A1272	A1336	G1537	G1538	U1599	G1722	U1786	A1848	U1911	U1971	A2031	A2094
A1142	G1211	U1273	C1337	G1471	U1539	G1601	C1726	C1788	G1850	A1912	G1972	G2032	A2095
U1143	C1212	A1274	G1401	U1539	G1601	U1602	C1727	A1789	U1851	C1913	G1973	A2033	C2096
A1144	A1213	A1275	U1402	G1473	U1602	A1664	U1728	A1789	U1851	C1914	C1974	U2034	A2097
C1145	G1214	G1276	A1403	C1472	A1603	A1665	U1729	C1790	U1852	U1915	G1975	G2035	U2098
U1146	G1215	A1277	A1404	U1476	A1603	A1666	U1730	A1791	A1853	A1916	U1976	C2036	C2099
A1147	G1216	C1278	U1405	G1543	C1605	G1667	C1730	G1792	A1854	U1917	A1977	A2037	G2100



- 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 images	8375	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	161000	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	0.72	0/1736	1.06	11/2340 (0.5%)
10	AK	0.75	0/894	1.17	11/1207 (0.9%)
11	AL	0.78	0/969	1.24	13/1300 (1.0%)
12	AM	0.75	0/884	1.29	13/1181 (1.1%)
13	AN	0.78	0/817	1.22	10/1088 (0.9%)
14	AO	0.73	0/722	1.14	9/964 (0.9%)
15	AP	0.78	0/648	1.21	7/870 (0.8%)
16	AQ	0.69	0/658	1.21	11/883 (1.2%)
17	AR	0.83	0/463	1.23	7/623 (1.1%)
18	AS	0.76	0/653	1.17	7/879 (0.8%)
19	AT	0.70	0/672	1.11	7/890 (0.8%)
2	AC	0.75	0/1651	1.13	14/2225 (0.6%)
20	AU	0.83	0/431	1.39	7/572 (1.2%)
21	AA	1.52	2/36759 (0.0%)	2.22	1945/57346 (3.4%)
22	A1	1.52	0/1668	2.16	80/2595 (3.1%)
23	A2	1.51	0/343	2.27	22/531 (4.1%)
24	A3	1.54	0/1722	2.21	92/2685 (3.4%)
25	BC	0.76	0/2121	1.32	27/2852 (0.9%)
26	BD	0.69	0/1586	1.14	10/2134 (0.5%)
27	BE	0.68	0/1571	1.18	13/2113 (0.6%)
28	BF	0.76	0/1444	1.15	11/1937 (0.6%)
29	BG	0.69	0/1343	1.16	9/1816 (0.5%)
3	AD	0.78	0/1665	1.20	20/2227 (0.9%)
30	BH	0.67	0/1122	1.14	6/1515 (0.4%)
31	BI	0.67	0/1046	1.04	3/1410 (0.2%)
32	BJ	0.75	0/1152	1.20	9/1551 (0.6%)
33	BK	0.72	0/947	1.25	11/1268 (0.9%)
34	BL	0.75	0/1054	1.38	15/1403 (1.1%)
35	BM	0.76	0/1093	1.25	14/1460 (1.0%)
36	BN	0.77	0/973	1.28	13/1301 (1.0%)
37	BO	0.75	0/902	1.25	13/1209 (1.1%)
38	BP	0.74	0/929	1.26	12/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.82	0/960	1.35	17/1278 (1.3%)
4	AE	0.70	0/1119	1.01	8/1506 (0.5%)
40	BR	0.72	0/829	1.14	6/1107 (0.5%)
41	BS	0.66	0/864	1.18	6/1156 (0.5%)
42	BT	0.67	0/744	1.15	4/994 (0.4%)
43	BU	0.69	0/787	1.16	5/1051 (0.5%)
44	BV	0.74	0/766	1.13	4/1025 (0.4%)
45	BW	0.76	0/604	1.33	9/799 (1.1%)
46	BX	0.76	0/635	1.27	9/848 (1.1%)
47	BY	0.69	0/510	1.26	6/677 (0.9%)
48	BZ	0.70	0/453	1.24	5/605 (0.8%)
49	B0	0.74	0/450	1.17	3/599 (0.5%)
5	AF	0.74	0/835	1.16	8/1128 (0.7%)
50	B1	0.72	0/417	1.15	4/556 (0.7%)
51	B2	0.83	0/380	1.65	11/498 (2.2%)
52	B3	0.75	0/513	1.25	5/676 (0.7%)
53	B4	0.71	0/303	1.34	5/397 (1.3%)
54	BA	1.40	0/69796	2.21	4043/108888 (3.7%)
55	BB	1.41	0/2800	2.18	152/4367 (3.5%)
56	B5	0.67	0/1673	1.09	10/2255 (0.4%)
6	AG	0.74	0/1188	1.21	15/1593 (0.9%)
7	AH	0.71	0/989	1.03	6/1326 (0.5%)
8	AI	0.82	0/1035	1.31	19/1377 (1.4%)
9	AJ	0.71	0/797	1.18	8/1079 (0.7%)
All	All	1.28	2/160085 (0.0%)	2.00	6820/239402 (2.8%)

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
2	AC	0	1
21	AA	0	369
22	A1	0	10
23	A2	0	4
24	A3	0	19
37	BO	0	1
52	B3	0	1
54	BA	0	715
55	BB	0	28
6	AG	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	AH	0	1
All	All	0	1150

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1533	C	C4-N4	-5.16	1.29	1.33
21	AA	942	G	C5'-C4'	5.05	1.57	1.51

The worst 5 of 6820 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	704	A	N1-C6-N6	-13.07	110.76	118.60
54	BA	1274	A	N1-C6-N6	-12.32	111.21	118.60
34	BL	41	ARG	NE-CZ-NH1	12.26	126.43	120.30
54	BA	910	A	N1-C6-N6	-12.23	111.26	118.60
21	AA	913	A	N1-C6-N6	-12.01	111.40	118.60

There are no chirality outliers.

5 of 1150 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	6	G	Sidechain
21	AA	7	A	Sidechain
2	AC	172	VAL	Peptide
6	AG	3	ARG	Sidechain
7	AH	76	ARG	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AF	818	0	808	2	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
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	0	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	16520	2	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	1	0
29	BG	1323	0	1374	0	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	1	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	2	0
39	BQ	947	0	1022	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	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
53	B4	302	0	343	0	0
54	BA	62317	0	31345	1	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	99663	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)
28:BF:151:LEU:H	28:BF:151:LEU:HD13	1.75	0.51
9:AJ:57:VAL:HG23	9:AJ:58:ASN:H	1.77	0.50
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.50
21:AA:565:U:H2'	21:AA:566:G:C8	2.48	0.47
21:AA:940:C:H2'	21:AA:941:G:C8	2.50	0.46

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%)	198 (91%)	16 (7%)	4 (2%)	11	53
2	AC	205/208 (99%)	188 (92%)	8 (4%)	9 (4%)	3	33
3	AD	203/206 (98%)	182 (90%)	18 (9%)	3 (2%)	13	57
4	AE	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	4	35
5	AF	99/101 (98%)	84 (85%)	9 (9%)	6 (6%)	2	26
6	AG	150/152 (99%)	130 (87%)	14 (9%)	6 (4%)	4	35
7	AH	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	24	69
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	12	56
9	AJ	98/100 (98%)	92 (94%)	2 (2%)	4 (4%)	3	35
10	AK	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	21	67
11	AL	121/124 (98%)	107 (88%)	13 (11%)	1 (1%)	24	69
12	AM	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	3	33
13	AN	98/101 (97%)	87 (89%)	10 (10%)	1 (1%)	19	65
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	16	61
15	AP	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	15	60
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	7	46
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	11	53
18	AS	79/81 (98%)	67 (85%)	9 (11%)	3 (4%)	4	37
19	AT	84/86 (98%)	78 (93%)	4 (5%)	2 (2%)	7	47
20	AU	51/53 (96%)	33 (65%)	14 (28%)	4 (8%)	1	20
25	BC	270/273 (99%)	237 (88%)	25 (9%)	8 (3%)	5	42
26	BD	207/209 (99%)	181 (87%)	17 (8%)	9 (4%)	3	34
27	BE	199/201 (99%)	180 (90%)	12 (6%)	7 (4%)	4	39
28	BF	176/179 (98%)	161 (92%)	8 (4%)	7 (4%)	4	35
29	BG	174/177 (98%)	158 (91%)	11 (6%)	5 (3%)	6	43
30	BH	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	9	51
31	BI	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
32	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	38
33	BK	121/123 (98%)	103 (85%)	12 (10%)	6 (5%)	3	31
34	BL	141/144 (98%)	122 (86%)	10 (7%)	9 (6%)	2	25
35	BM	134/136 (98%)	121 (90%)	8 (6%)	5 (4%)	4	38
36	BN	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	6	45
39	BQ	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	7	45
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	9	51
41	BS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	4	38
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	8	49
43	BU	101/104 (97%)	79 (78%)	16 (16%)	6 (6%)	2	27
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	7	45
46	BX	75/79 (95%)	69 (92%)	6 (8%)	0	100	100
47	BY	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	12	56
48	BZ	56/59 (95%)	47 (84%)	4 (7%)	5 (9%)	1	17
49	B0	54/57 (95%)	50 (93%)	2 (4%)	2 (4%)	4	38
50	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	9	51
51	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
52	B3	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	25
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	205 (93%)	15 (7%)	1 (0%)	34	77
All	All	5876/6008 (98%)	5258 (90%)	453 (8%)	165 (3%)	10	44

5 of 165 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	206	ILE
2	AC	4	VAL
3	AD	54	LEU
4	AE	105	ILE
5	AF	59	TYR

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%)	175 (97%)	5 (3%)	51	78
2	AC	170/171 (99%)	166 (98%)	4 (2%)	57	82
3	AD	172/173 (99%)	168 (98%)	4 (2%)	58	83
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	85 (98%)	2 (2%)	58	83
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	102 (98%)	2 (2%)	65	86
8	AI	105/105 (100%)	100 (95%)	5 (5%)	31	67
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	88 (98%)	2 (2%)	60	83
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	82 (99%)	1 (1%)	78	90
14	AO	76/77 (99%)	75 (99%)	1 (1%)	76	89
15	AP	65/65 (100%)	63 (97%)	2 (3%)	47	77
16	AQ	74/74 (100%)	74 (100%)	0	100	100
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%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	212 (98%)	4 (2%)	65	86
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	161 (98%)	4 (2%)	57	82
28	BF	149/150 (99%)	146 (98%)	3 (2%)	63	85
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	107 (98%)	2 (2%)	66	87
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	84	93
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	107 (98%)	2 (2%)	66	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	100 (100%)	0	100	100
37	BO	86/87 (99%)	83 (96%)	3 (4%)	43	74
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	91 (98%)	2 (2%)	60	83
42	BT	80/80 (100%)	79 (99%)	1 (1%)	76	89
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	77 (99%)	1 (1%)	76	89
45	BW	59/59 (100%)	55 (93%)	4 (7%)	20	57
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4763 (98%)	79 (2%)	72	88

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	BC	191	LEU
28	BF	134	GLN
49	B0	2	VAL
26	BD	32	ASN
27	BE	78	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	AF	14	GLN

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Mol	Chain	Res	Type
27	BE	46	GLN
35	BM	97	GLN
37	BO	29	HIS
49	B0	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	229 (14%)	86 (5%)
22	A1	73/76 (96%)	14 (19%)	5 (6%)
23	A2	15/15 (100%)	5 (33%)	4 (26%)
24	A3	76/77 (98%)	17 (22%)	6 (7%)
54	BA	2902/2903 (99%)	457 (15%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	4 (3%)
All	All	4711/4722 (99%)	740 (15%)	222 (4%)

5 of 740 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	27	G
21	AA	28	A
21	AA	32	A
21	AA	35	G

5 of 222 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A3	73	A
54	BA	503	A
54	BA	2564	A
54	BA	91	A
54	BA	228	C

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	15,26,27	1.90	3 (20%)	18,37,40	3.09	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.95	1 (5%)	15,36,39	1.27	1 (6%)
22	7MG	A1	46	22	20,26,27	2.21	3 (15%)	23,39,42	2.11	2 (8%)
22	5MU	A1	54	22	13,22,23	1.04	1 (7%)	16,32,35	4.65	2 (12%)
22	PSU	A1	55	22	15,21,22	1.08	1 (6%)	16,30,33	3.50	4 (25%)
22	4SU	A1	7	22	12,21,22	0.94	0	15,30,33	2.24	2 (13%)
24	H2U	A3	21	24	17,21,22	1.42	2 (11%)	23,30,33	1.32	4 (17%)
24	OMC	A3	33	24	15,22,23	1.03	0	20,31,34	0.87	0
24	5MU	A3	55	24	13,22,23	1.14	1 (7%)	16,32,35	4.44	2 (12%)
24	PSU	A3	56	24	15,21,22	1.19	1 (6%)	16,30,33	3.46	5 (31%)
24	4SU	A3	8	24	12,21,22	1.18	2 (16%)	15,30,33	2.28	1 (6%)

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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.31	1.33	1.45
22	A1	34	CM0	O5-C5	-5.83	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C4-N3	-3.40	1.32	1.37
24	A3	21	H2U	C2-N3	-3.25	1.31	1.38
22	A1	46	7MG	C8-N7	-2.77	1.30	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-12.75	114.64	125.35
24	A3	55	5MU	C5-C4-N3	-12.43	114.92	125.35
24	A3	8	4SU	C5-C4-N3	-8.18	114.89	123.56
22	A1	7	4SU	C5-C4-N3	-7.70	115.39	123.56
22	A1	46	7MG	C5-C6-N1	-6.71	113.39	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	5,6,7	0.63	0	5,7,9	2.08	1 (20%)
58	FME	BA	3001	57	8,9,10	0.72	0	5,9,11	1.24	0

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	-	0/4/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-4.20	114.21	125.69

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.