



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:20 PM BST

PDB ID : 4V70
EMDB ID: : EMD-1718
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate pre-translocation state (pre3)
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 : 17.00 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

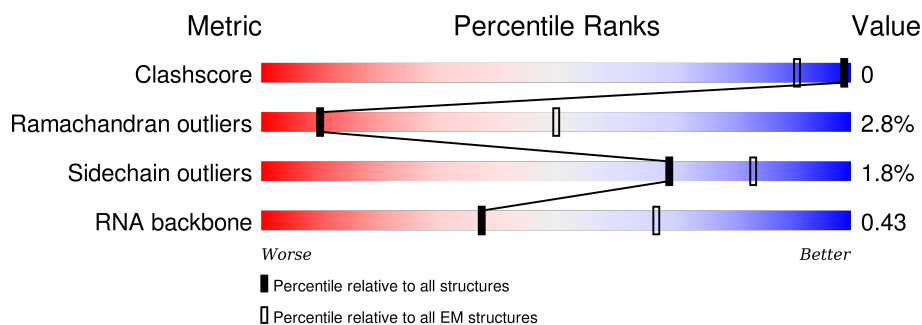
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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.













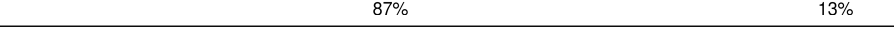
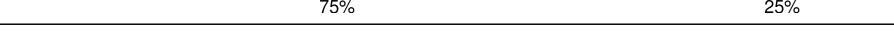
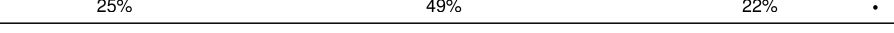


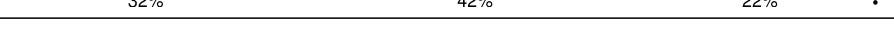









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	93% 7%
2	AC	208	87% 13%
3	AD	206	89% 10%
4	AE	152	94% 6%
5	AF	101	85% 15%
6	AG	152	88% 11% .
7	AH	130	92% 8% .
8	AI	128	85% 13% .













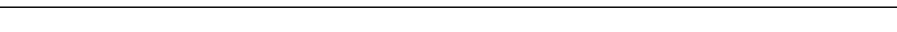



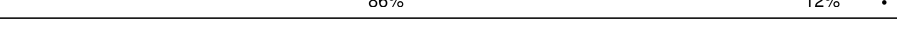




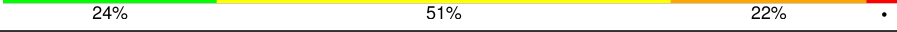
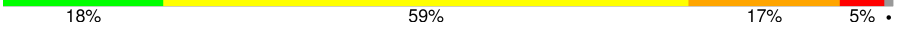
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Mol	Chain	Length	Quality of chain
9	AJ	100	 85% 14% .
10	AK	118	 92% 8%
11	AL	124	 86% 12% ..
12	AM	115	 82% 17% .
13	AN	101	 85% 12% ..
14	AO	89	 89% 10% .
15	AP	81	 89% 10% .
16	AQ	82	 89% 11%
17	AR	57	 89% 11%
18	AS	81	 89% 11%
19	AT	86	 87% 13%
20	AU	53	 75% 25%
21	AA	1533	 25% 49% 22% .
22	A1	76	 33% 47% 16% .
23	A2	15	 27% 33% 27% 13%
24	A3	77	 32% 42% 22% .
25	BC	273	 87% 12%
26	BD	209	 87% 12% .
27	BE	201	 92% 8%
28	BF	179	 89% 11% .
29	BG	177	 93% 6% ..
30	BH	149	 93% 7%
31	BI	142	 94% 6% .
32	BJ	142	 89% 11% .
33	BK	123	 89% 11%

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Mol	Chain	Length	Quality of chain
34	BL	144	 86% 13% .
35	BM	136	 89% 10% .
36	BN	121	 83% 17%
37	BO	117	 87% 12% .
38	BP	115	 86% 12% ..
39	BQ	118	 84% 14% ..
40	BR	103	 91% 9%
41	BS	110	 89% 10% .
42	BT	94	 89% 11%
43	BU	104	 85% 13% ...
44	BV	94	 91% 9%
45	BW	80	 83% 16% .
46	BX	79	 77% 13% 8% .
47	BY	63	 92% 5% .
48	BZ	59	 90% 8% .
49	B0	57	 86% 12% .
50	B1	52	 87% 13%
51	B2	46	 74% 26%
52	B3	65	 86% 11% ..
53	B4	38	 89% 11%
54	BA	2903	 24% 51% 22% .
55	BB	118	 18% 59% 17% 5% .
56	B5	234	 88% 7% 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*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		

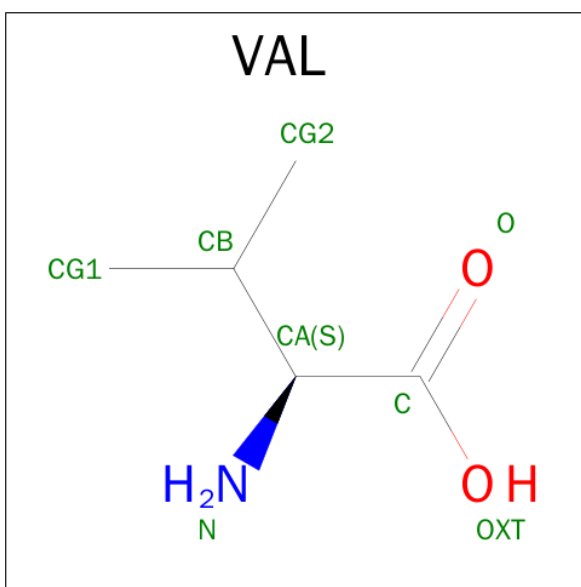
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

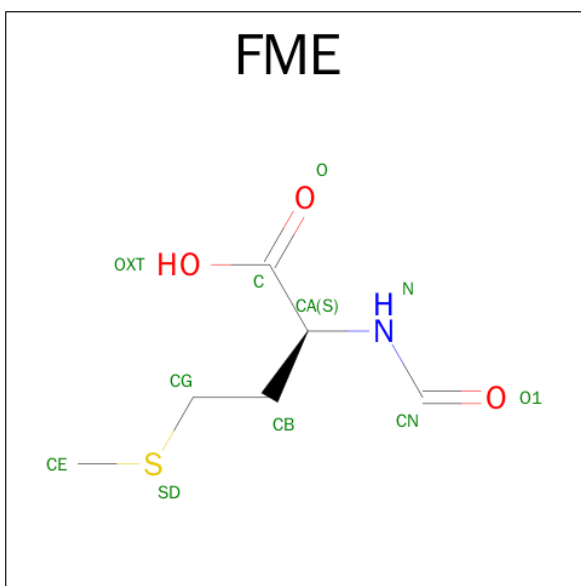
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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: C₆H₁₁NO₃S).

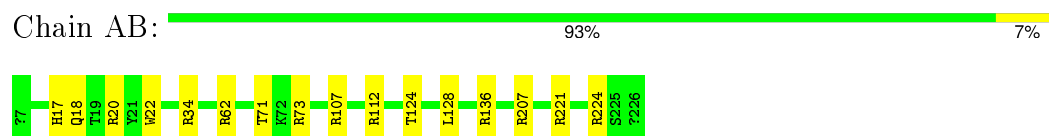


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

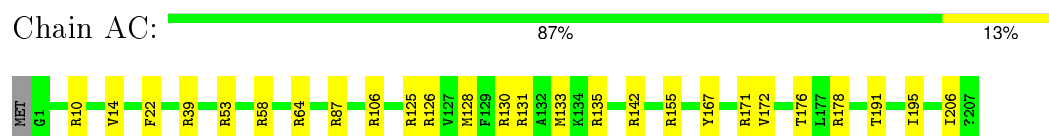
3 Residue-property plots

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.

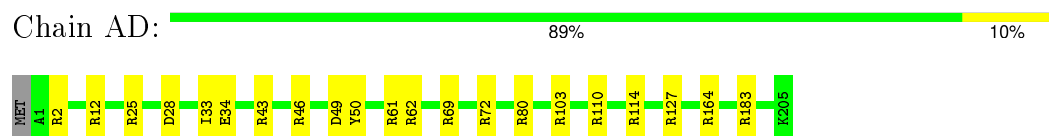
- Molecule 1: 30S ribosomal protein S2



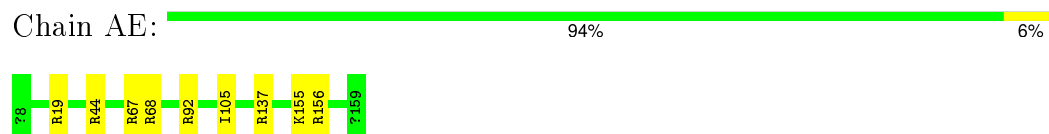
- Molecule 2: 30S ribosomal protein S3



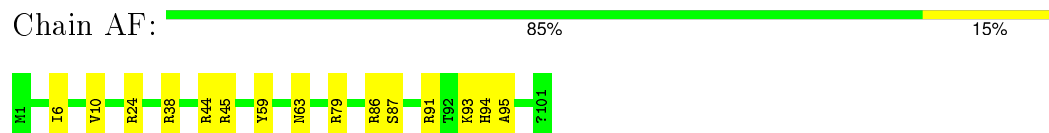
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





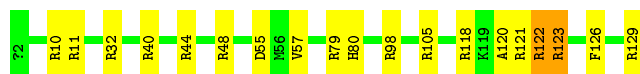
- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 85% 13%



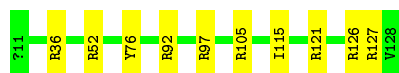
- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 14%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 86% 12%



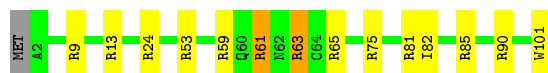
- Molecule 12: 30S ribosomal protein S13

Chain AM: 82% 17%



- Molecule 13: 30S ribosomal protein S14

Chain AN: 85% 12%



- Molecule 14: 30S ribosomal protein S15

Chain AO:  89% 10%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  89% 10%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  89% 11%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 11%




- Molecule 18: 30S ribosomal protein S19

Chain AS:  89% 11%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  87% 13%



- Molecule 20: 30S ribosomal protein S21

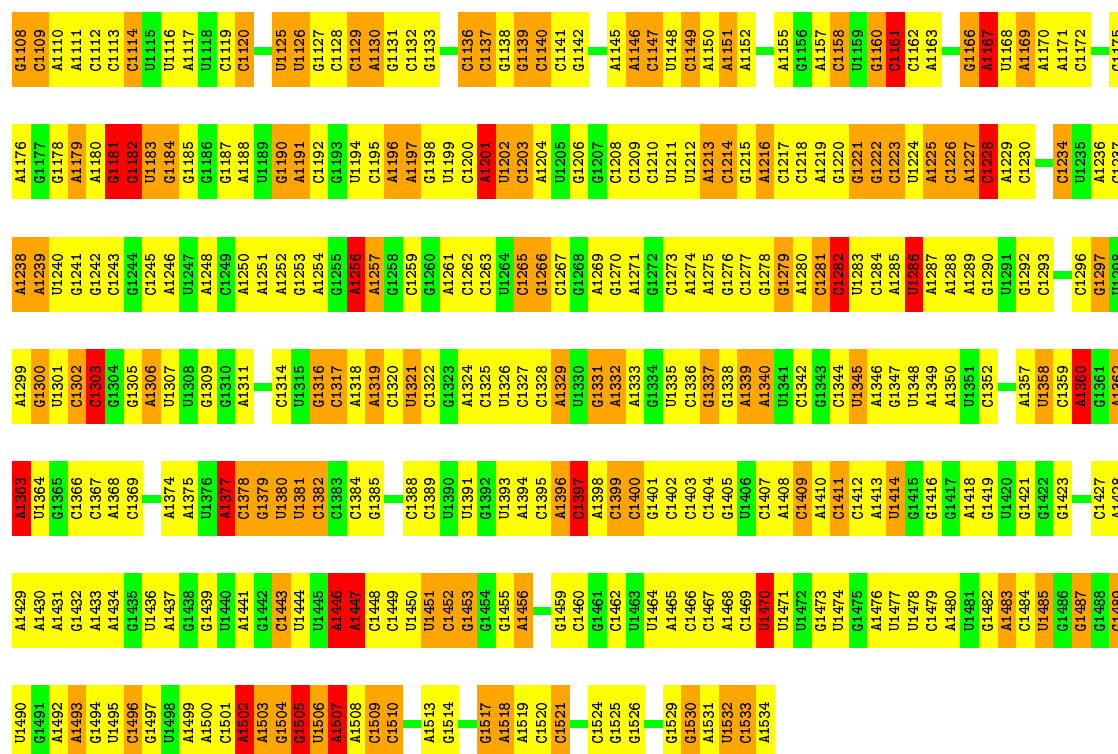
Chain AU:  75% 25%



- Molecule 21: 16S ribosomal RNA

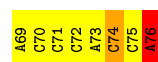
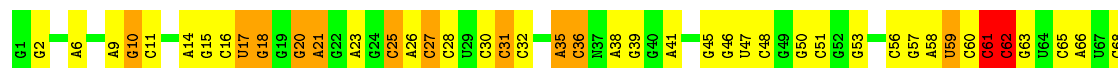
Chain AA:  25% 49% 22%





• 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% 33% 27% 13%

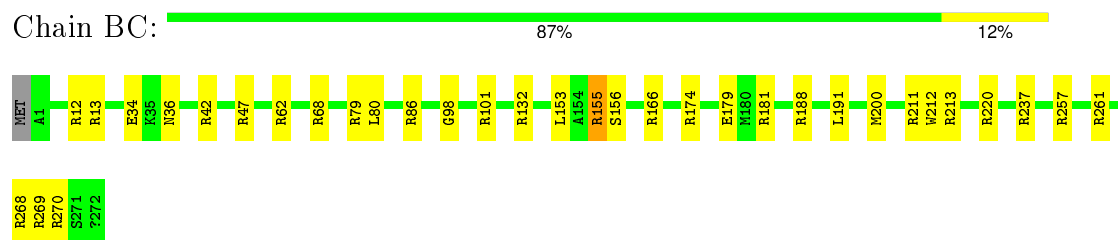


• Molecule 24: tRNA-fMet

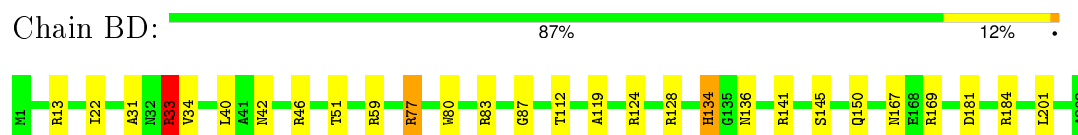
Chain A3: 32% 42% 22%



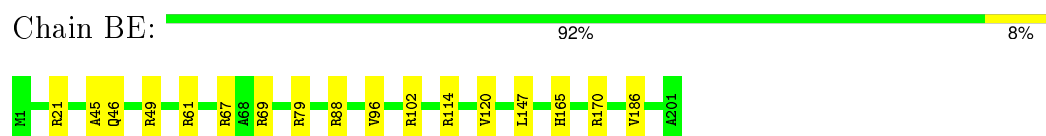
• Molecule 25: 50S ribosomal protein L2



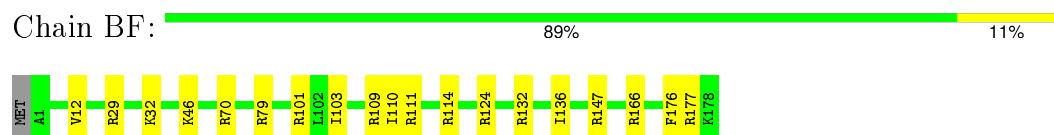
- Molecule 26: 50S ribosomal protein L3



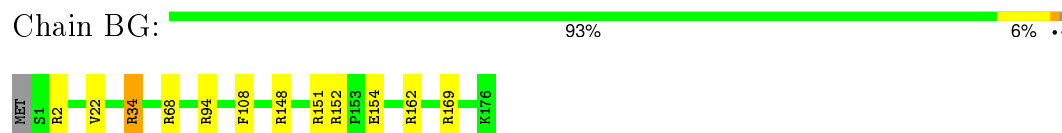
- Molecule 27: 50S ribosomal protein L4



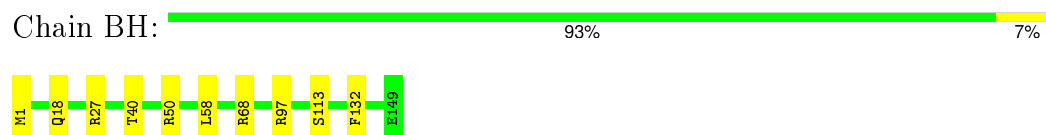
- Molecule 28: 50S ribosomal protein L5



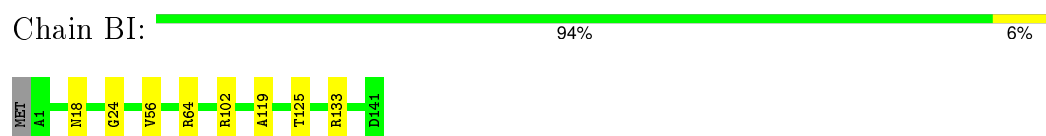
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  89% 11%



- Molecule 33: 50S ribosomal protein L14

Chain BK:  89% 11%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  86% 13%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  89% 10%




- Molecule 36: 50S ribosomal protein L17

Chain BN:  83% 17%




- Molecule 37: 50S ribosomal protein L18

Chain BO:  87% 12%




- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  84% 14%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 91% 9%



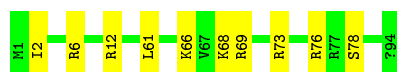
- Molecule 41: 50S ribosomal protein L22

Chain BS: 89% 10%



- Molecule 42: 50S ribosomal protein L23

Chain BT: 89% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 85% 13%



- Molecule 44: 50S ribosomal protein L25

Chain BV: 91% 9%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 83% 16%

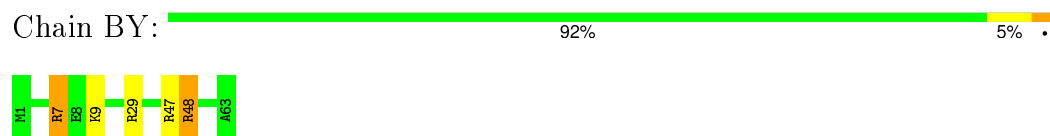


- Molecule 46: 50S ribosomal protein L28

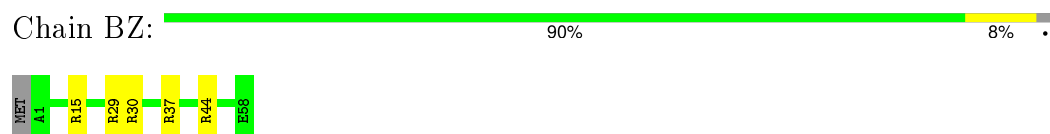
Chain BX: 77% 13% 8%



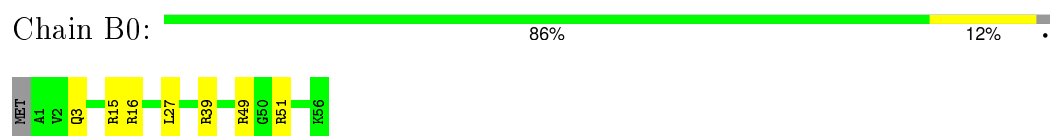
- Molecule 47: 50S ribosomal protein L29



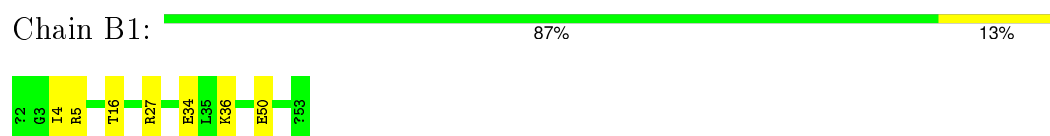
- Molecule 48: 50S ribosomal protein L30



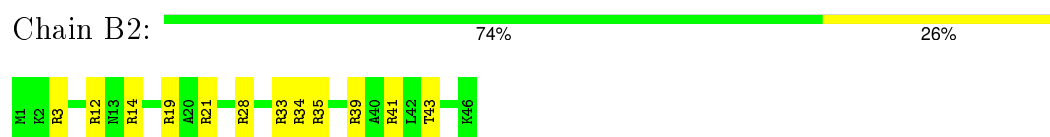
- Molecule 49: 50S ribosomal protein L32



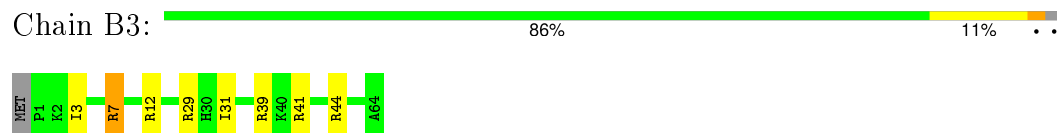
- Molecule 50: 50S ribosomal protein L33



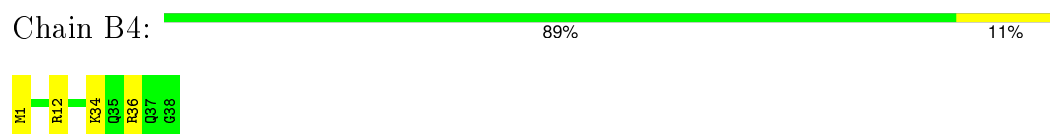
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36

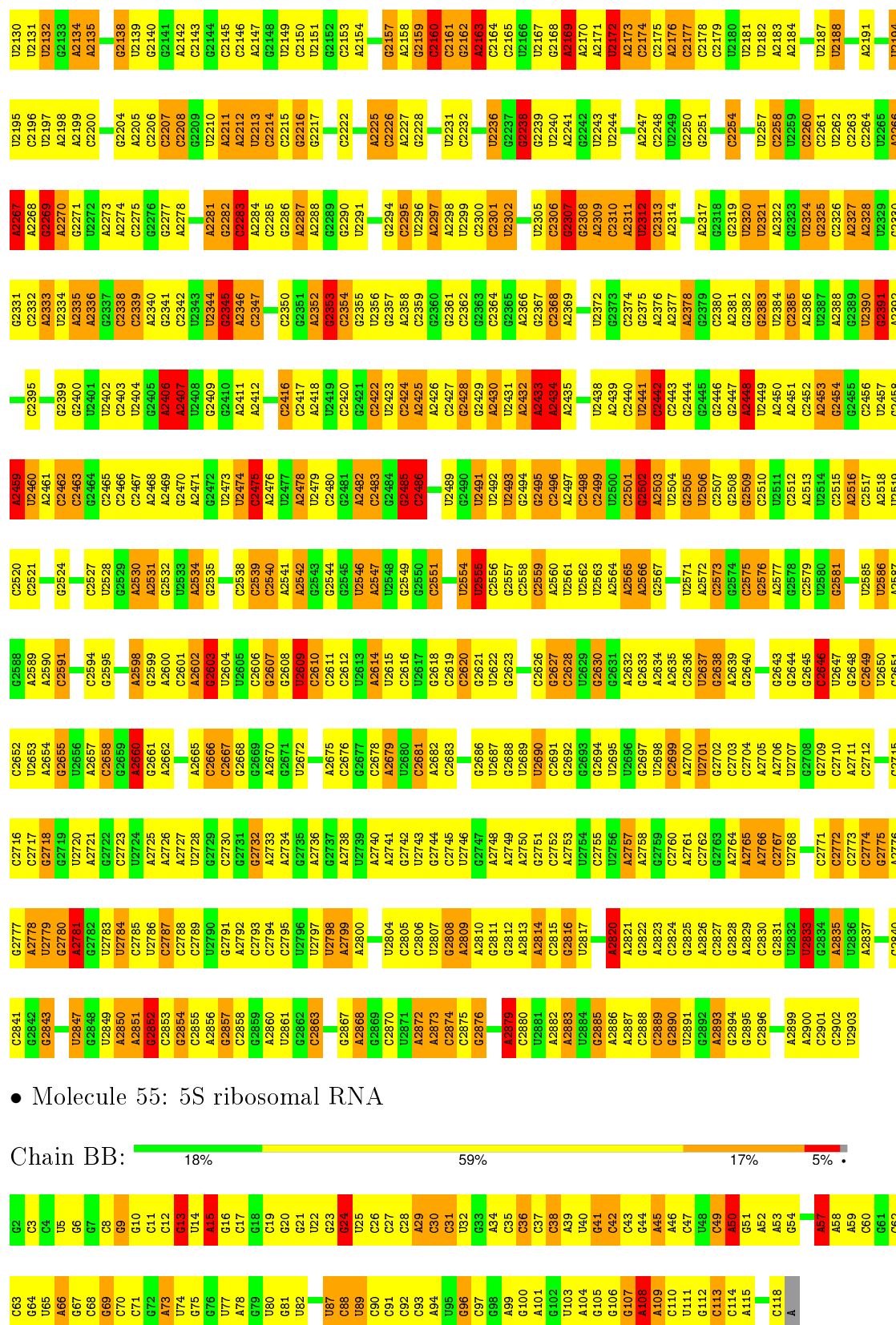


- Molecule 54: 23S ribosomal RNA





C2063	C1999	A1936	C1874	A1810	C1748	C1685	G1623	U1562	A1495	A1427	G1358	C1295	U1231	G1162	A1095
C2064	C2000	A1937	G1875	G1811	A1749	C1686	U1624	U1563	A1496	C1428	G1359	G1296	G1232	G1163	A1096
C2065	C2001	A1938	A1876	G1812	G1750	G1687	C1625	C1564	C1497	G1429	G1360	C1297	C1233	C1164	A1097
C2066	G2002	U1939	A1877	G1813	U1751	U1688	A1626	C1565	C1498	G1430	G1361	C1298	U1234	A1165	A1098
C2067	A2003	G1940	G1878	G1814	C1752	A1689	G1627	A1566	C1499	A1431	C1362	G1299	G1235	C1166	G1099
C2068	G2004	C1941	C1879	A1815	G1753	A1690	G1628	G1567	G1499	G1432	C1363	G1300	G1236	C1167	C1100
G2069	A2005	C1942	U1880	C1816	A1754	C1691	U1629	G1568	A1502	A1433	G1364	A1301	A1237	G1168	U1101
A2070	C2006	U1943	C1881	G1817	A1755		A1630	A1569	A1503	A1434	A1365	A1302	G1238	A1169	C1102
A2071	U2007	U1944	G1818	G1818	G1756	C1694	G1631	A1570	A1504		A1366	G1303	G1239	C1170	C1103
C2072	C2008	G1945	U1883	A1819	A1757	G1695	A1632	A1571	U1505	C1437	A1367	A1304	U1240	G1171	G1107
C2073	A2009	U1946	G1884	G1820	U1758	G1696	G1633	A1572	U1506	U1438		A1305	A1241	C1172	
C2074	G2010	C1947	A1885	A1821	A1759	A1697	A1634	G1573	C1507	A1439	G1370	C1306	U1242	U1173	A1111
U2075	U2011	G1948	U1886	C1822	C1760	A1698	A1635	C1574	A1508	U1440	G1371	A1307	C1243	U1174	
U2076	G2012		C1887	G1825	C1761	G1699	U1636	C1575	A1509	G1441	U1372	A1308	A1244	A1175	A1111
A2077	A2013	U1951	G1888	G1824	A1762	A1700	A1637	U1576	C1512	U1442	A1373	G1309	G1245	U1176	A1112
C2078	A2014	A1952	A1889	U1825	G1763	A1701	C1638	C1577	U1513	G1445	C1376	G1310	A1246	G1177	U1113
U2079	A2015	A1953	G1889	G1826	C1764	G1702	C1639	U1578	G1514	G1446	G1377	U1312	A1247	C1178	C1114
A2080	U2016	G1954	U1827	G1831	U1765	G1703	A1640	A1579	G1514	C1447	U1378	U1313	G1248	G1115	
U2081	U2017	U1955	G1828	G1828	C1774	C1704	A1641	A1580	A1515		U1379	U1314		U1181	G1116
A2082	G2018	U1956	G1829	A1829	C1768	A1705	G1642	G1581	C1518	G1450	U1379	C1314	C1251	G1182	C1117
G2083	C2083	C1957	C1894	C1830	U1769	G1706	G1643	G1582		G1451	U1380	C1315	C1252	G1183	
C2084	A2020	C1958	G1831	G1831	G1770	G1707	C1644	A1583	G1521	C1452	G1381	U1316	A1253	G1185	U1119
U2085	C2021	G1959	G1832	C1832	C1771	G1708	G1645	U1584	G1521	G1453	G1382	G1317	A1254	G1186	G1120
C2086	U2022	A1960	G1833	C1833	A1772	U1709	C1646	C1585	A1522	A1454	A1383	U1318	U1255	G1187	C1121
G2087	C2023	C1961	U1834	U1834	A1773	G1710	U1647	A1586		C1455	A1384	C1319	G1256	U1188	G1122
A2088	G2024	C1962	G1835	G1835	C1774	U1711	U1648	G1587	A1525	G1455	A1385	C1320	C1257	A1189	C1123
C2089	C2025	U1963	C1836	C1836	U1775	U1712	G1649	G1588			C1386	A1321	U1258		
A2090	A2030	G1964	C1837	C1837	U1776	A1713	A1650	U1589	G1527	U1458	U1387	U1322	G1259	A1194	A1126
C2091	G2032	C1965	U1838	G1838	G1776	G1714	G1651	A1590	A1528	G1459	G1388	C1323	A1260	G1195	A1127
G2093	A2031	A1966	G1839	G1839	U1779	G1715	A1652	A1591		U1460	G1389	G1324	C1261	C1196	G1128
A2094	C2033	C1967	G1840	G1840	U1780	U1716	G1653	C1592	G1531	C1461	U1390	U1325	A1262	U1129	A1129
U2095	U2034	G1968	U1841	U1841	U1781	A1717	A1654	A1593	A1532	C1462	U1391	U1326	U1263	U1130	U1130
C2096	C2035	A1970	G1842	G1842	U1782	U1720	A1655	U1594	C1533	C1463	A1392	A1327	A1264	U1201	G1131
A2097	G2036	U1971	C1843	C1843	A1783	G1721	C1656	C1595	U1534	G1464	U1393	A1328	A1265	G1202	U1132
	A2037	G1972	G1845	G1845	A1785	A1722	U1657	A1596	A1535	G1465	U1394	U1329	G1266	U1203	A1133
	G2038	G1973	G1846	G1846	A1786	U1725	G1658	A1597	C1536	U1466	A1395	C1330	U1267	A1204	A1134
	U2039		A1847	A1847	A1787	C1726	G1659	A1598	G1537		U1396	G1331	A1268	A1205	G1135
C2103	G2040	A1976	C1726	A1848	A1788	C1727	G1660	U1599	G1538	A1469	U1397		A1269	G1206	
C2104	U2041	A1977	C1727		A1789	G1728	A1664	C1600	U1539	G1470	C1398	C1335	C1270	G1207	G1139
U2105	A2042	A1978	C1790	U1851	C1788	G1729	A1665	U1602	G1540	C1471	C1399	A1336	G1271	C1208	C1140
C2043	C2043		A1791	U1852	A1790	U1729	G1666	A1603	C1541	C1472	U1400		U1272	U1209	U1141
C2044	G2045	A1981	G1792	A1853	G1791	G1730	G1667	C1604	U1542		G1401	G1339	U1273	G1210	A1142
C2045	C2046	U1982	C1793	A1854	C1793	G1731	A1668	C1605	G1543	G1475	U1402	U1340	A1274	G1211	A1143
U2111	C2047	G1983	A1794	U1855	A1794	C1732	A1669	C1606	A1544	U1476	A1403	A1341	A1275	G1212	A1144
		G1984	C1795		C1795	G1733	A1670	U1607	A1545	A1477	C1404	A1342	G1276	A1213	C1145
C2050	C2050	C1985	U1796	A1858	U1796	G1734	C1671	A1608	G1546		U1405	G1343	C1277	A1214	C1146
A2051	A2051	C1986	G1797	U1859	A1735	G1734	A1672	C1607	C1547	C1480		U1344	C1278	A1147	A1147
A2052	A2052	A1987	U1798	G1860	U1736	U1736	A1673	A1609	A1548	U1481	U1412	C1345	G1218	G1148	U1148
G2053	G2053	G1988	G1799	G1861	G1799	G1738	G1674	C1611	C1550	G1482	C1414	A1347	A1284	U1219	C1150
A2054	A2054	C1989	C1800		C1800	U1738	C1675	C1612	A1551	U1485	U1415	C1348	A1285	G1220	A1151
C2055	C2055	U1990	A1801	U1865	A1801	A1739	A1676	G1613	A1552	U1486	G1416	C1349	A1286	C1221	C1152
C2056	G2056	U1991	A1802	A1866	A1802	G1740	A1677	A1614	A1553	U1487	C1417	C1350	A1287	U1222	C1153
G2057	G2057	G1992	G1803	G1867	A1803	C1741	A1678	C1615		C1488	G1418	C1351	G1288	G1223	G1154
U2058	U2058	C1993	C1804	G1869	A1804	U1742	A1679	A1616	C1489	A1419	C1419	U1352	C1289	U1224	A1155
A2059	A2059	U1994	A1805	G1869	A1805	G1743	U1680	C1617	C1556	A1490	A1420	A1353	G1290	G1225	A1156
A2060	A2060	G1995	C1806	C1870	C1806	A1744	G1681	A1618		G1491		A1354	C1291	A1226	G1157
G2127	G2127	C1996	G1807	A1871	G1807	U1745	G1682	U1621	C1557	G1492	G1424	G1355	G1292	C1229	C1158
C2129	C2129	A1998	A1808	U1872	A1808	A1746	U1683	G1622	U1559	C1493	G1425	C1357		A1230	



Response	Percentage
Yes, the U.S. is a democracy	88%
No, the U.S. is not a democracy	7%
Don't know	5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	2648	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	0.74	0/1736	1.04	11/2340 (0.5%)
10	AK	0.77	0/894	1.18	9/1207 (0.7%)
11	AL	0.78	0/969	1.23	14/1300 (1.1%)
12	AM	0.77	0/884	1.30	16/1181 (1.4%)
13	AN	0.80	0/817	1.35	12/1088 (1.1%)
14	AO	0.74	0/722	1.20	9/964 (0.9%)
15	AP	0.80	0/648	1.15	5/870 (0.6%)
16	AQ	0.72	0/658	1.10	7/883 (0.8%)
17	AR	0.82	0/463	1.18	5/623 (0.8%)
18	AS	0.78	0/653	1.12	6/879 (0.7%)
19	AT	0.71	0/672	1.18	8/890 (0.9%)
2	AC	0.75	0/1651	1.19	17/2225 (0.8%)
20	AU	0.86	0/431	1.59	9/572 (1.6%)
21	AA	1.52	0/36759	2.22	1943/57346 (3.4%)
22	A1	1.54	0/1668	2.18	94/2595 (3.6%)
23	A2	1.50	0/343	2.20	15/531 (2.8%)
24	A3	1.51	0/1722	2.19	80/2685 (3.0%)
25	BC	0.76	0/2121	1.28	25/2852 (0.9%)
26	BD	0.71	0/1586	1.19	12/2134 (0.6%)
27	BE	0.70	0/1571	1.14	9/2113 (0.4%)
28	BF	0.77	0/1444	1.16	12/1937 (0.6%)
29	BG	0.72	0/1343	1.14	9/1816 (0.5%)
3	AD	0.80	0/1665	1.19	16/2227 (0.7%)
30	BH	0.70	0/1122	1.11	5/1515 (0.3%)
31	BI	0.69	0/1046	1.08	4/1410 (0.3%)
32	BJ	0.76	0/1152	1.12	6/1551 (0.4%)
33	BK	0.73	0/947	1.20	10/1268 (0.8%)
34	BL	0.75	0/1054	1.29	14/1403 (1.0%)
35	BM	0.78	0/1093	1.23	12/1460 (0.8%)
36	BN	0.79	0/973	1.35	16/1301 (1.2%)
37	BO	0.76	0/902	1.29	15/1209 (1.2%)
38	BP	0.76	0/929	1.27	9/1242 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.80	0/960	1.30	15/1278 (1.2%)
4	AE	0.73	0/1119	1.04	7/1506 (0.5%)
40	BR	0.75	0/829	1.12	6/1107 (0.5%)
41	BS	0.68	0/864	1.19	11/1156 (1.0%)
42	BT	0.68	0/744	1.17	5/994 (0.5%)
43	BU	0.73	0/787	1.15	7/1051 (0.7%)
44	BV	0.74	0/766	1.17	6/1025 (0.6%)
45	BW	0.78	0/604	1.34	10/799 (1.3%)
46	BX	0.78	0/635	1.35	10/848 (1.2%)
47	BY	0.71	0/510	1.22	5/677 (0.7%)
48	BZ	0.72	0/453	1.27	5/605 (0.8%)
49	B0	0.74	0/450	1.22	5/599 (0.8%)
5	AF	0.76	0/835	1.17	8/1128 (0.7%)
50	B1	0.76	0/417	1.09	2/556 (0.4%)
51	B2	0.82	0/380	1.56	13/498 (2.6%)
52	B3	0.75	0/513	1.26	8/676 (1.2%)
53	B4	0.68	0/303	1.13	2/397 (0.5%)
54	BA	1.40	1/69796 (0.0%)	2.21	4048/108888 (3.7%)
55	BB	1.41	0/2800	2.18	153/4367 (3.5%)
56	B5	0.68	0/1673	1.13	11/2255 (0.5%)
6	AG	0.77	0/1188	1.19	13/1593 (0.8%)
7	AH	0.71	0/989	1.03	8/1326 (0.6%)
8	AI	0.83	0/1035	1.33	19/1377 (1.4%)
9	AJ	0.75	0/797	1.24	12/1079 (1.1%)
All	All	1.28	1/160085 (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
10	AK	0	1
2	AC	0	1
21	AA	0	365
22	A1	0	13
23	A2	0	5
24	A3	0	17
25	BC	0	1
43	BU	0	1
54	BA	0	636
55	BB	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	AI	0	1
9	AJ	0	1
All	All	0	1062

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	945	A	N3-C4	5.58	1.38	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	330	A	O4'-C1'-N9	12.97	118.58	108.20
54	BA	2270	A	N1-C6-N6	-12.77	110.94	118.60
54	BA	900	A	N1-C6-N6	-12.68	110.99	118.60
54	BA	1069	A	N1-C6-N6	-12.45	111.13	118.60
54	BA	1616	A	N1-C6-N6	-12.33	111.20	118.60

There are no chirality outliers.

5 of 1062 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	5	U	Sidechain
2	AC	172	VAL	Peptide
8	AI	123	ARG	Peptide
9	AJ	37	ARG	Sidechain
10	AK	115	ILE	Peptide

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	1	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	1	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	16522	0	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	1	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	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	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	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	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	1	0
54	BA	62317	0	31345	6	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99665	12	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 12 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)
35:BM:126:ILE:H	35:BM:126:ILE:HD13	1.74	0.53
54:BA:2105:U:HO2'	56:B5:2:ALA:N	2.13	0.46
54:BA:2352:A:C5	54:BA:2353:G:H1'	2.53	0.43
24:A3:24:C:H2'	24:A3:25:U:C6	2.53	0.43
54:BA:480:A:H3'	54:BA:481:G:C5'	2.48	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%)	198 (91%)	17 (8%)	3 (1%)	14	58
2	AC	205/208 (99%)	185 (90%)	15 (7%)	5 (2%)	7	47
3	AD	203/206 (98%)	189 (93%)	11 (5%)	3 (2%)	13	57
4	AE	150/152 (99%)	137 (91%)	12 (8%)	1 (1%)	26	71
5	AF	99/101 (98%)	83 (84%)	10 (10%)	6 (6%)	2	26
6	AG	150/152 (99%)	134 (89%)	11 (7%)	5 (3%)	5	40
7	AH	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	24	69
8	AI	126/128 (98%)	109 (86%)	12 (10%)	5 (4%)	4	35
9	AJ	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	5	42
10	AK	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
11	AL	121/124 (98%)	107 (88%)	10 (8%)	4 (3%)	5	40
12	AM	112/115 (97%)	98 (88%)	11 (10%)	3 (3%)	6	45
13	AN	98/101 (97%)	84 (86%)	13 (13%)	1 (1%)	19	65
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	16	61
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	2	30
16	AQ	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	15	60
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	15	60
19	AT	84/86 (98%)	78 (93%)	3 (4%)	3 (4%)	4	38
20	AU	51/53 (96%)	40 (78%)	7 (14%)	4 (8%)	1	20
25	BC	270/273 (99%)	242 (90%)	25 (9%)	3 (1%)	17	63
26	BD	207/209 (99%)	176 (85%)	16 (8%)	15 (7%)	1	22
27	BE	199/201 (99%)	174 (87%)	17 (8%)	8 (4%)	4	35
28	BF	176/179 (98%)	158 (90%)	11 (6%)	7 (4%)	4	35
29	BG	174/177 (98%)	148 (85%)	24 (14%)	2 (1%)	17	63
30	BH	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
31	BI	139/142 (98%)	121 (87%)	14 (10%)	4 (3%)	6	43
32	BJ	140/142 (99%)	127 (91%)	8 (6%)	5 (4%)	4	38
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	7	46
34	BL	141/144 (98%)	125 (89%)	10 (7%)	6 (4%)	3	34
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	49
36	BN	119/121 (98%)	105 (88%)	10 (8%)	4 (3%)	5	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	105 (92%)	8 (7%)	1 (1%)	21	67
38	BP	112/115 (97%)	97 (87%)	11 (10%)	4 (4%)	4	38
39	BQ	115/118 (98%)	103 (90%)	8 (7%)	4 (4%)	4	39
40	BR	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	5	42
41	BS	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	10	52
42	BT	92/94 (98%)	81 (88%)	7 (8%)	4 (4%)	3	34
43	BU	101/104 (97%)	87 (86%)	5 (5%)	9 (9%)	1	17
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	17	63
45	BW	78/80 (98%)	58 (74%)	17 (22%)	3 (4%)	4	37
46	BX	75/79 (95%)	62 (83%)	8 (11%)	5 (7%)	1	24
47	BY	61/63 (97%)	55 (90%)	3 (5%)	3 (5%)	3	31
48	BZ	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	10	52
50	B1	50/52 (96%)	46 (92%)	1 (2%)	3 (6%)	2	26
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	B3	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	5	41
53	B4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
56	B5	221/234 (94%)	206 (93%)	12 (5%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5263 (90%)	450 (8%)	163 (3%)	10	44

5 of 163 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	206	ILE
6	AG	11	ILE
9	AJ	75	ASP
11	AL	43	LYS

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%)	176 (98%)	4 (2%)	60	83
2	AC	170/171 (99%)	167 (98%)	3 (2%)	66	87
3	AD	172/173 (99%)	169 (98%)	3 (2%)	68	87
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	86	94
7	AH	104/105 (99%)	102 (98%)	2 (2%)	65	86
8	AI	105/105 (100%)	104 (99%)	1 (1%)	82	92
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%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	80 (96%)	3 (4%)	42	74
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	37	71
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	67 (96%)	3 (4%)	35	70
19	AT	65/65 (100%)	63 (97%)	2 (3%)	47	77
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	208 (96%)	8 (4%)	41	73
26	BD	164/164 (100%)	159 (97%)	5 (3%)	48	77
27	BE	165/165 (100%)	165 (100%)	0	100	100
28	BF	149/150 (99%)	149 (100%)	0	100	100
29	BG	137/138 (99%)	135 (98%)	2 (2%)	72	88
30	BH	114/114 (100%)	108 (95%)	6 (5%)	28	64
31	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
32	BJ	116/116 (100%)	110 (95%)	6 (5%)	29	65
33	BK	103/103 (100%)	103 (100%)	0	100	100
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%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	96 (97%)	3 (3%)	48	77
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	79 (99%)	1 (1%)	76	89
43	BU	83/84 (99%)	80 (96%)	3 (4%)	42	74
44	BV	78/78 (100%)	77 (99%)	1 (1%)	76	89
45	BW	59/59 (100%)	56 (95%)	3 (5%)	29	66
46	BX	67/68 (98%)	60 (90%)	7 (10%)	9	36
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%)	43 (96%)	2 (4%)	35	69
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%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4755 (98%)	87 (2%)	69	87

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	BD	134	HIS
30	BH	113	SER
49	B0	3	GLN
26	BD	136	ASN
30	BH	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	AF	58	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	271 (17%)	84 (5%)
22	A1	73/76 (96%)	11 (15%)	3 (4%)
23	A2	14/15 (93%)	6 (42%)	2 (14%)
24	A3	77/77 (100%)	13 (16%)	1 (1%)
54	BA	2902/2903 (99%)	460 (15%)	131 (4%)
55	BB	116/118 (98%)	21 (18%)	4 (3%)
All	All	4711/4722 (99%)	782 (16%)	225 (4%)

5 of 782 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	17	U

5 of 225 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	244	A
54	BA	750	A
54	BA	2459	A
54	BA	330	A
54	BA	506	G

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	1.79	3 (20%)	18,37,40	3.19	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	6MZ	A1	37	22	17,25,26	0.91	0	15,36,39	1.24	1 (6%)
22	7MG	A1	46	22	20,26,27	2.19	4 (20%)	23,39,42	2.11	2 (8%)
22	5MU	A1	54	22	13,22,23	1.17	1 (7%)	16,32,35	4.65	2 (12%)
22	PSU	A1	55	22	15,21,22	1.23	2 (13%)	16,30,33	3.31	3 (18%)
22	4SU	A1	7	22	12,21,22	1.00	1 (8%)	15,30,33	2.26	2 (13%)
24	H2U	A3	21	24	17,21,22	1.40	2 (11%)	23,30,33	1.27	3 (13%)
24	OMC	A3	33	24	15,22,23	1.10	0	20,31,34	0.87	1 (5%)
24	5MU	A3	55	24	13,22,23	1.00	1 (7%)	16,32,35	4.41	2 (12%)
24	PSU	A3	56	24	15,21,22	1.16	1 (6%)	16,30,33	3.55	5 (31%)
24	4SU	A3	8	24	12,21,22	1.08	1 (8%)	15,30,33	2.17	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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.02	1.33	1.45
22	A1	34	CM0	O5-C5	-5.39	1.26	1.37
24	A3	21	H2U	C4-N3	-3.39	1.32	1.37
24	A3	21	H2U	C2-N3	-3.31	1.31	1.38
22	A1	46	7MG	C8-N7	-2.75	1.30	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
22	A1	54	5MU	C5-C4-N3	-12.87	114.55	125.35
24	A3	55	5MU	C5-C4-N3	-12.27	115.05	125.35
24	A3	8	4SU	C5-C4-N3	-8.09	114.98	123.56
22	A1	7	4SU	C5-C4-N3	-7.58	115.52	123.56
22	A1	46	7MG	C5-C6-N1	-6.80	113.27	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 [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	5,6,7	0.61	0	5,7,9	1.59	1 (20%)
58	FME	BA	3001	57	8,9,10	0.73	0	5,9,11	1.20	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($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-3.14	117.12	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.