



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:21 PM BST

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

This is a wwPDB 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

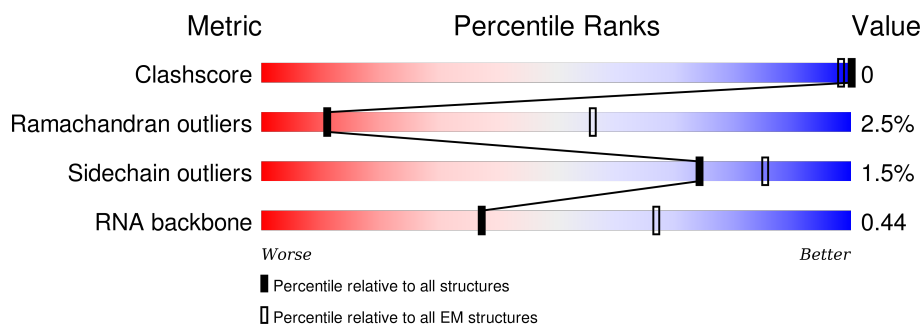
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.












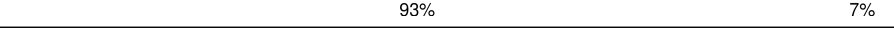

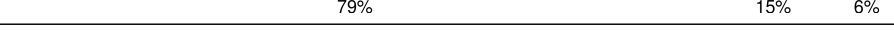
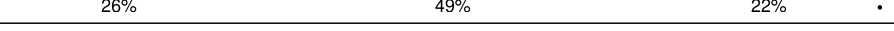


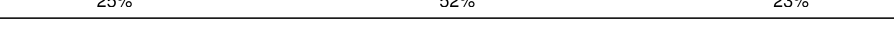



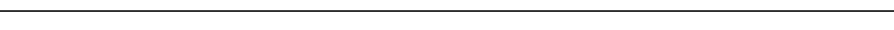

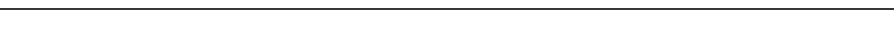
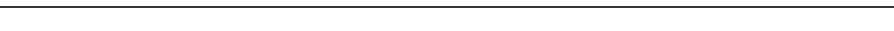


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	97% .
2	AC	208	91% 8%
3	AD	206	89% 11%
4	AE	152	89% 11%
5	AF	101	87% 13%
6	AG	152	88% 11% .
7	AH	130	94% 5% .
8	AI	128	85% 15%

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

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

2 Entry composition

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

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

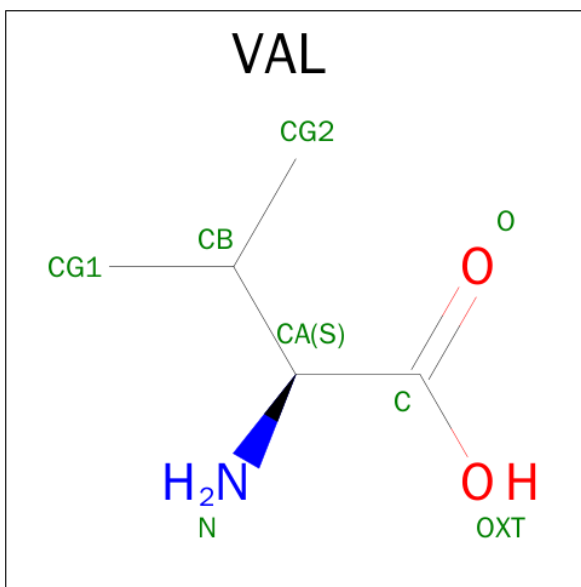
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

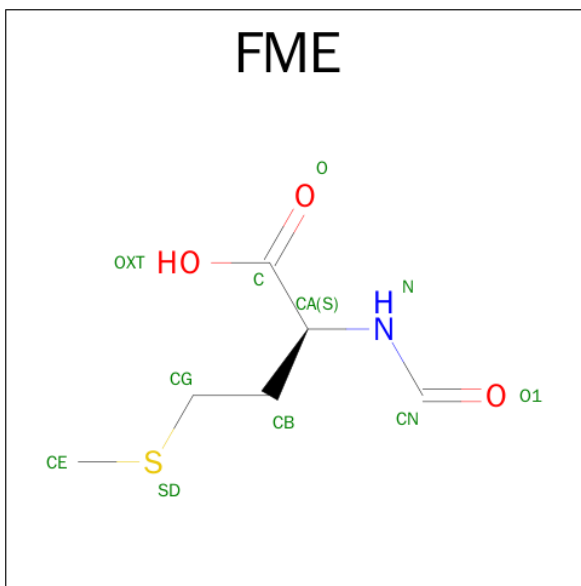
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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

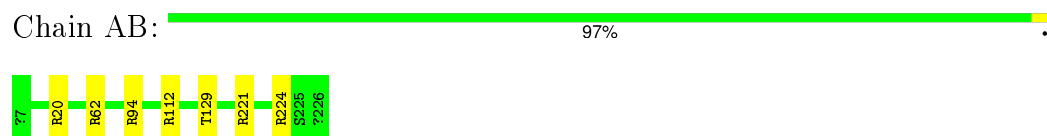


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

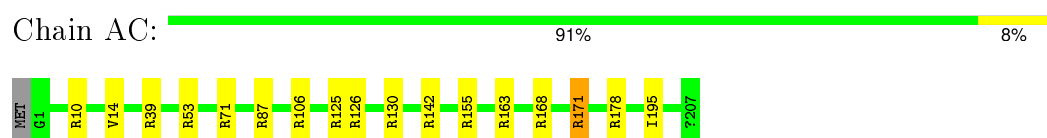
3 Residue-property plots [i](#)

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

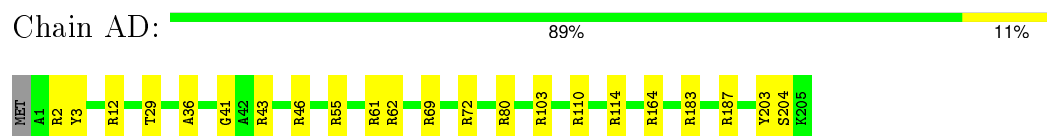
- Molecule 1: 30S ribosomal protein S2



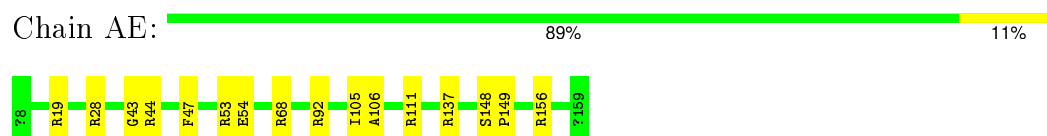
- Molecule 2: 30S ribosomal protein S3



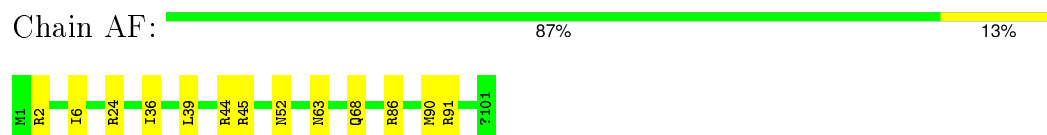
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 94% 5%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 85% 15%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 87% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 91% 9%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 89% 10%



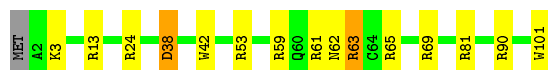
- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 84% 13%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  85% 13%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  86% 14%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  89% 9%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 11%



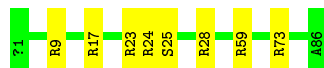
- Molecule 18: 30S ribosomal protein S19

Chain AS:  93% 7%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  91% 9%



- Molecule 20: 30S ribosomal protein S21

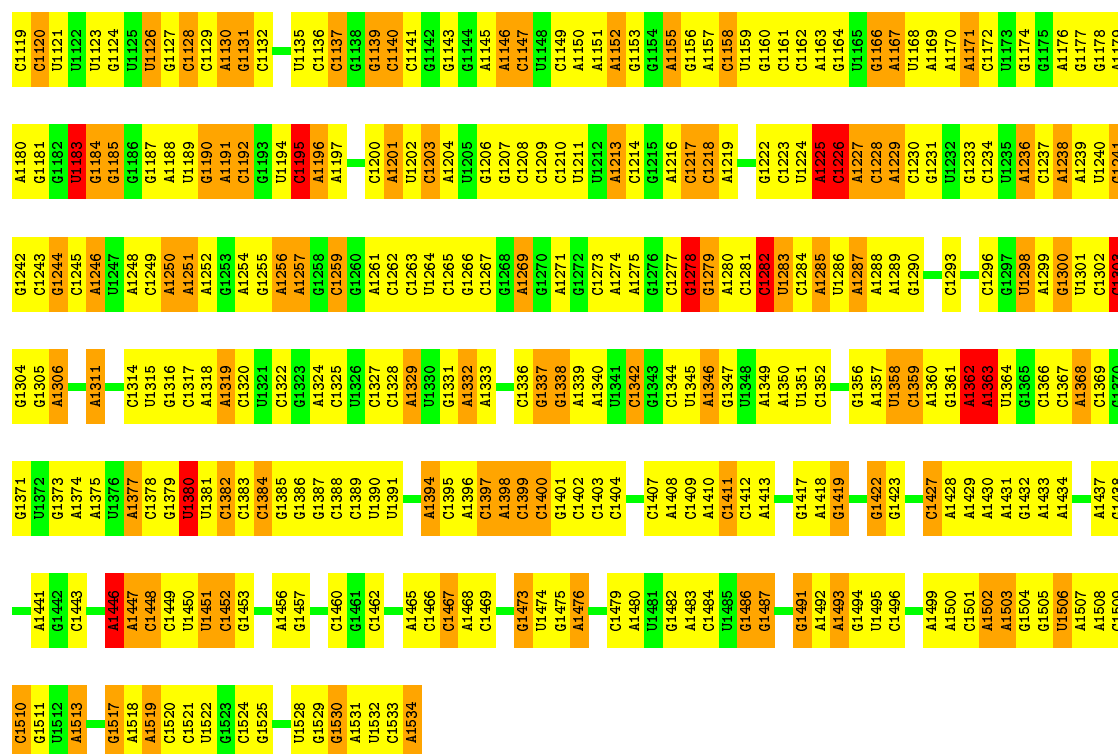
Chain AU:  79% 15% 6%



- Molecule 21: 16S ribosomal RNA

Chain AA:  26% 49% 22%

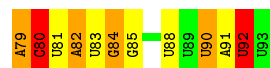
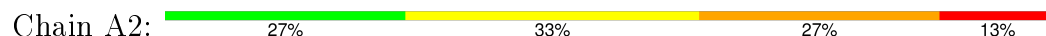
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U1052	C985	C857	G724	U853	C586	C522	A460	U398	U333	A270	A205	G68	A
G1063	C986	C858	G725	G854	C589	G523	A461	G399	C334	C271	C206	G69	U
C1054	C987	C859	G726	A855	U589	A824	G462	C400	C335	C272	C207	U70	G6
A1055	C990	A860	G727	G856	C525	C526	U463	C401	A336	A273	U208	A71	A7
U1056	C991	G861	A728	U857	G592	G527	U464	G402	G337	A274	U209	A72	A8
C1059	U991	C862	A729	C858	U593	G527	A465	C403	A338	C275	C210	C73	A9
U1062	U992	U863	G730	U859	U594	C528	A466	C404	C339	C276	G211	A74	G9
C1063	C993	U864	G731	C860	A595	G529	U467	U405	U340	C277	G212	G75	A10
G1064	A996	A865	G732	G861	A596	C532	A468	G406	C341	G278	U150	G76	U13
U1065	U997	G866	G736	G864	C599	U534	C470	U407	C342	A279	C214	A77	U14
C1066	C998	C867	C737	A865	G601	A535	U471	A408	U343	C280	C215	A78	U15
A1067	C999	G868	C737	G866	A602	C536	G474	A411	C344	G281	U151	G79	G15
G1068	A1000	G869	G738	G866	A602	C537	G475	A412	G346	U283	U152	A80	A16
C1069	C1001	A872	C739	G867	A602	G538	U476	G413	G347	C284	U153	A81	U17
U1070	A1004	A873	U740	G868	U605	G539	C477	A414	G348	C285	U154	A82	U18
C1071	A1005	G874	G741	U872	G606	G540	A478	G415	A349	C286	G158	U84	U20
G1072	U1005	U875	G742	A873	A607	G541	U479	G416	C350	U287	C222	U85	G21
U1073	C1010	C876	A743	A874	A608	G542	U480	G417	G351	A288	A160	G86	G22
G1077	C1011	C877	C744	G873	A609	G542	U481	C418	C352	G289	U161	C87	C23
U1078	A1012	A878	G745	G874	U610	C545	U482	C419	A353	C290	C162	U88	U24
G1079	G1013	C880	A746	A875	C611	C546	C483	U421	G354	U291	G226	U89	C25
A1080	A1014	C881	A747	A876	C612	A547	C484	G422	C355	G292	G227	C90	A26
U1081	U1015	C882	G748	C879	C613	G548	U485	G423	A356	G293	A228	G91	G27
A1082	G1016	A883	C750	C880	C614	C549	U486	G424	C357	U294	U229	U91	G28
G1083	U1017	C884	U751	A881	C618	C549	A487	G425	U358	C295	G230	C95	G31
U1084	C1018	G885	G752	G888	U619	A553	C488	U426	G361	C296	G168	U96	A32
A1085	A1019	C886	A753	G889	C620	A554	C489	U427	C362	C297	U170	G97	A33
U1086	G1020	U820	C754	C889	A621	U555	C490	U428	A363	G298	A171	A98	A34
G1087	U1021	G821	G755	A622	C622	C556	G491	A430	A364	G300	U173	C99	G35
A1092	A1022	U822	C756	A623	A623	G557	C492	A431	U365	G301	A236	G106	U37
G1093	U1023	C823	U757	A624	C624	C558	A493	A432	A366	G302	C175	G107	G38
A1094	G1024	A896	G758	A625	U625	A559	G494	G433	U367	A303	C176	G108	C40
U1095	U1025	C893	A759	U626	G626	A560	A495	U434	U368	G241	G241	C409	C41
C1096	G1026	A898	C764	G627	G627	U561	A496	A435	G369	C307	G242	G109	G42
G1097	C1027	C897	G765	C628	G628	U562	C497	C436	C370	C308	A243	A109	A44
U1098	U1028	C898	A766	A630	A630	C564	A498	U437	A371	A309	U180	G110	G47
C1099	G1029	C899	A767	C631	C631	U565	A499	U438	C372	A310	U244	G111	G42
G1100	U1030	A900	A768	U632	U632	G566	C501	U440	A373	G311	U245	G112	A44
A1101	C1031	A901	G769	G633	G633	G567	A502	A441	A374	C312	A246	G113	G47
U1102	G1032	G902	C770	G634	G634	G568	C503	G442	C379	C313	G247	U114	C48
C1103	A1035	A906	G773	U636	U636	G570	C504	C443	G380	A314	U248	G115	C49
G1104	U1036	A907	G774	C637	C637	G571	C507	G445	C381	C315	A250	G116	A50
A1105	C1037	A908	G775	U638	U638	A572	U508	G446	A382	G316	G251	A119	A51
G1106	U1038	C910	G776	G639	G639	A573	A509	G447	A383	U252	C188	A120	C52
C1107	G1039	C911	A777	A640	A640	G574	A510	G448	G384	A189	G252	U121	A53
U1108	U1040	U911	G778	U641	U641	G575	C511	G449	C385	A190	G253	G122	C54
C1109	A1041	C912	C779	A642	A642	C576	U512	G450	C386	G191	U256	U123	A55
G1110	G1042	A913	A780	C643	C643	G577	C513	A451	A389	C194	C193	C124	C58
A1111	U1043	G846	A781	U644	U644	C578	C514	A452	U390	A325	A252	A129	A59
C1112	A1044	G847	A782	G646	G646	A579	G515	G453	G391	G326	G263	A130	A60
G1113	U1045	C848	C783	C647	C647	C580	U516	G454	G392	C264	A197	A131	G63
C1114	A1046	G849	A784	A648	A648	G581	G517	G455	A393	C328	G265	C132	C63
A1117	U1049	C852	G786	C649	C649	G582	C518	G456	G394	A329	G266	U133	G64
U1118	G1050	C853	A787	G720	G720	A583	C519	G457	C395	C330	C267	G134	A65
		U920		G722	C651	G584	A520	U458	C396	G331	U268	C135	A66



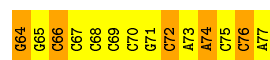
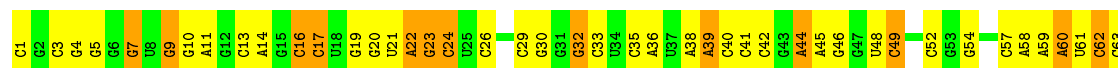
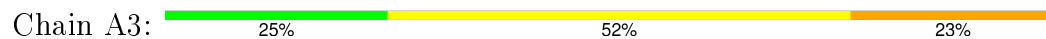
- Molecule 22: fMet-Val-tRNA-Val



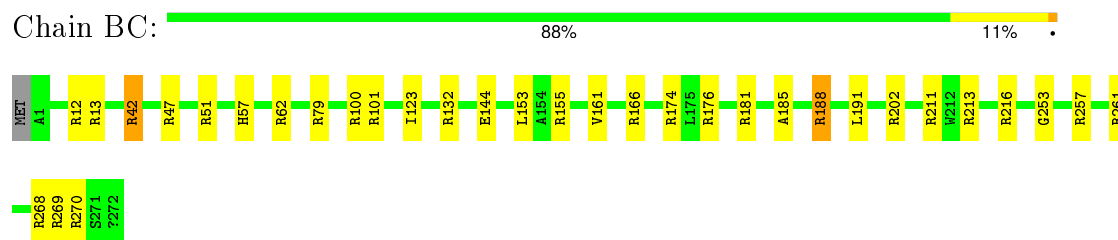
● Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'



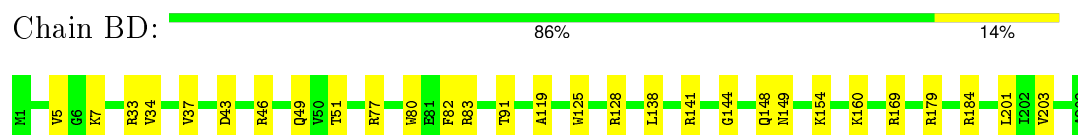
- Molecule 24: tRNA-fMet



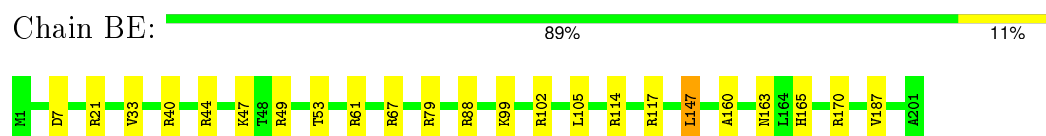
- Molecule 25: 50S ribosomal protein L2



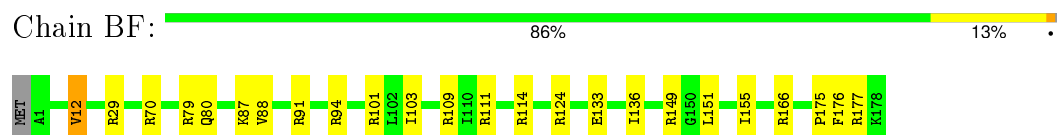
- Molecule 26: 50S ribosomal protein L3



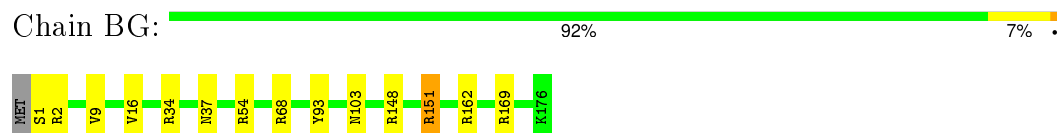
- Molecule 27: 50S ribosomal protein L4



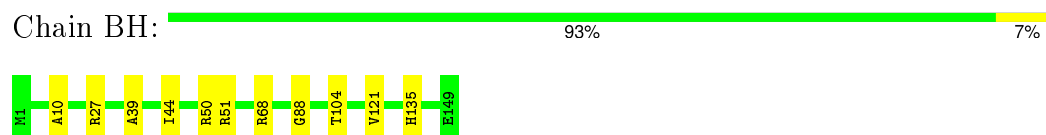
- Molecule 28: 50S ribosomal protein L5



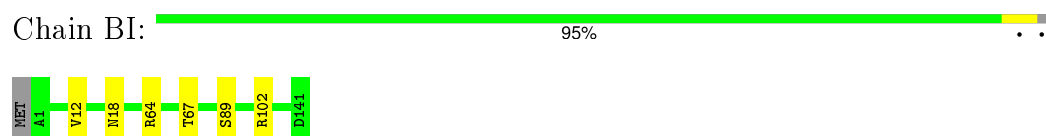
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  92% 8%




- Molecule 33: 50S ribosomal protein L14

Chain BK:  88% 11%



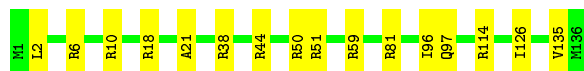
- Molecule 34: 50S ribosomal protein L15

Chain BL:  82% 17%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  88% 12%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  85% 15%




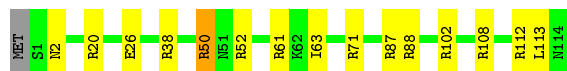
- Molecule 37: 50S ribosomal protein L18

Chain BO:  89% 10%



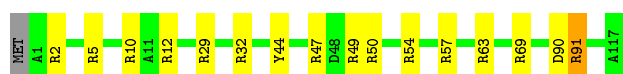
- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  86% 13%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 90% 10%



- Molecule 41: 50S ribosomal protein L22

Chain BS: 93% 7%



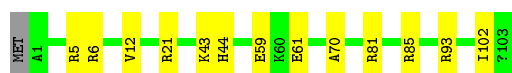
- Molecule 42: 50S ribosomal protein L23

Chain BT: 90% 10%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 87% 13%



- Molecule 44: 50S ribosomal protein L25

Chain BV: 90% 10%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 11%

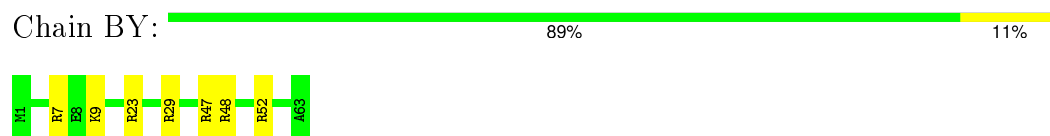


- Molecule 46: 50S ribosomal protein L28

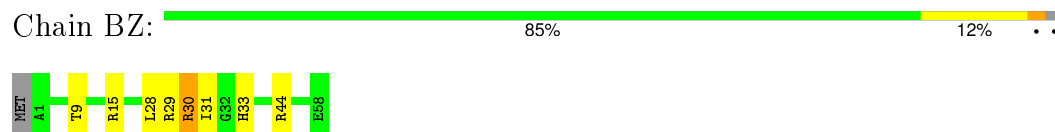
Chain BX: 82% 14%



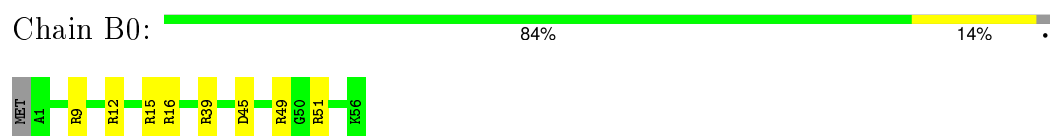
- Molecule 47: 50S ribosomal protein L29



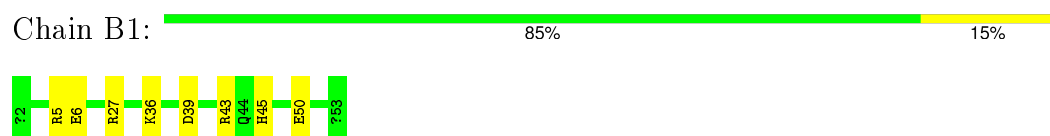
- Molecule 48: 50S ribosomal protein L30



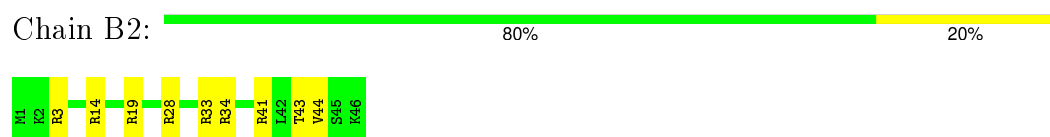
- Molecule 49: 50S ribosomal protein L32



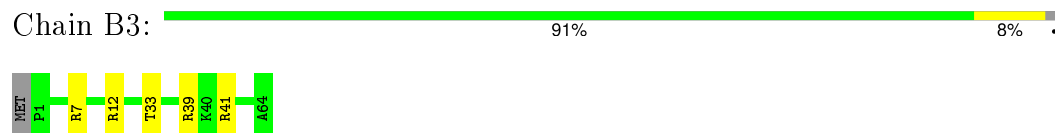
- Molecule 50: 50S ribosomal protein L33



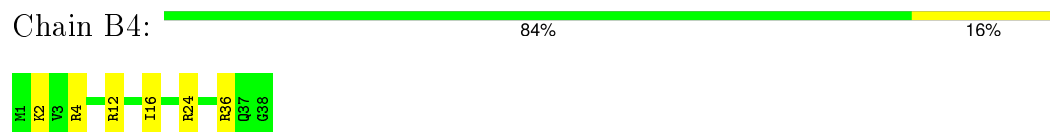
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36

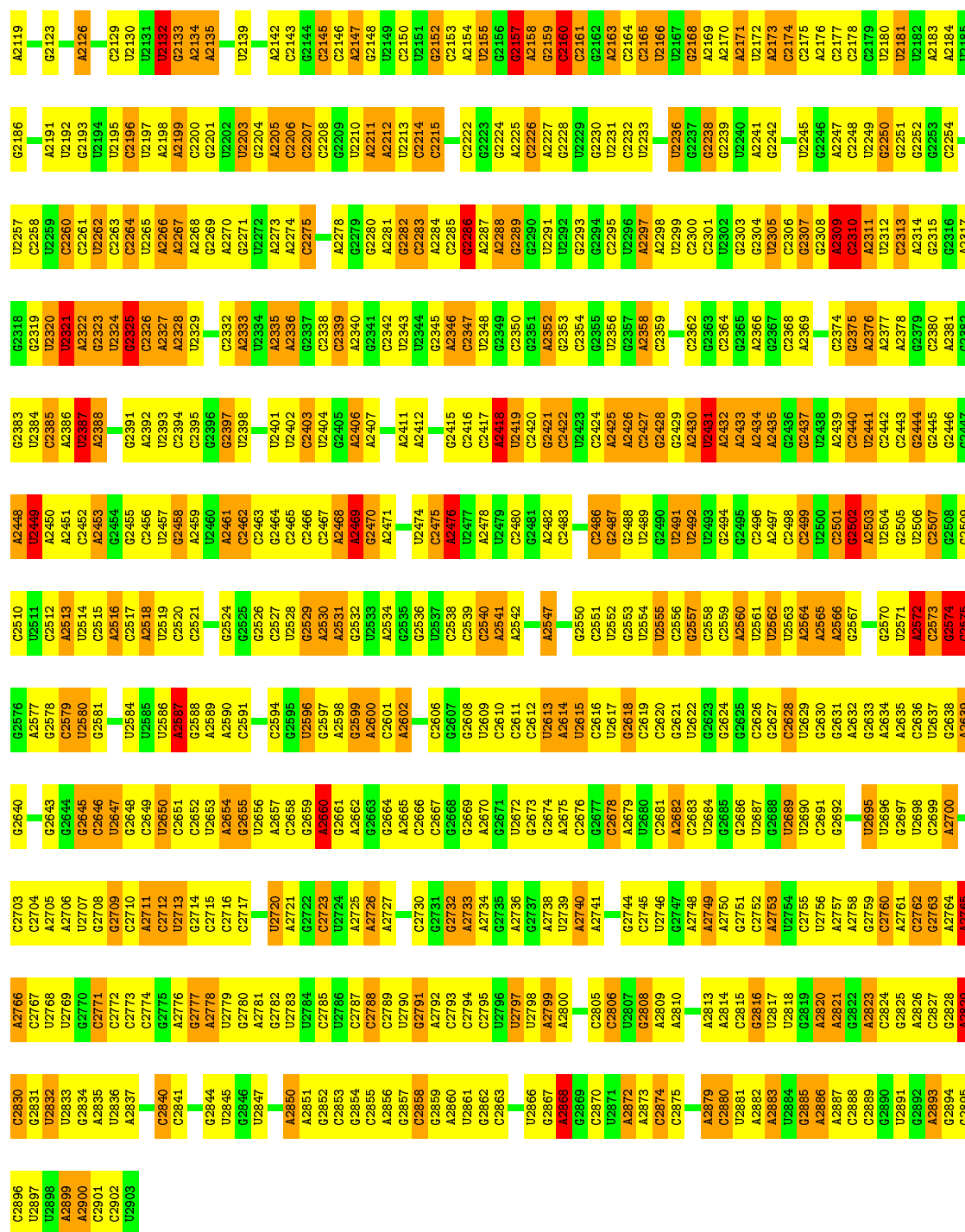


- Molecule 54: 23S ribosomal RNA



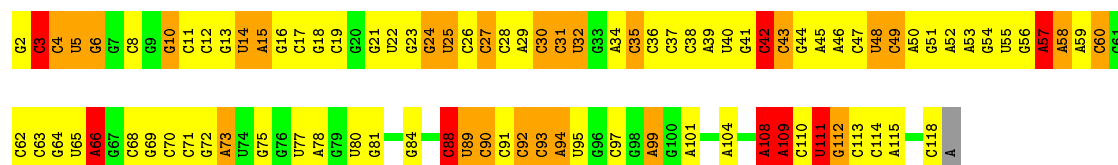
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G1036	A974	A910	A845	A781	A716	C545	A582	C516	A453	G388	A322	G258	A198	U72	A71	U3
G1037	G975	A911	A846	A782	C717	G647	A583	C517	A454	G389	C323	G259	A199	U74	U72	U4
A1038	A979	C912	U846	A783	C718	G647	C584	G518	C455	U390	A324		U200	A73	A73	A5
A1040	A980	G914	U847	A784	C719	C650	A586	G520	A457	U392	C327	A262	C201	A74	A74	A6
	A981	C915	A849	G785	U720		C587	U521	A458	C393	U328	C263	U202	C75	C75	G7
C1043	C982	G916	U850	C786	A721	U653	U588	A522	A459	C394	U329	A264	A203	C140	C140	C8
C1044	A983	A917	C851	C787	A722	A654	U589	C523	U459	C395	G329	A265	A204	G141	C76	C9
C1045	A984	A918	C852	A788	C723	A655	A590	G524	C461	U395	A330	C266	U206	C143	G77	A10
A1046	C985	U919	C853	A789	U724	A656	U591	G525	G462		C331	C267	U207	C144	C79	C11
G1047	C986	A920	C854	U790	G725	U657	A592	U526	G463	C398	A332	C268	A208	C145	U12	U12
A1048	C987	C921		C791	G726	U658	A593	A527	U464	U399	G333	C269	C207	A146	A13	A13
C1049	A988	C922	G858	A792	G727	U659	C595	C527	U465	G400	C334	A270	C209	C147	A84	A84
A1050	C989	G923	C859	A793	G728	C660	U596	A528	A466	A401	C335	G271	C210	U148	G85	G15
G1051	A990	G924	U860	A794	G729	A661	G597	A529		A402	C336	A272	C211	A149	G86	C16
C1052	C991	A925	A861	C795	A730	G662	U598	G530	U470	U403	A343	U280	A218	U150	U87	U87
C1053	C992	G926	G862	C796	G731	G663	A599	A532	A471	U404	A344	C281	A219	C151	G88	A19
A1054	C993	A927	A863		G732	G664	G600	G533	A472	U405	A345	A282	A221	U152	A89	C20
G1055	C994	A928	G864		G733	U665	C601		G473	G407	C341	G277	A222	U153	U90	A21
G1056	C995		C865	G801	A734	A666	A602	A538	G474	G406	A342	A278	A217	U154	A91	
A1057	A996	U931	A866	A802	A735	U667	A603	G539	C475	G411	C343	U279	A218	A155	U92	U25
G997	C997	U932	C867	U803	C736	G668	U606	G540	G476	A412	A346	A283	A223	C157	A94	A94
C998	C998	A933	U868	A804	C737	A670	U607	A541	A477	C413	A347	G283	A224	U158	A95	A28
U999	U999	U934	G869	G805	G738	A671		C542	A478	C414	A348	U284	A225	G96	C96	U29
A1000	A1000	C935	U870	C806	A739	C671	A608	G543	A479	A415	U349	G285	A226	A160	C97	G30
G1062	A1001	A936	U871	U807	C740	C672	A609	G544	A480	U416	G350	U286	U224	A161	G98	C31
G1063	G1002	C937	U872	G808	U741	C673	C610	U545	G481	C417	G351	G287	U225	U162	U99	C32
C1064	G1003		G873	G809	A742	G674	C611	U546	A482	C418	C352	U288	A226	C163	U100	C33
U1065	U1004	A941		U810	A743	A675	G612	A547	A483	U419	A353	U289	A227	C164	A101	U34
U1066	C942	G942	C876	U811	U744	A676	A613	G548	C484	C420	C353	G289	A228	A165	U102	
A1067	A943	A943	A877	C812	U745	A677	A614	G549	C485	A421	A354	U290	C228	U166	A103	A38
G1068	C944	C944	A878	U813	U746	C678	U615	C550	C486	A422	C357	U292	C229	G168	C105	G39
A1069	A1008	A945		C814	U747	C679	A616		C487	A423		U293	G230	G169	C106	U40
A1070	A1009	A946	C883	C815	G748	C680	G617	U554	G488	G426	U360	A294	A231	U170	G107	C51
G1071	A1010	A947	C884	C816	A749	C681		G555	G489	U427	G361	G295	A233	U171	A42	A42
C1072	G1011	C948	C885	C817	A750	U683	G620	A556	C490	U428	A362	G296	A234	U172	A43	A43
A1073			A886	G818	A751	G684	A621	C557	G491	A429	G363	A299	U235	A173	C109	
G1074	C1013	C951	U887	A819	A752	A885	G622	U558	A492	A430	C364	A300	C236	U174	A111	
C1075	U1015	G952	C888	A820	A753	U686	C623	G559	G493	U431	U365	G301	C237	G175	U112	C47
C1076	U1016	G953	C889	A821	U754	C687	C624	G560	G494	A432	C366	G302	C238	A176	U113	G48
A1077	G1017	G954	C890	G822	U755	U688	G625	G561	G495	C433	G367	G303	C239	G177	U114	A49
U1078	G1017	U955	G891	C823	U756	A689	A626	U562	G496	C434	A368	U304	C240	G178	C115	
C1079	U1018	G956	G892	U824	G757	G690	A627	A563	A497	U435	U369	C305	A241	G179	C116	A52
A1080	U1019	C957	C893	A825	C758	C691	G628	C564		C436	U370	U306	G242	G180	G117	A53
U1081	A1020	U958	U894	U826	G759	C692	G629	C565	A501	C437	A371	G307	U243	A118	A118	G54
U1082	A1021	A959	U895	G760	G760	A693	G630	U566	A502	G439	G372	G308	A244	A182	A119	G55
U1083	G1022	A960	C896	U828	A761	U694	A631	U567	A503	C440	U373	A309	G245	C183	U120	A56
A1084	U1023	C961	C897	U829	U762	U694	A632	U568	A504	U441	A374	A310	G246	C184	G121	C57
A1085	G1024	G962	C898		G763	C698	A633	U571		G442	G375	A311	G247	G187	G122	
A1086	G1025	U963	A899	A764	A764	A699	C634	G572	A505	G443	G376	G312	G248	A125	C61	C61
G1087	G1026	C964	C900	C765	C765	U702	C635	A573	G506	C444	C378	G313	C249	A126	U62	U62
A1088	A1027	C965	C901	G834	U766	U703	G636	A574	A507	C445	G379	G314	G250	A191	A127	A63
A1089	A1028	G966	C902	C835	U767	G704	G637	A575	A508	G446		G315	G251	A192	C128	A64
A1090	A1029	U967	C903	G836		G705	G638	U576	C509	A447	A382	C316	G252	C192	C129	G65
G1091	C1030	C968	G904	C837	C772	A705	U639	U577	C510	U448	C383	G317	G253	A193	C130	C56
C1092	G1031	G969	A905	C838	G773	A706	C640	G577	U511	U449	A394	G318	G254	G194	C130	
G1093	A1032	U970	U906	U839	G774		U641	G578	G512	A450	C385	G319	G255	A195	A131	
U1094	U1033	G971	G907	C840	G775	U709	U642	G579	A513	G450						



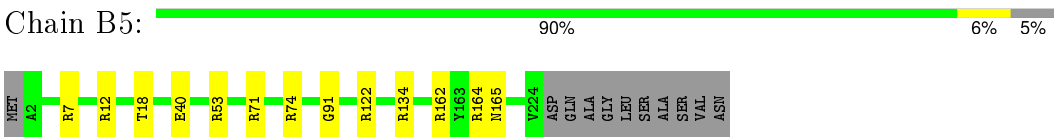



• Molecule 55: 5S ribosomal RNA

Chain BB: 20% 50% 22% 7%



● 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	13207	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	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	0.70	0/1736	0.99	6/2340 (0.3%)
10	AK	0.74	0/894	1.23	11/1207 (0.9%)
11	AL	0.74	0/969	1.22	13/1300 (1.0%)
12	AM	0.76	0/884	1.30	14/1181 (1.2%)
13	AN	0.78	0/817	1.25	11/1088 (1.0%)
14	AO	0.72	0/722	1.19	8/964 (0.8%)
15	AP	0.77	0/648	1.19	8/870 (0.9%)
16	AQ	0.70	0/658	1.14	7/883 (0.8%)
17	AR	0.81	0/463	1.22	5/623 (0.8%)
18	AS	0.74	0/653	1.08	5/879 (0.6%)
19	AT	0.69	0/672	1.12	8/890 (0.9%)
2	AC	0.73	0/1651	1.13	16/2225 (0.7%)
20	AU	0.83	0/431	1.51	9/572 (1.6%)
21	AA	1.53	0/36759	2.21	1951/57346 (3.4%)
22	A1	1.55	0/1668	2.23	94/2595 (3.6%)
23	A2	1.46	1/343 (0.3%)	2.24	14/531 (2.6%)
24	A3	1.52	0/1722	2.20	88/2685 (3.3%)
25	BC	0.74	0/2121	1.26	28/2852 (1.0%)
26	BD	0.69	0/1586	1.17	11/2134 (0.5%)
27	BE	0.67	0/1571	1.18	13/2113 (0.6%)
28	BF	0.75	0/1444	1.24	15/1937 (0.8%)
29	BG	0.69	0/1343	1.17	10/1816 (0.6%)
3	AD	0.75	0/1665	1.16	16/2227 (0.7%)
30	BH	0.65	0/1122	1.07	4/1515 (0.3%)
31	BI	0.66	0/1046	1.00	2/1410 (0.1%)
32	BJ	0.71	0/1152	1.14	8/1551 (0.5%)
33	BK	0.70	0/947	1.28	11/1268 (0.9%)
34	BL	0.73	0/1054	1.32	13/1403 (0.9%)
35	BM	0.74	0/1093	1.15	10/1460 (0.7%)
36	BN	0.77	0/973	1.27	14/1301 (1.1%)
37	BO	0.73	0/902	1.28	12/1209 (1.0%)
38	BP	0.76	0/929	1.28	12/1242 (1.0%)

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

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

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

All (2) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 1084 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 11 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
21:AA:730:G:C5	21:AA:731:G:H1'	2.48	0.48
6:AG:148:LYS:HE3	10:AK:60:PHE:CZ	2.48	0.47
26:BD:125:TRP:CE3	26:BD:160:LYS:HE3	2.48	0.47
29:BG:1:SER:HA	54:BA:2749:A:OP1	2.18	0.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AB	218/220 (99%)	202 (93%)	15 (7%)	1 (0%)	34 77
2	AC	205/208 (99%)	190 (93%)	12 (6%)	3 (2%)	13 57
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	9 51
4	AE	150/152 (99%)	135 (90%)	11 (7%)	4 (3%)	6 45
5	AF	99/101 (98%)	90 (91%)	4 (4%)	5 (5%)	2 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AG	150/152 (99%)	130 (87%)	18 (12%)	2 (1%)	15	60
7	AH	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	24	69
8	AI	126/128 (98%)	114 (90%)	11 (9%)	1 (1%)	24	69
9	AJ	98/100 (98%)	92 (94%)	3 (3%)	3 (3%)	5	42
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	67
11	AL	121/124 (98%)	108 (89%)	11 (9%)	2 (2%)	11	55
12	AM	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	11	53
13	AN	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	9	51
14	AO	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	4	39
15	AP	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	4	37
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	7	46
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53
18	AS	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	15	60
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	36 (71%)	12 (24%)	3 (6%)	2	27
25	BC	270/273 (99%)	241 (89%)	22 (8%)	7 (3%)	7	45
26	BD	207/209 (99%)	172 (83%)	20 (10%)	15 (7%)	1	22
27	BE	199/201 (99%)	179 (90%)	17 (8%)	3 (2%)	13	57
28	BF	176/179 (98%)	142 (81%)	25 (14%)	9 (5%)	2	30
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	11	55
30	BH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	5	40
31	BI	139/142 (98%)	128 (92%)	9 (6%)	2 (1%)	14	58
32	BJ	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	14	58
33	BK	121/123 (98%)	102 (84%)	15 (12%)	4 (3%)	5	40
34	BL	141/144 (98%)	111 (79%)	19 (14%)	11 (8%)	1	20
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	49
36	BN	119/121 (98%)	108 (91%)	9 (8%)	2 (2%)	11	55
37	BO	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	6	45
39	BQ	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	7	45
40	BR	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BS	108/110 (98%)	95 (88%)	13 (12%)	0	100	100
42	BT	92/94 (98%)	77 (84%)	12 (13%)	3 (3%)	5	40
43	BU	101/104 (97%)	83 (82%)	12 (12%)	6 (6%)	2	27
44	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	17	63
45	BW	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	2	30
46	BX	75/79 (95%)	66 (88%)	8 (11%)	1 (1%)	15	60
47	BY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	12	56
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	29
49	B0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
50	B1	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	19
51	B2	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	8	48
52	B3	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	B4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	28
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	34	77
All	All	5876/6008 (98%)	5234 (89%)	497 (8%)	145 (2%)	11	46

5 of 145 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	180 (100%)	0	100	100
2	AC	170/171 (99%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	112 (99%)	1 (1%)	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%)	103 (99%)	1 (1%)	82	92
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%)	101 (98%)	2 (2%)	65	86
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	78 (94%)	5 (6%)	24	60
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88
20	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
25	BC	216/217 (100%)	214 (99%)	2 (1%)	84	93
26	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
27	BE	165/165 (100%)	156 (94%)	9 (6%)	27	63
28	BF	149/150 (99%)	146 (98%)	3 (2%)	63	85
29	BG	137/138 (99%)	135 (98%)	2 (2%)	72	88
30	BH	114/114 (100%)	112 (98%)	2 (2%)	66	87
31	BI	109/110 (99%)	107 (98%)	2 (2%)	66	87
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BN	100/100 (100%)	98 (98%)	2 (2%)	63	85
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	57 (97%)	2 (3%)	44	75
46	BX	67/68 (98%)	64 (96%)	3 (4%)	34	69
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	61	84
49	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
50	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
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%)	4769 (98%)	73 (2%)	74	88

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

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

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

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	251 (16%)	84 (5%)
22	A1	73/76 (96%)	10 (13%)	4 (5%)
23	A2	14/15 (93%)	8 (57%)	2 (14%)
24	A3	76/77 (98%)	13 (17%)	2 (2%)
54	BA	2902/2903 (99%)	462 (15%)	119 (4%)
55	BB	117/118 (99%)	18 (15%)	6 (5%)
All	All	4712/4722 (99%)	762 (16%)	217 (4%)

5 of 762 RNA backbone outliers are listed below:

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

5 of 217 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	119	A
54	BA	818	G
54	BA	2573	C
54	BA	180	G
54	BA	503	A

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	1.82	3 (20%)	18,37,40	3.15	2 (11%)

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	0.96	0	15,36,39	1.49	2 (13%)
22	7MG	A1	46	22	20,26,27	2.23	4 (20%)	23,39,42	2.10	2 (8%)
22	5MU	A1	54	22	13,22,23	1.20	2 (15%)	16,32,35	4.70	2 (12%)
22	PSU	A1	55	22	15,21,22	1.08	1 (6%)	16,30,33	3.28	4 (25%)
22	4SU	A1	7	22	12,21,22	1.01	0	15,30,33	2.13	1 (6%)
24	H2U	A3	21	24	17,21,22	1.35	2 (11%)	23,30,33	1.49	4 (17%)
24	OMC	A3	33	24	15,22,23	1.04	0	20,31,34	0.76	0
24	5MU	A3	55	24	13,22,23	0.94	1 (7%)	16,32,35	4.74	2 (12%)
24	PSU	A3	56	24	15,21,22	1.11	1 (6%)	16,30,33	3.51	5 (31%)
24	4SU	A3	8	24	12,21,22	1.21	2 (16%)	15,30,33	2.12	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	-8.32	1.33	1.45
22	A1	34	CM0	O5-C5	-5.63	1.26	1.37
24	A3	21	H2U	C4-N3	-3.33	1.32	1.37
24	A3	21	H2U	C2-N3	-3.15	1.32	1.38
22	A1	46	7MG	C8-N7	-2.86	1.30	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
24	A3	55	5MU	C5-C4-N3	-13.25	114.23	125.35
22	A1	54	5MU	C5-C4-N3	-12.76	114.64	125.35
22	A1	7	4SU	C5-C4-N3	-7.53	115.58	123.56
24	A3	8	4SU	C5-C4-N3	-7.36	115.75	123.56
22	A1	46	7MG	C5-C6-N1	-6.79	113.28	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	VAL	A1	101	58,22	5,6,7	0.61	0	5,7,9	1.78	1 (20%)
58	FME	BA	3001	57	8,9,10	0.72	0	5,9,11	1.57	2 (40%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	BA	3001	FME	O-C-CA	-2.67	118.39	125.69
58	BA	3001	FME	O1-CN-N	-2.17	121.47	124.80
57	A1	101	VAL	C-CA-N	3.57	117.84	109.95

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.