



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:24 PM BST

PDB ID : 4V78
EMDB ID: : EMD-2475
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3a)
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 : 20.00 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

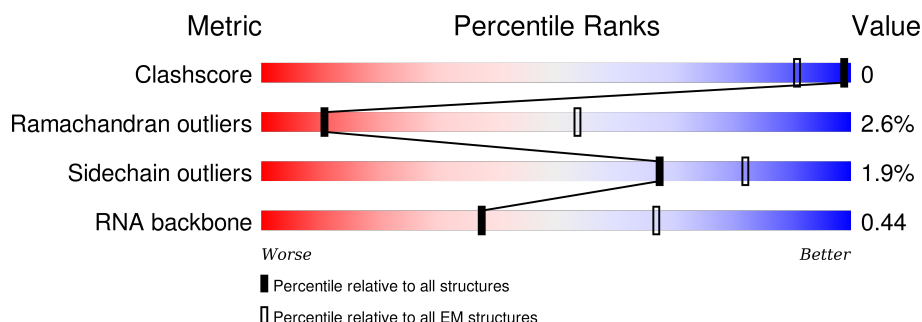
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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.















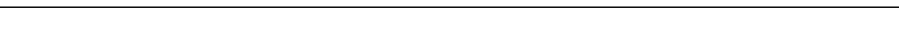

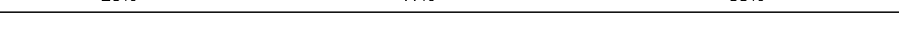

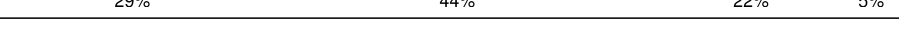





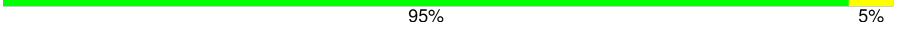
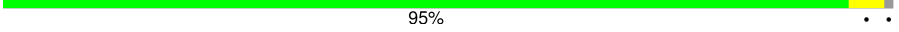

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	94% 5% .
2	AC	208	87% 13%
3	AD	206	86% 12% .
4	AE	152	94% 6%
5	AF	101	87% 13%
6	AG	152	88% 11% .
7	AH	130	92% 8% .
8	AI	128	84% 16%











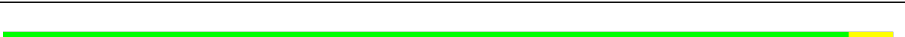


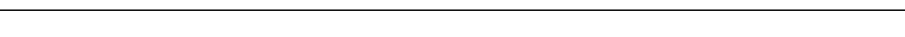
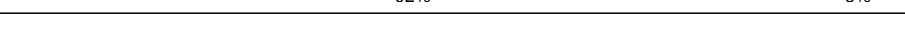
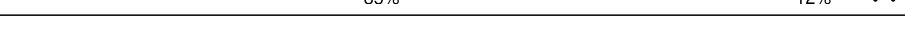

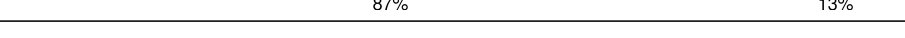

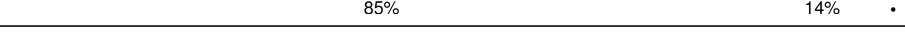

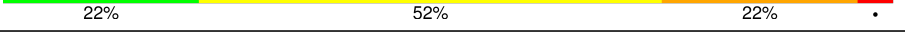
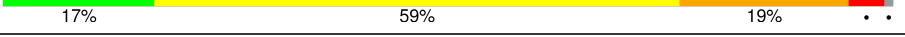
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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 7% .
11	AL	124	 85% 15% .
12	AM	115	 90% 10% .
13	AN	101	 87% 10% ..
14	AO	89	 88% 11% .
15	AP	81	 78% 22%
16	AQ	82	 90% 9% .
17	AR	57	 84% 16%
18	AS	81	 90% 9% .
19	AT	86	 86% 13% .
20	AU	53	 75% 25%
21	AA	1533	 23% 50% 22% .
22	A1	76	 26% 41% 33%
23	A2	15	 60% 27% 13%
24	A3	77	 29% 44% 22% 5%
25	BC	273	 89% 9% .
26	BD	209	 90% 9%
27	BE	201	 89% 10%
28	BF	179	 89% 10% ..
29	BG	177	 89% 10% .
30	BH	149	 95% 5%
31	BI	142	 95% . .
32	BJ	142	 90% 10%
33	BK	123	 89% 11%

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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*P*AP*UP*U)-3'.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

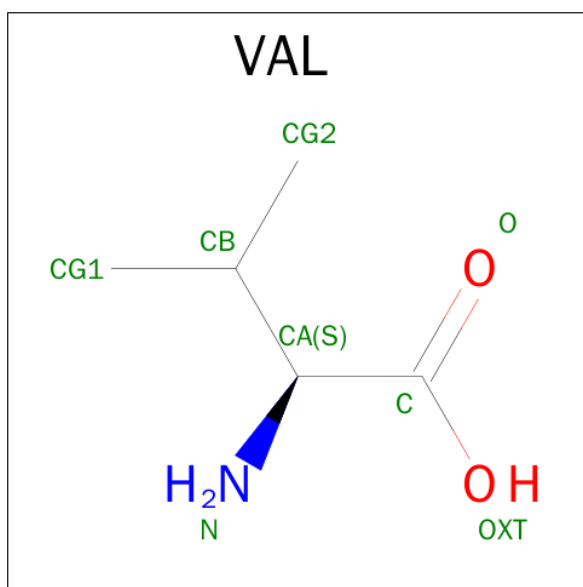
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

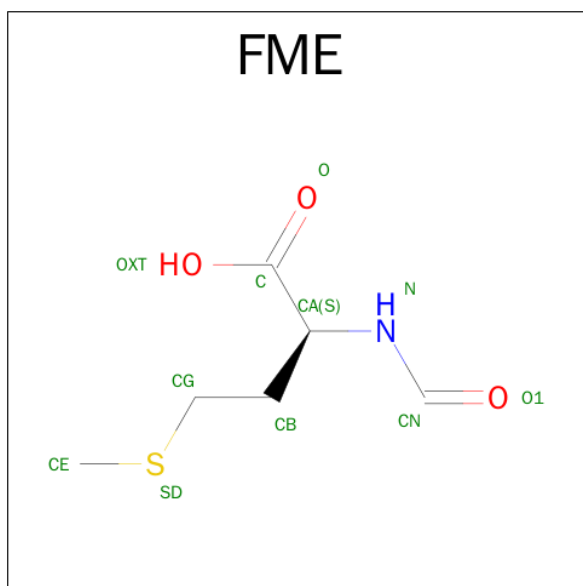
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

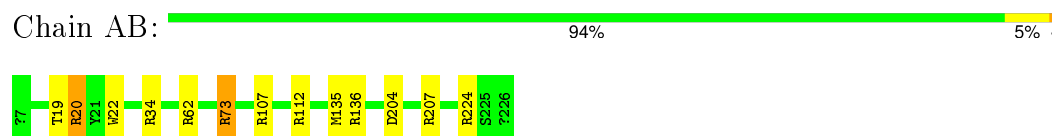


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

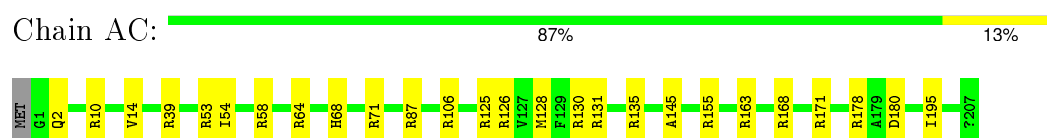
3 Residue-property plots

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

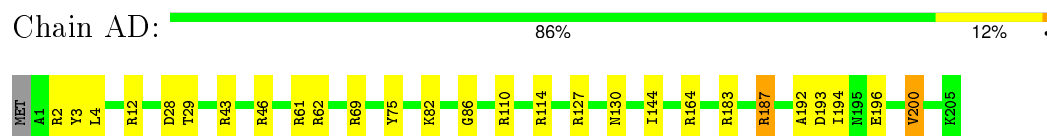
- Molecule 1: 30S ribosomal protein S2



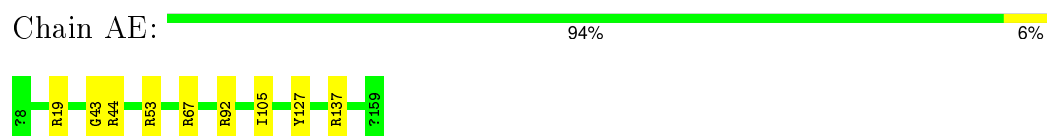
- Molecule 2: 30S ribosomal protein S3



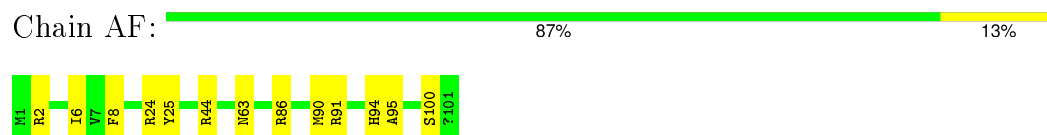
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 84% 16%



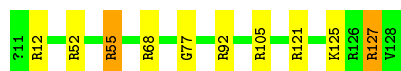
- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 7%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 90% 10%

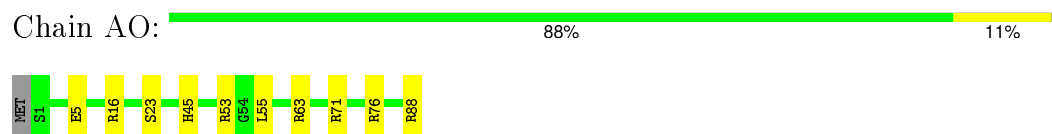


- Molecule 13: 30S ribosomal protein S14

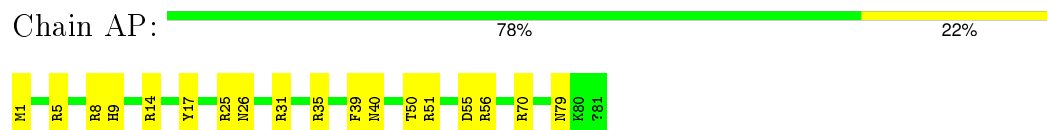
Chain AN: 87% 10%



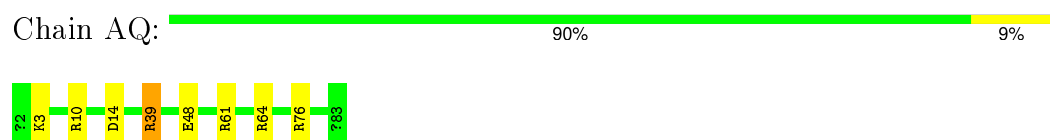
- Molecule 14: 30S ribosomal protein S15



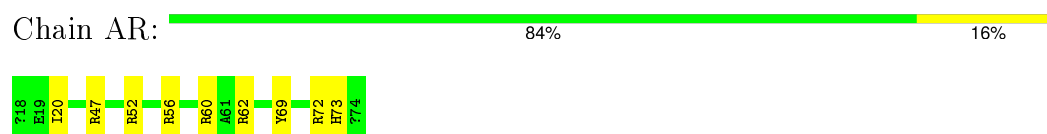
- Molecule 15: 30S ribosomal protein S16



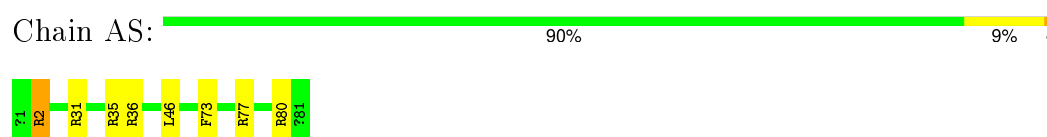
- Molecule 16: 30S ribosomal protein S17



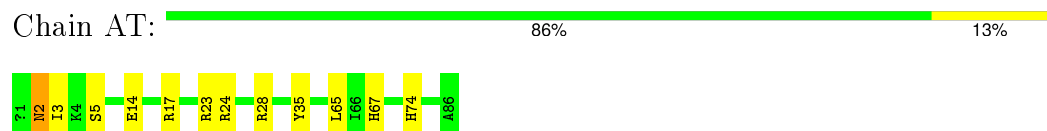
- Molecule 17: 30S ribosomal protein S18



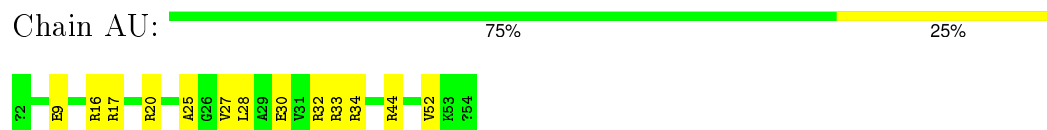
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



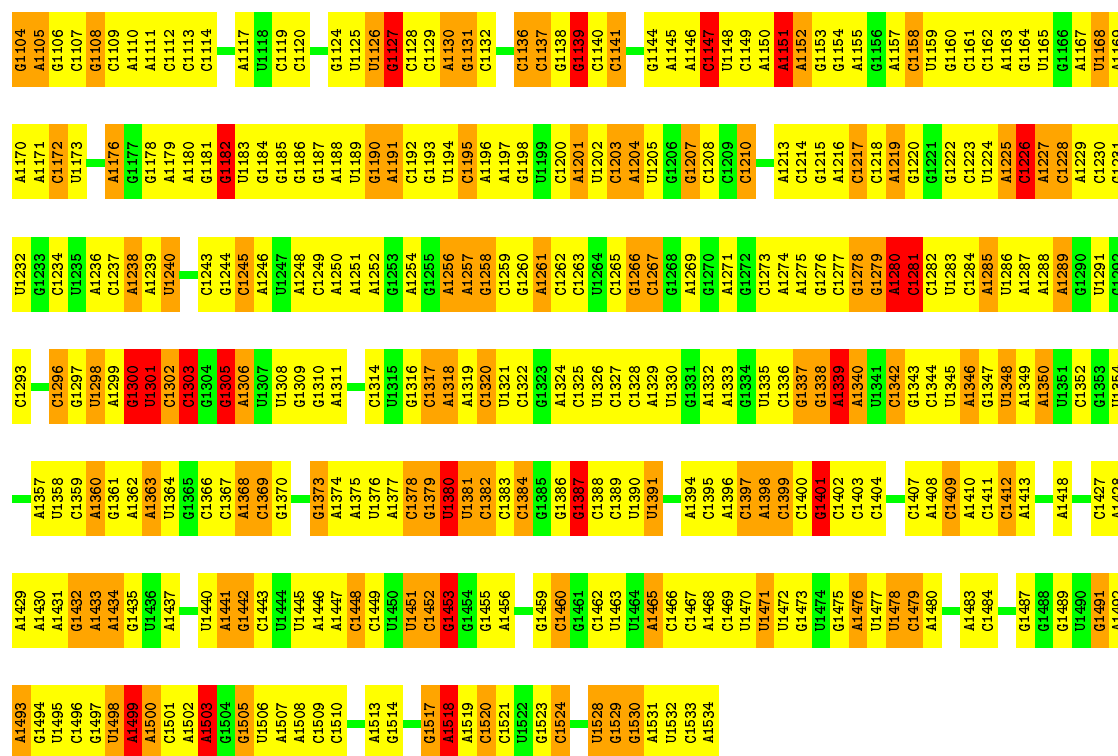
- Molecule 20: 30S ribosomal protein S21



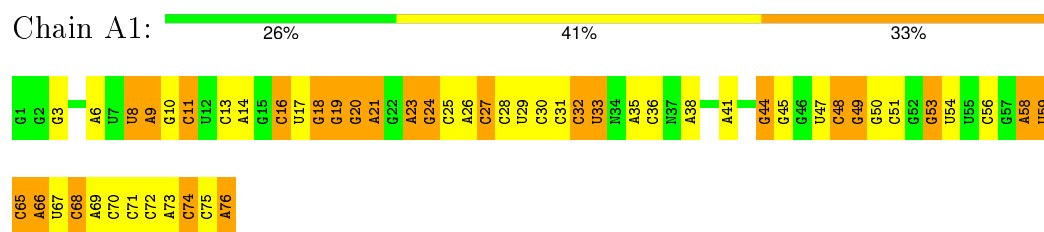
- Molecule 21: 16S ribosomal RNA



A	A	U	U5	G6	A7	G9	A10	G11	U12	U13	U14	A16	A17	G18	A19	U20	U21	G22	C23	U24	C25	A26	G27	A28	U29	U30	G31	A32	G33	G34	G35	C36	U37	G38	C40	G41	C43	A44		C47	C48	U49	A50	A51	C52	A53	C54	G55		C58	A59	A60	G61	U62	C63					
G64	A65	A66	C67	G68	G69	U70	A71	C72	A74		A77	G78	A80	U81	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95	U96	G97	G98	C99	G100	A101	G102	C106	G107	G108	A109		C110	G111	G112		G115	A116	C117	A119	A120	U121		C124	U125	A128	G128	A129	U130	C132	
A131	C132		G135	C136	U137	G138	A139	U140	G141	G142	A143	G148	A149	C143	U150	A151	C152	C153	U154	A155	C156	U157	U158	G158	C159	A160	U161	C162		U166	G167	G168	C169	G100	A171	U172	A173	C175	G176	G178	A179	U180	G181	A182	C183	U185	A186	A187	U188	C188		C192	A190	G191	A192	C193	U194			
A195	G259	C222	U233	G234	A235	G236	A237	C238	C239	C240	C241	A205	C206	C207	U208	U209	C210	G211	G212	C213	C214	C215	C223	U224	C225	G226	C227	A228	C229	U231	G230	U231	G232	C233	C234	C235	C236	A238	U239	G241	G242	A243	U244	U245	A246	C247	C248	U249	A250	C251	U252	A253	C254	G255	G319	A321				
G259	A262	C263	A264	G265	C266	C267	U268	C269	A270	C271	C272	U273	A274	G275	C276	C277	U278	A279	C280	G281	A282	U283	C284	C285	C286	U287	A288	C289	C290	U291	G292		G293	C294	A300		A303	U304	G305	C306	A307	C308	A309	G310	C311	C312	A313	C314	A315	C316	U317	G318	C319	A321						
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A389	U390	C391	C392	A393	G394	C395	C396	A397	U398	C399	C400	G402	C403	G404	U405	G406	U407	A408	U409	A410	A411	A412	G413	U414	A415	G416	C417	C418	C419	U420	U421	C422	A423	G424	G425	U426	U427	G428	U429	A430	A431	U432	G433	U434	A435	C436	U437	A438	C439	U440	A441	C442	C443	G444	G445	A448	C449			
G450	A451	A452	A453	G454	G455	A456	A459	A460	A461	G462	U463	U464	A465	A466	U467	A468	C469	C470	U471	U472	U473	G474	C475	U476	C477	A478	U479	A482	C483	A484	U485	U486	A487	C488	C489	C490	A491	C492	A493	A494	A495	A496	A497	A498	A499	G500	C501	A502	A503	C504	G505	G506	C507	U508	A509	A510	C511			
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A640	U641	A642	C643	G646	C647	A648	A649	G650	C651	A655	G656	U657	C658	U659	U660	U661	U662	A663	G664	A665	G666	G667	G668	G669	G670	A673	G674	A675	A676	U677	U678	C679	C680	A681	A687	A688	G689	C690	A691	A692	A693	A694	A695	A696	U697	G698	C699	U700	U701	A702	G703	A704	G705	A706	U707	C708				
U709	G710	G711	A712	G713	C714	A715	A716	U717	A718	C719	G720	G721	G722	U723	G724	C725	G726	G727	A728	U729	C730	G731	G732	G733	C734	C735	C736	C737	C738	C739	U740	G741	G742	A743	C744	G745	A746	A747	G748	A749	C750	U751	G752	A753	C754	G755	C756			A759	U760	G761	C764	U765	A766	U767	A768	G769	C770	
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A908	A909	U910	U911	C912	A913	A914	A915	A918	A919	A920	U921	G922	A923	C924	C925	G926	G927	G928	G929	C930	C931	C932	C933	C934	A935	A936	A938	C939	C940	G941	G942	G945	A946	G947	C948	A949	U950	G951	G954	A958	A959	U960	U961	C962	G963	A964	U965	U966	A967	A968	A969	C970	C971	C972						
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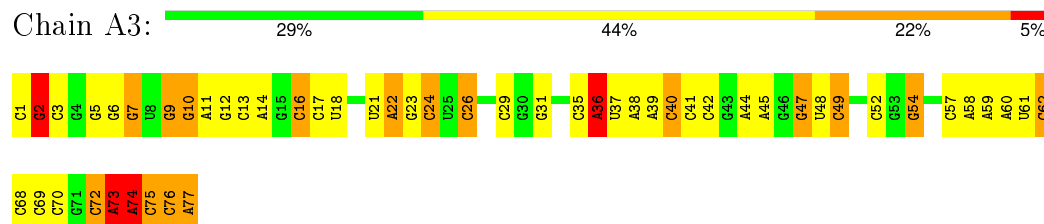
• Molecule 22: fMet-Val-tRNA-Val



• 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





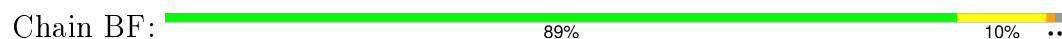
- Molecule 26: 50S ribosomal protein L3



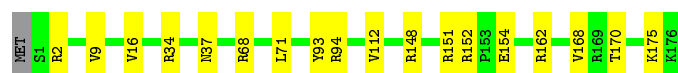
- Molecule 27: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L5



- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



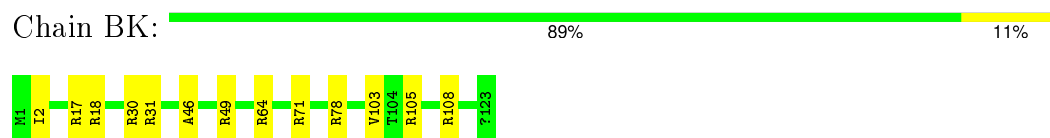
- Molecule 31: 50S ribosomal protein L11



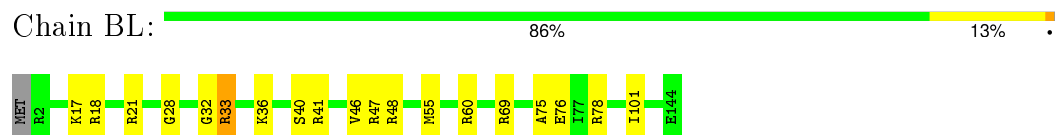
- Molecule 32: 50S ribosomal protein L13



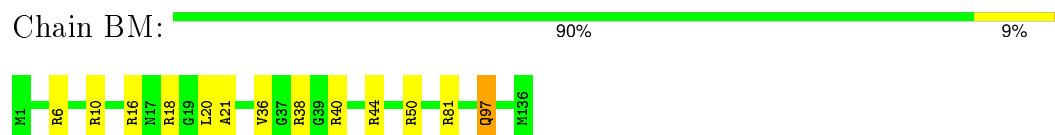
- Molecule 33: 50S ribosomal protein L14



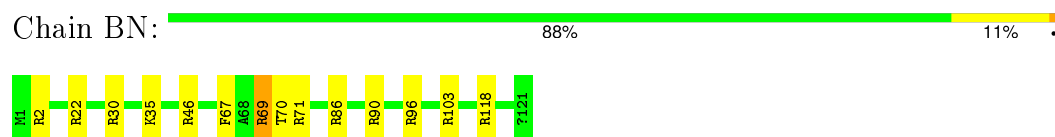
- Molecule 34: 50S ribosomal protein L15



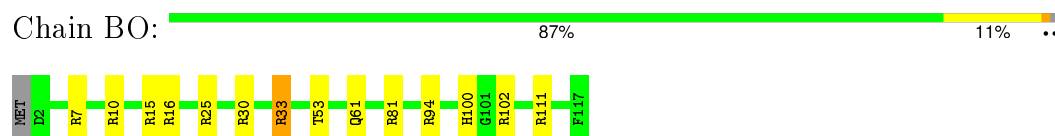
- Molecule 35: 50S ribosomal protein L16



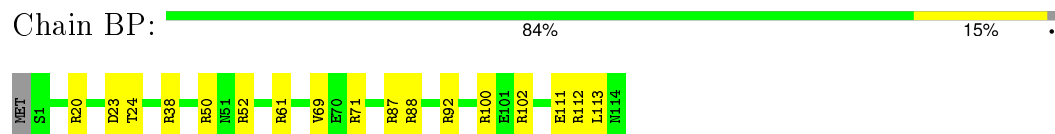
- Molecule 36: 50S ribosomal protein L17



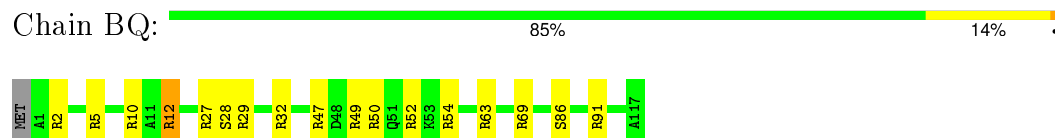
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20



- Molecule 40: 50S ribosomal protein L21

Chain BR:  92% 8%



- Molecule 41: 50S ribosomal protein L22

Chain BS:  92% 7%




- Molecule 42: 50S ribosomal protein L23

Chain BT:  91% 7%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  88% 12%



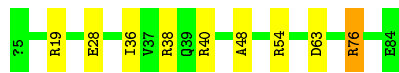
- Molecule 44: 50S ribosomal protein L25

Chain BV:  95% 5%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  89% 10%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  86% 11%



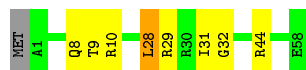
- Molecule 47: 50S ribosomal protein L29

Chain BY:  92% 8%



- Molecule 48: 50S ribosomal protein L30

Chain BZ: 85% 12% . .



- Molecule 49: 50S ribosomal protein L32

Chain B0: 77% 21% .



- Molecule 50: 50S ribosomal protein L33

Chain B1: 87% 13%



- Molecule 51: 50S ribosomal protein L34

Chain B2: 78% 22%



- Molecule 52: 50S ribosomal protein L35

Chain B3: 85% 14% .



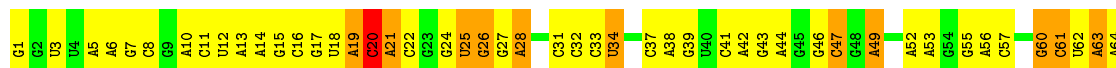
- Molecule 53: 50S ribosomal protein L36

Chain B4: 87% 13%



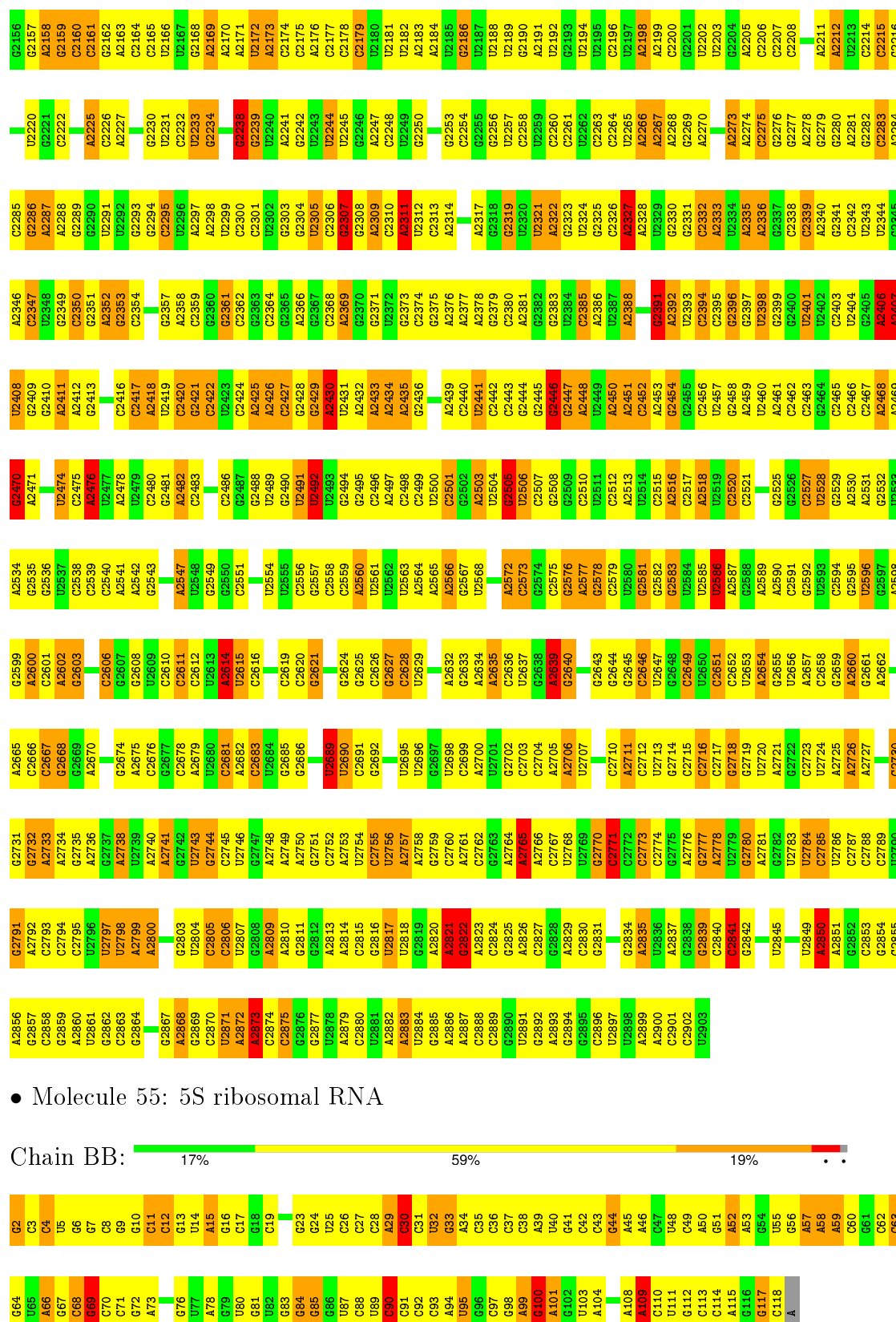
- Molecule 54: 23S ribosomal RNA

Chain BA: 22% 52% 22% .



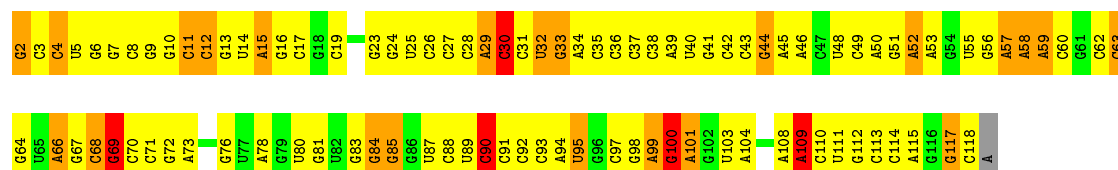
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U1082	U1019	C958	U767	G704	U641	G579	A513	C445	C382	C318	C257	A197	C129	C66
U1083	A1020	U958	G768	A705	U642	G580	A514	G446	C383	G319	G258	C198	C130	U67
A1084	A1021	A959		A706	A643	C581	A515	A447	C384	A320	G259	A199	A131	G68
A1085	A1022	G836	C772	U709	A644	A582	C516	U448	A384	U321	G260	U200	G132	C69
A1086	G1023	C961	C773	U710	C645	G583	C517	U449	C385	A322	G261	C201	U133	G70
G1087	G1024	C962	G774	G711	U646	C584	U518	G450	G386	C323	A262	U202	G134	A71
A1088	G1025	C963	G775		U647	G585	A522	U451	U387	A324	G263	A203	U135	U72
A1089	G1026	C964	G776	U714	G648	G586	C523	G452	G388	G325	C264	A204		A73
A1090	A1027	C965	G777	A715	C649	C587	C524	A453	G389	G326	A265	G205	U138	A74
G1091	A1028	U967		A716	C650	C588	G525	A454	U390	G327	G266	U206	U139	G75
C1092	A1029	C968	G780	C717	U651	U589	U525	C455	A391		C267	A207	C140	C76
	A1030	G943	A781	A717	A652	A590	U526	C456	U392	A330	C268	C208	G141	G77
	G1031	A845	A782	C718	A653	U591	C527	A457	C393	C331	C269	C209	A142	U78
	A1032	C948	A783	C719	U654	A592	A528	G458	C394	A332	A270	C210	C143	C79
	U1033	G949	G784	U720	U655		A529	U459		G333	G271	C211	A144	
	G1034	A910	G785	A721	U656	C595	G530	A460	U397	C334	A272	G212	C145	G80
	U1035	A911	G786	A722	U657	U596	G531	C461	C398	C335	G273	A213	A146	G81
		C912	G787	C723	C660	G597	A532	C462	U399	C336	G274	G214	C147	U82
		C913	U724	U724	A661	U598		C463	G400	C337	C275	G215	U148	A83
		G914	A730		U658	G600	G535	U464	A401	G338	C276	A216	A149	A84
		G915	C731		U659	C601	G536	A465	A402	U339	G277	A217	U150	G85
		G916	C732		U660	A602	G537	A466	U403	A340	A278	A218	C151	U87
		A917	G733		U661	A603	A538		A404	C341	A279	A219	A152	G88
		A918	G734		U662	G604	C540	A470		C342	U280	G220	A155	A89
		A919	C735		U663	G605	A541	A471	G408	C343	C281	A221	A156	U90
		U919	C736		U664	C606	C542	A472	G409	A344	A282	A222	A157	A91
		G920	C737		U665	U607	C543	G473	G410	A345	G283	A223	C157	
		C921	C738		U666	A608	C544	A477	G411	A346	U284	U224	U158	A94
		G922	A739		U667	C609	C550	A478	G412	A347	U285	C225	G159	A95
		G923	C740		U668	A610	C551	A479	G413	A348	U286	A226	A160	C96
		A924	U741		U669	A611	U552	C485	C420	U355		A227	A161	C97
		G925	A742		U670	A612	G553	C486	C421	G356		C228	U162	G98
		G926	U744		U671	G617		C487	A422	C357	U296	U235	U170	C105
		U931			U672	G618	A556	G488	A423		G297	U236	U171	C106
		U932			U673	A620	C557			U360	G298	C237	A172	
		A933			U674	G621	U558	C490	C426	G361	A299	C238	A173	C109
		C935			U675	A622	C559	C491	U427	A362	A300	C239	U174	G110
		A936			U676	C623	C560	C492	A428	G363	G301	C240	G175	A111
		C937			U677	C624		C493	A429	C364	C302	A241	U112	U113
		G940			U678	G625	A563	A497	U431	U365	G303	U242	G177	U114
		A941			U679	A626	C564		U432	C366	U304	C305	G178	U115
		G942			U680	A627	C565		U433	U367	U305	A244	C179	C115
		A943			U681	G628	U566		C433	U368	U306	G245	G180	C116
		G944			U682	A630		A501	U434	G369	G307	C246	A181	G117
		C945			U683	G631	U569	A502		C370	G308	G247	A182	A118
		A946			U684	A632	G570	A503	C435	A371	A309	C248	C183	A119
		C947			U685	A633	U571	A504	C436	G372	A310	C249	C184	U120
		G948			U686	G634	U572	A505	U437	U373	A311	G250	G121	G122
		A949			U687	C635	U573	A506	G438	A374	G312	A251	A190	
		C950			U688	G636	A574	A507	C439	G375	G313	G252	A191	
		G951			U689	A637	U575	A508	C440	G376	G314	G253	C192	A125
		U952			U690	G638	U576	C509	U441	G377	G315	G254	A126	A127
		G953			U691	A639		C510	U442	C378	C316	A255	A195	
		C954			U692	U639	G577	U511	A443					







• Molecule 55: 5S ribosomal RNA

Chain BB:



• Molecule 56: 50S ribosomal protein L1

Chain B5:  88% 7% 5%

MET	A2	R7	M8	R9	R12	N24	V42	G49	I50	R53	R60	R71	R74	G91	R122	R134	R164	N168	V224	ASP	GLN	ALA	GLY	LEU	SER	ALA	SER	VAL	ASN
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	0.67	0/1736	1.06	12/2340 (0.5%)
10	AK	0.73	0/894	1.10	8/1207 (0.7%)
11	AL	0.73	0/969	1.29	17/1300 (1.3%)
12	AM	0.72	0/884	1.36	14/1181 (1.2%)
13	AN	0.75	0/817	1.18	10/1088 (0.9%)
14	AO	0.70	0/722	1.18	7/964 (0.7%)
15	AP	0.74	0/648	1.27	11/870 (1.3%)
16	AQ	0.66	0/658	1.17	7/883 (0.8%)
17	AR	0.76	0/463	1.17	6/623 (1.0%)
18	AS	0.72	0/653	1.19	7/879 (0.8%)
19	AT	0.67	0/672	1.13	6/890 (0.7%)
2	AC	0.70	0/1651	1.18	18/2225 (0.8%)
20	AU	0.83	0/431	1.48	7/572 (1.2%)
21	AA	1.61	27/36759 (0.1%)	2.23	2065/57346 (3.6%)
22	A1	1.63	0/1668	2.16	80/2595 (3.1%)
23	A2	1.49	0/343	2.31	18/531 (3.4%)
24	A3	1.64	0/1722	2.26	102/2685 (3.8%)
25	BC	0.73	0/2121	1.28	21/2852 (0.7%)
26	BD	0.65	0/1586	1.19	14/2134 (0.7%)
27	BE	0.66	0/1571	1.22	14/2113 (0.7%)
28	BF	0.72	0/1444	1.18	12/1937 (0.6%)
29	BG	0.65	0/1343	1.14	9/1816 (0.5%)
3	AD	0.74	0/1665	1.20	17/2227 (0.8%)
30	BH	0.62	0/1122	1.08	5/1515 (0.3%)
31	BI	0.63	0/1046	1.03	4/1410 (0.3%)
32	BJ	0.71	0/1152	1.22	10/1551 (0.6%)
33	BK	0.70	0/947	1.23	10/1268 (0.8%)
34	BL	0.72	0/1054	1.29	10/1403 (0.7%)
35	BM	0.71	0/1093	1.19	9/1460 (0.6%)
36	BN	0.75	0/973	1.34	12/1301 (0.9%)
37	BO	0.71	0/902	1.27	13/1209 (1.1%)
38	BP	0.70	0/929	1.22	11/1242 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.76	0/960	1.30	16/1278 (1.3%)
4	AE	0.66	0/1119	1.03	7/1506 (0.5%)
40	BR	0.68	0/829	1.18	8/1107 (0.7%)
41	BS	0.63	0/864	1.22	10/1156 (0.9%)
42	BT	0.62	0/744	1.19	7/994 (0.7%)
43	BU	0.65	0/787	1.21	6/1051 (0.6%)
44	BV	0.66	0/766	1.06	4/1025 (0.4%)
45	BW	0.71	0/604	1.26	7/799 (0.9%)
46	BX	0.72	0/635	1.28	7/848 (0.8%)
47	BY	0.65	0/510	1.24	5/677 (0.7%)
48	BZ	0.67	0/453	1.23	5/605 (0.8%)
49	B0	0.72	0/450	1.30	7/599 (1.2%)
5	AF	0.71	0/835	1.12	7/1128 (0.6%)
50	B1	0.68	0/417	1.10	2/556 (0.4%)
51	B2	0.79	0/380	1.49	9/498 (1.8%)
52	B3	0.70	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.35	5/397 (1.3%)
54	BA	1.48	61/69796 (0.1%)	2.23	4183/108888 (3.8%)
55	BB	1.48	1/2800 (0.0%)	2.19	150/4367 (3.4%)
56	B5	0.62	0/1673	1.09	11/2255 (0.5%)
6	AG	0.72	0/1188	1.27	17/1593 (1.1%)
7	AH	0.69	0/989	1.07	8/1326 (0.6%)
8	AI	0.77	0/1035	1.21	13/1377 (0.9%)
9	AJ	0.71	0/797	1.16	9/1079 (0.8%)
All	All	1.34	89/160085 (0.1%)	2.01	7075/239402 (3.0%)

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
21	AA	0	374
22	A1	0	20
23	A2	0	5
24	A3	0	13
25	BC	0	1
26	BD	0	1
3	AD	0	1
31	BI	0	1
35	BM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	BN	0	1
54	BA	0	623
55	BB	0	30
All	All	0	1072

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2507	C	C4-N4	-5.63	1.28	1.33
21	AA	742	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.57	1.28	1.33
54	BA	2164	C	C4-N4	-5.44	1.29	1.33
21	AA	984	C	C4-N4	-5.43	1.29	1.33

The worst 5 of 7075 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1617	C	N3-C2-O2	-16.02	110.69	121.90
54	BA	640	C	N3-C2-O2	-15.80	110.84	121.90
24	A3	73	A	N1-C6-N6	-13.57	110.46	118.60
54	BA	1847	A	N1-C6-N6	-13.18	110.69	118.60
54	BA	323	C	O4'-C1'-N1	12.86	118.49	108.20

There are no chirality outliers.

5 of 1072 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	25	C	Sidechain
21	AA	26	A	Sidechain
21	AA	5	U	Sidechain
3	AD	75	TYR	Sidechain
10	AK	127	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	1	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	0	0
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	1	0
9	AJ	790	0	832	0	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	1	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16457	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	839	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
53	B4	302	0	343	0	0
54	BA	62317	0	31205	8	0
55	BB	2504	0	1269	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	99454	17	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 17 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)
54:BA:1068:G:H1'	54:BA:1069:A:C6	2.45	0.51
54:BA:1131:G:C5	54:BA:2025:C:H4'	2.50	0.46
22:A1:53:G:C8	22:A1:54:5MU:H72	2.50	0.46
18:AS:46:LEU:HD23	18:AS:46:LEU:H	1.81	0.46
3:AD:86:GLY:H	3:AD:200:VAL:HG23	1.81	0.45

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%)	200 (92%)	15 (7%)	3 (1%)	14	58
2	AC	205/208 (99%)	188 (92%)	12 (6%)	5 (2%)	7	47
3	AD	203/206 (98%)	190 (94%)	7 (3%)	6 (3%)	5	42
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	51
5	AF	99/101 (98%)	83 (84%)	12 (12%)	4 (4%)	4	35
6	AG	150/152 (99%)	133 (89%)	14 (9%)	3 (2%)	9	51
7	AH	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
8	AI	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	7	47
9	AJ	98/100 (98%)	87 (89%)	6 (6%)	5 (5%)	2	30
10	AK	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11	55
11	AL	121/124 (98%)	109 (90%)	8 (7%)	4 (3%)	5	40
12	AM	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
13	AN	98/101 (97%)	86 (88%)	9 (9%)	3 (3%)	5	42
14	AO	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	8	48
15	AP	79/81 (98%)	64 (81%)	9 (11%)	6 (8%)	1	20
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	15	60
17	AR	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	11	53
18	AS	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	15	60
19	AT	84/86 (98%)	75 (89%)	5 (6%)	4 (5%)	3	32
20	AU	51/53 (96%)	34 (67%)	13 (26%)	4 (8%)	1	20
25	BC	270/273 (99%)	241 (89%)	21 (8%)	8 (3%)	5	42
26	BD	207/209 (99%)	181 (87%)	18 (9%)	8 (4%)	4	36
27	BE	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	3	33
28	BF	176/179 (98%)	151 (86%)	20 (11%)	5 (3%)	6	44
29	BG	174/177 (98%)	151 (87%)	16 (9%)	7 (4%)	4	35
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	14	58
31	BI	139/142 (98%)	128 (92%)	10 (7%)	1 (1%)	26	71
32	BJ	140/142 (99%)	123 (88%)	14 (10%)	3 (2%)	9	50
33	BK	121/123 (98%)	104 (86%)	13 (11%)	4 (3%)	5	40
34	BL	141/144 (98%)	110 (78%)	23 (16%)	8 (6%)	2	28
35	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8	49
36	BN	119/121 (98%)	102 (86%)	16 (13%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	BP	112/115 (97%)	96 (86%)	12 (11%)	4 (4%)	4	38
39	BQ	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	21	67
40	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
41	BS	108/110 (98%)	95 (88%)	12 (11%)	1 (1%)	21	67
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	8	49
43	BU	101/104 (97%)	83 (82%)	13 (13%)	5 (5%)	3	31
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	30
46	BX	75/79 (95%)	68 (91%)	5 (7%)	2 (3%)	6	45
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2	29
49	B0	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	4	38
50	B1	50/52 (96%)	42 (84%)	4 (8%)	4 (8%)	1	19
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	48
52	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	5	41
53	B4	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	6	44
56	B5	221/234 (94%)	207 (94%)	11 (5%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5232 (89%)	490 (8%)	154 (3%)	11	45

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	73	ARG
2	AC	14	VAL
3	AD	82	LYS
9	AJ	77	VAL
15	AP	79	ASN

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%)	178 (99%)	2 (1%)	80	91
2	AC	170/171 (99%)	169 (99%)	1 (1%)	90	95
3	AD	172/173 (99%)	167 (97%)	5 (3%)	50	78
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	101 (97%)	3 (3%)	50	78
8	AI	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	58	83
10	AK	90/90 (100%)	89 (99%)	1 (1%)	80	91
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	62 (95%)	3 (5%)	33	68
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	46 (96%)	2 (4%)	36	70
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
20	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
27	BE	165/165 (100%)	160 (97%)	5 (3%)	48	77
28	BF	149/150 (99%)	146 (98%)	3 (2%)	63	85
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
35	BM	109/109 (100%)	108 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	97 (97%)	3 (3%)	48	77
37	BO	86/87 (99%)	82 (95%)	4 (5%)	32	68
38	BP	99/100 (99%)	95 (96%)	4 (4%)	38	71
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83
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%)	77 (99%)	1 (1%)	76	89
45	BW	59/59 (100%)	58 (98%)	1 (2%)	68	87
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	46 (96%)	2 (4%)	36	70
49	B0	47/48 (98%)	43 (92%)	4 (8%)	13	48
50	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
51	B2	38/38 (100%)	38 (100%)	0	100	100
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%)	4750 (98%)	92 (2%)	67	86

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	BC	190	THR
28	BF	142	TYR
49	B0	32	THR
25	BC	191	LEU
27	BE	67	ARG

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

Mol	Chain	Res	Type
2	AC	184	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	254 (16%)	77 (5%)
22	A1	73/76 (96%)	10 (13%)	3 (4%)
23	A2	14/15 (93%)	8 (57%)	5 (35%)
24	A3	76/77 (98%)	15 (19%)	5 (6%)
54	BA	2902/2903 (99%)	474 (16%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	2 (1%)
All	All	4710/4722 (99%)	779 (16%)	209 (4%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	15	G
21	AA	16	A
21	AA	22	G

5 of 209 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	125	A
54	BA	686	U
54	BA	2430	A
54	BA	278	A
54	BA	571	U

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	15,26,27	1.83	3 (20%)	18,37,40	3.19	3 (16%)

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	1.01	1 (5%)	15,36,39	1.03	1 (6%)
22	7MG	A1	46	22	20,26,27	2.22	3 (15%)	23,39,42	2.13	2 (8%)
22	5MU	A1	54	22	13,22,23	1.07	1 (7%)	16,32,35	4.73	2 (12%)
22	PSU	A1	55	22	15,21,22	1.10	1 (6%)	16,30,33	3.27	4 (25%)
22	4SU	A1	7	22	12,21,22	1.05	1 (8%)	15,30,33	2.16	1 (6%)
24	H2U	A3	21	24	17,21,22	1.36	2 (11%)	23,30,33	1.26	4 (17%)
24	OMC	A3	33	24	15,22,23	1.08	0	20,31,34	0.76	0
24	5MU	A3	55	24	13,22,23	1.09	1 (7%)	16,32,35	4.64	2 (12%)
24	PSU	A3	56	24	15,21,22	1.22	2 (13%)	16,30,33	3.21	4 (25%)
24	4SU	A3	8	24	12,21,22	1.08	0	15,30,33	2.27	2 (13%)

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

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

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.64	1.32	1.45
22	A1	34	CM0	O5-C5	-5.49	1.26	1.37
24	A3	21	H2U	C4-N3	-3.47	1.32	1.37
24	A3	21	H2U	C2-N3	-3.31	1.31	1.38
22	A1	46	7MG	C8-N7	-2.72	1.31	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
22	A1	54	5MU	C5-C4-N3	-12.85	114.56	125.35
24	A3	55	5MU	C5-C4-N3	-12.69	114.70	125.35
24	A3	8	4SU	C5-C4-N3	-8.18	114.89	123.56
22	A1	7	4SU	C5-C4-N3	-7.51	115.60	123.56
22	A1	46	7MG	C5-C6-N1	-6.83	113.22	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	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	0.49	0	5,7,9	1.79	1 (20%)
58	FME	BA	3001	57	8,9,10	0.62	0	5,9,11	1.28	1 (20%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-3.52	116.07	125.69
58	BA	3001	FME	O-C-CA	-2.06	120.06	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.