



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 31, 2017 – 02:40 PM EST

PDB ID : 5JBH
EMDB ID: : EMD-8149
Title : Cryo-EM structure of a full archaeal ribosomal translation initiation complex
in the P-IN conformation
Authors : COUREUX, P.-D.; SCHMITT, E.; MECHULAM, Y.
Deposited on : 2016-04-13
Resolution : 5.34 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : rb-20028442

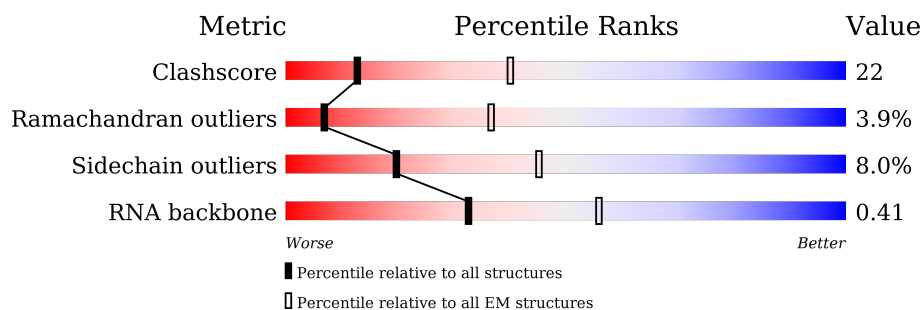
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.34 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.
























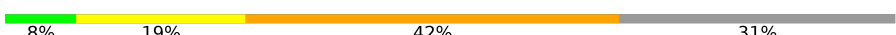



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	2	1518	31% 51% 15% . .
2	Z	210	79% 9% 11%
3	3	123	85% 14% .
4	L	102	67% 25% 7% .
5	O	148	86% 13% .
6	P	56	80% 16% .
7	S	67	85% 13% .
8	T	132	70% 14% 16%

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Mol	Chain	Length	Quality of chain
9	U	150	
10	X	71	
11	Y	50	
12	H	215	
13	K	135	
14	M	137	
15	N	147	
16	Q	158	
17	R	113	
18	A	198	
19	B	202	
20	V	99	
21	W	63	
22	D	180	
23	E	243	
24	F	236	
25	G	125	
26	I	130	
27	J	127	
28	C	57	
29	0	22	
30	5	26	
31	1	102	
32	4	76	
33	6	113	

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Mol	Chain	Length	Quality of chain
34	7	415	
35	8	139	
36	9	266	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	MET	4	101	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70653 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		

- Molecule 2 is a protein called 30S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	186	Total	C	N	O	S	0	0
			1459	933	271	251	4		

- Molecule 3 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	123	Total	C	N	O	S	0	0
			939	599	155	181	4		

- Molecule 4 is a protein called 30S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	102	Total	C	N	O	S	0	0
			822	507	159	152	4		

- Molecule 5 is a protein called 30S ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	148	Total	C	N	O	S	0	0
			1189	746	237	200	6		

- Molecule 6 is a protein called 30S ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	56	Total	C	N	O	S	0	0
			462	292	95	69	6		

- Molecule 7 is a protein called 30S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	67	Total	C	N	O	S	0	0
			556	353	105	95	3		

- Molecule 8 is a protein called 30S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	111	Total	C	N	O	S	0	0
			923	594	173	150	6		

- Molecule 9 is a protein called 30S ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	144	Total	C	N	O	S	0	0
			1175	758	212	204	1		

- Molecule 10 is a protein called 30S ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	71	Total	C	N	O	S	0	0
			568	345	115	107	1		

- Molecule 11 is a protein called 30S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	50	Total	C	N	O	S	0	0
			409	262	75	66	6		

- Molecule 12 is a protein called 30S ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 13 is a protein called 30S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	135	Total	C	N	O	S	0	0
			1072	671	205	190	6		

- Molecule 14 is a protein called 30S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	133	Total	C	N	O	S	0	0
			1004	623	200	179	2		

- Molecule 15 is a protein called 30S ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	145	Total	C	N	O	S	0	0
			1140	722	222	193	3		

- Molecule 16 is a protein called 30S ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	158	Total	C	N	O	S	0	0
			1310	834	250	221	5		

- Molecule 17 is a protein called 30S ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	113	Total	C	N	O	S	0	0
			934	592	177	160	5		

- Molecule 18 is a protein called 30S ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	190	Total	C	N	O	S	0	0
			1559	1007	273	274	5		

- Molecule 19 is a protein called 30S ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	202	Total	C	N	O	S	0	0
			1623	1046	282	290	5		

- Molecule 20 is a protein called 30S ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	99	Total	C	N	O	S	0	0
			823	532	134	154	3		

- Molecule 21 is a protein called 30S ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	63	Total	C	N	O	S	0	0
			478	306	85	81	6		

- Molecule 22 is a protein called 30S ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	172	Total	C	N	O	S	0	0
			1434	902	273	255	4		

- Molecule 23 is a protein called 30S ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	241	Total	C	N	O	S	0	0
			1976	1277	355	339	5		

- Molecule 24 is a protein called 30S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	217	Total	C	N	O	S	0	0
			1716	1084	319	305	8		

- Molecule 25 is a protein called 30S ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G	125	Total	C	N	O	S	0	0
			984	623	180	179	2		

- Molecule 26 is a protein called 30S ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 27 is a protein called 30S ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	J	127	Total	C	N	O	S	0	0
			1004	622	207	174	1		

- Molecule 28 is a protein called 30S ribosomal protein SX.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C	57	Total	C	N	O	0	0
			286	171	57	58		

- Molecule 29 is a protein called 30S ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	0	22	Total	C	N	O	S	0	0
			213	135	52	25	1		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	18	Total	C	N	O	P	0	0
			388	173	70	127	18		

- Molecule 31 is a protein called aIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1	80	Total	C	N	O	S	0	0
			632	399	112	117	4		

- Molecule 32 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	76	Total	C	N	O	P	0	0
			1621	723	291	531	76		

- Molecule 33 is a protein called aIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	95	Total	C	N	O	S	2	0
			792	504	150	135	3		

- Molecule 34 is a protein called aIF2-gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	409	Total	C	N	O	S	0	0
			3171	2028	541	590	12		

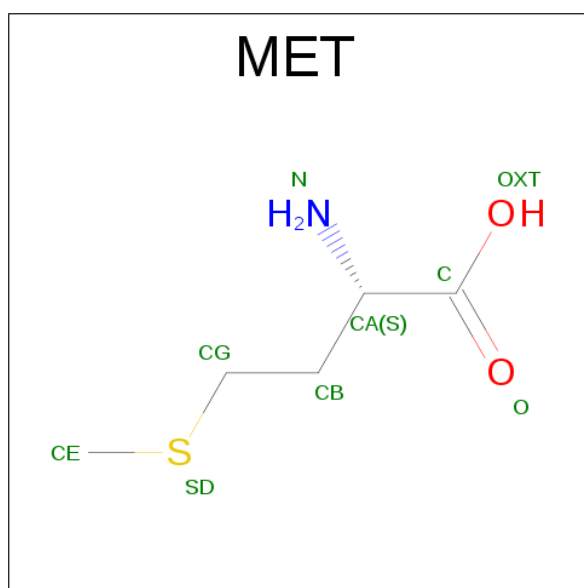
- Molecule 35 is a protein called aIF2-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	129	Total	C	N	O	S	0	0
			1033	659	172	192	10		

- Molecule 36 is a protein called aIF2-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	253	Total	C	N	O	S	0	0
			2025	1296	345	383	1		

- Molecule 37 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).

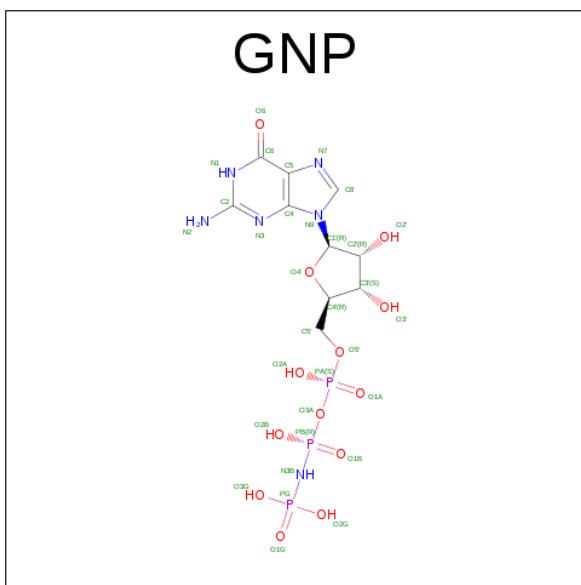


Mol	Chain	Residues	Atoms					AltConf
37	4	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	7	1	Total	Mg	0
			1	1	

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	

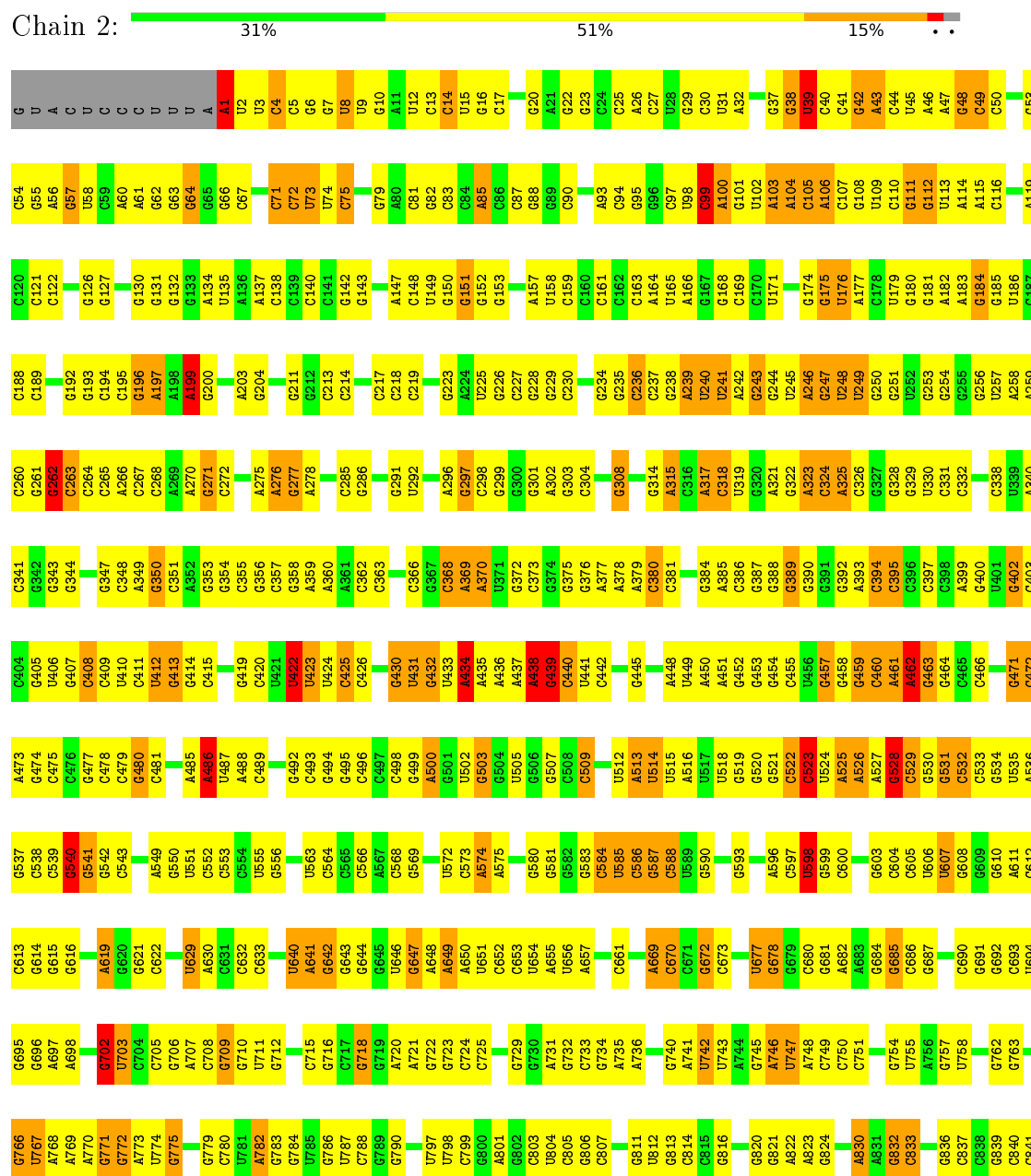
- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

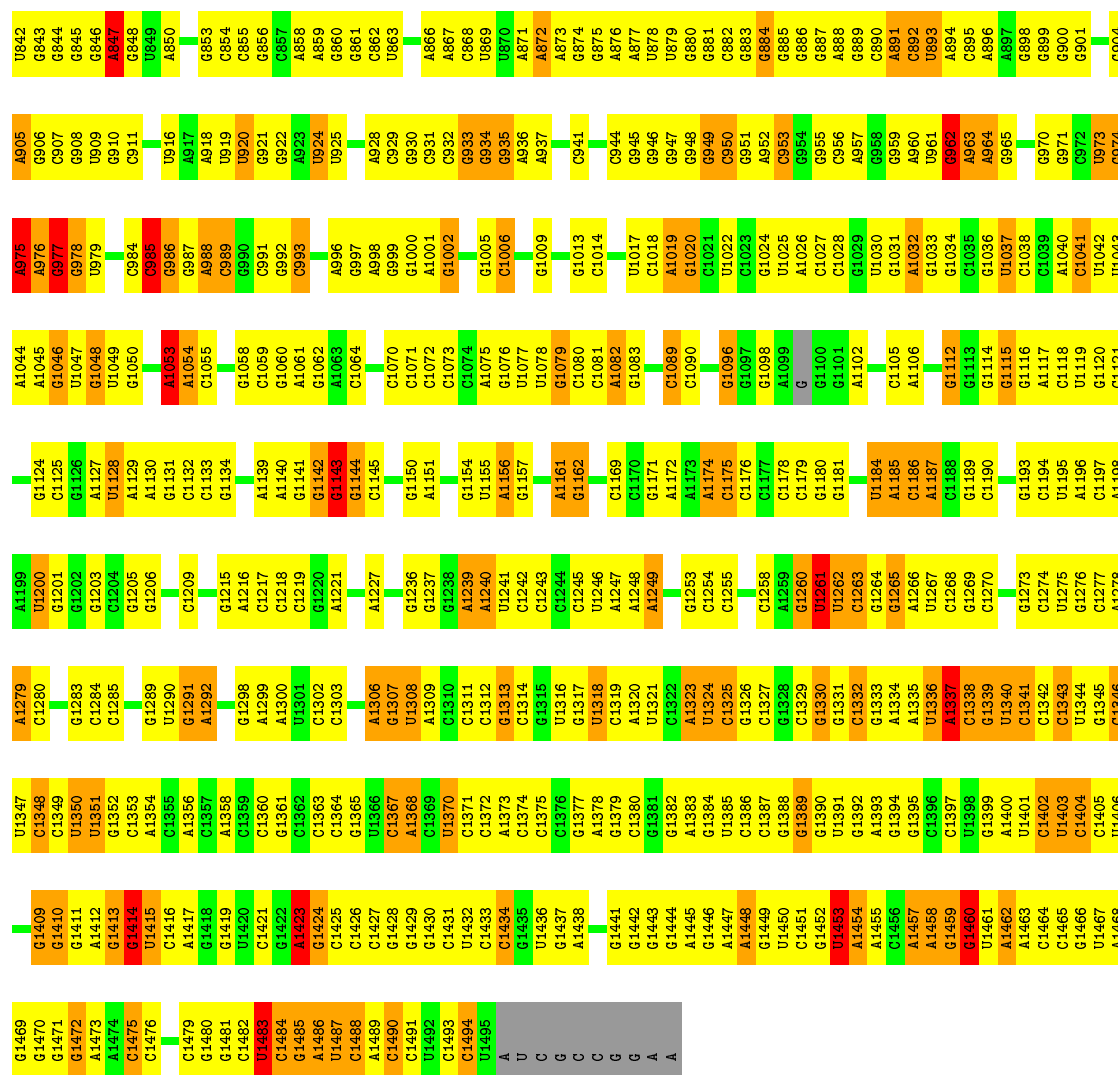
Mol	Chain	Residues	Atoms	AltConf
40	8	1	Total Zn 1 1	0

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.

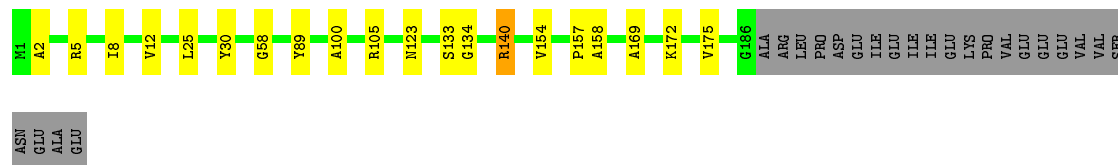
- Molecule 1: 16S ribosomal RNA





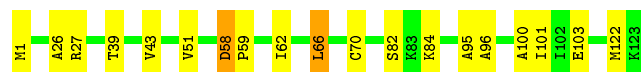
• Molecule 2: 30S ribosomal protein uS3

Chain Z: 79% 9% 11%

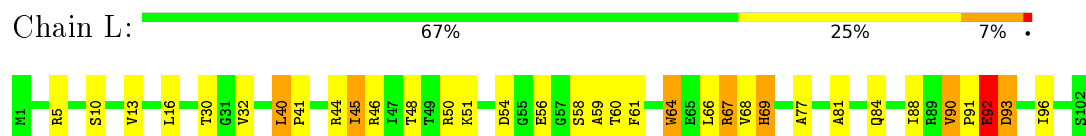


• Molecule 3: 50S ribosomal protein uL30

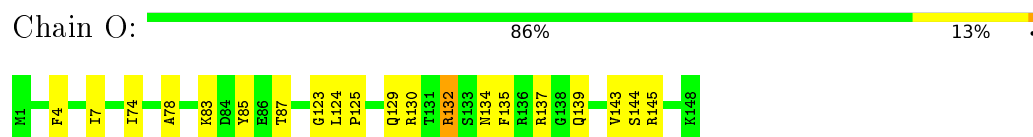
Chain 3: 85% 14%



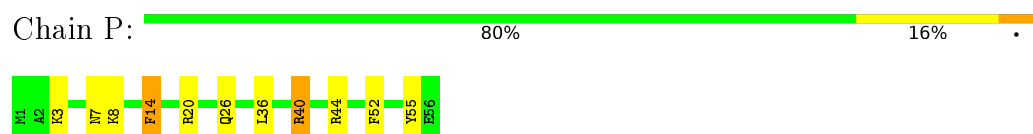
• Molecule 4: 30S ribosomal protein uS10



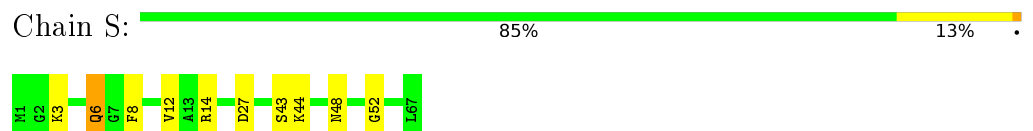
- Molecule 5: 30S ribosomal protein uS13



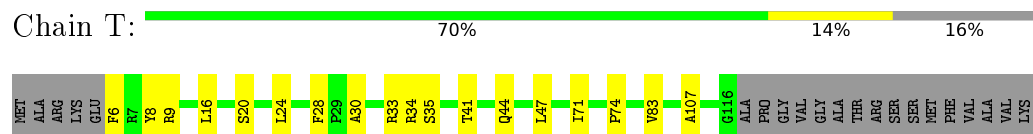
- Molecule 6: 30S ribosomal protein uS14



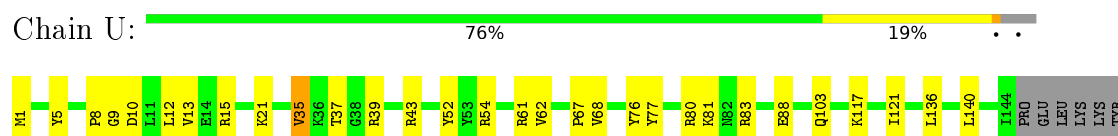
- Molecule 7: 30S ribosomal protein eS17



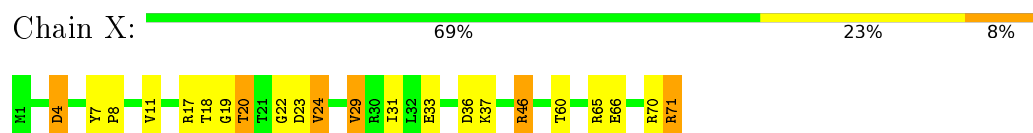
- Molecule 8: 30S ribosomal protein uS19



- Molecule 9: 30S ribosomal protein eS19



- Molecule 10: 30S ribosomal protein eS28



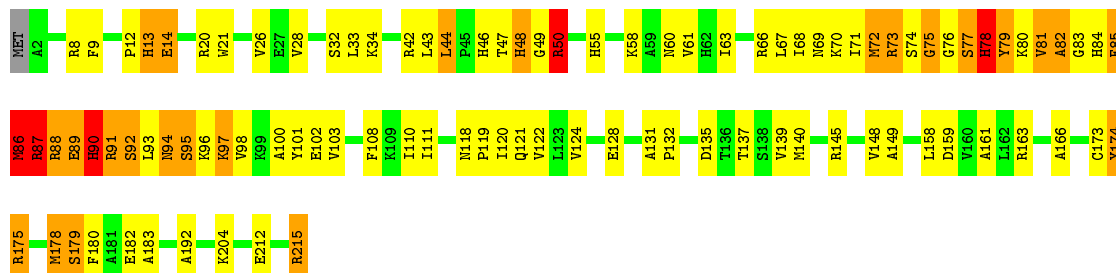
- Molecule 11: 30S ribosomal protein eS27





- Molecule 12: 30S ribosomal protein uS7

Chain H: 54% 32% 11% .



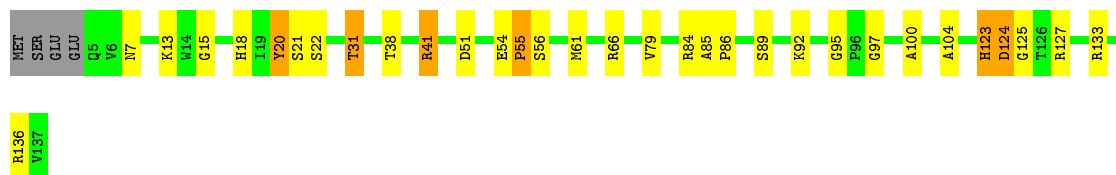
- Molecule 13: 30S ribosomal protein uS9

Chain K: 77% 21% .



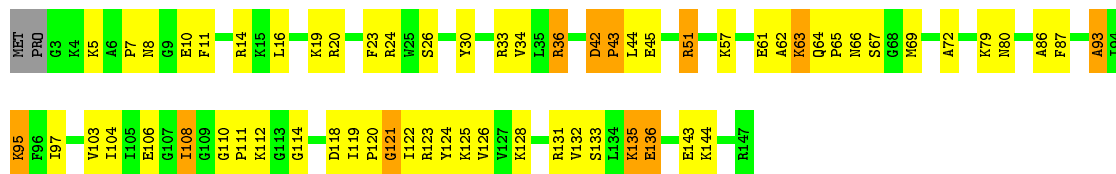
- Molecule 14: 30S ribosomal protein uS11

Chain M: 74% 19% . .



- Molecule 15: 30S ribosomal protein uS12

Chain N: 56% 35% 7% .



- Molecule 16: 30S ribosomal protein uS15

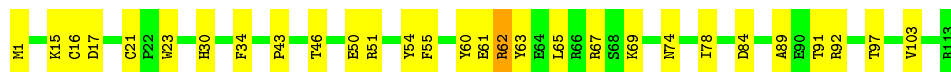
Chain Q: 75% 19% 6%





- Molecule 17: 30S ribosomal protein uS17

Chain R: 74% 25% .



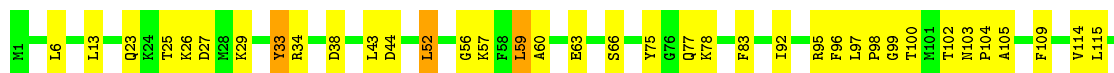
- Molecule 18: 30S ribosomal protein uS3

Chain A: 72% 22% . . .



- Molecule 19: 30S ribosomal protein uS2

Chain B: 73% 25% .



- Molecule 20: 30S ribosomal protein eS24

Chain V: 66% 28% . .



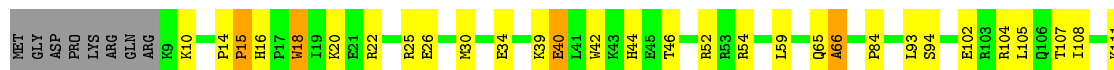
- Molecule 21: 30S ribosomal protein eS27

Chain W: 90% 10%



- Molecule 22: 30S ribosomal protein uS4

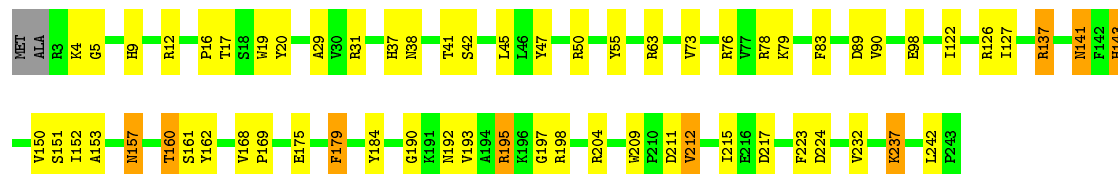
Chain D: 69% 23% . .





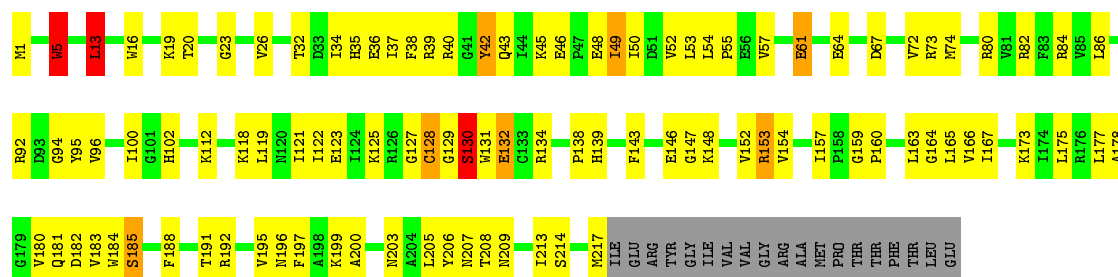
• Molecule 23: 30S ribosomal protein eS4

Chain E: 73% 22% ..



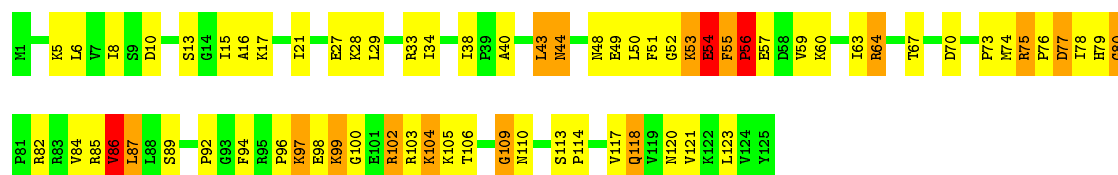
• Molecule 24: 30S ribosomal protein uS5

Chain F: 49% 39% 8% ..



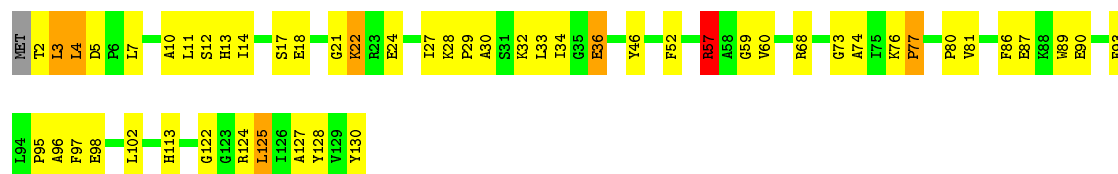
• Molecule 25: 30S ribosomal protein eS6

Chain G: 45% 41% 12% ..



• Molecule 26: 30S ribosomal protein uS8

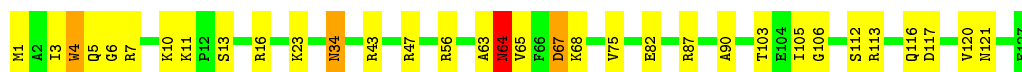
Chain I: 59% 35% 5% ..



• Molecule 27: 30S ribosomal protein eS8

Chain J: 74% 23% ..





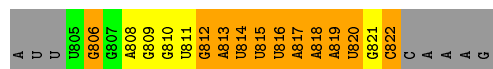
- Molecule 28: 30S ribosomal protein SX



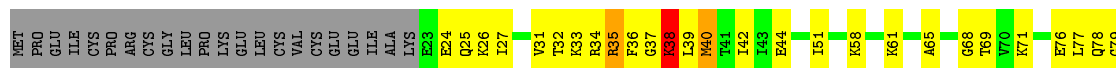
- Molecule 29: 30S ribosomal protein eL41



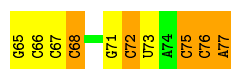
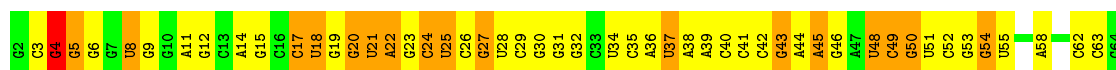
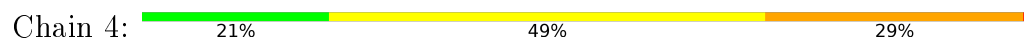
- Molecule 30: mRNA



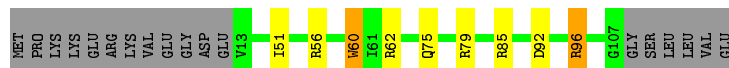
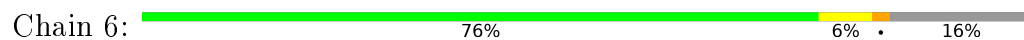
- Molecule 31: aIF1



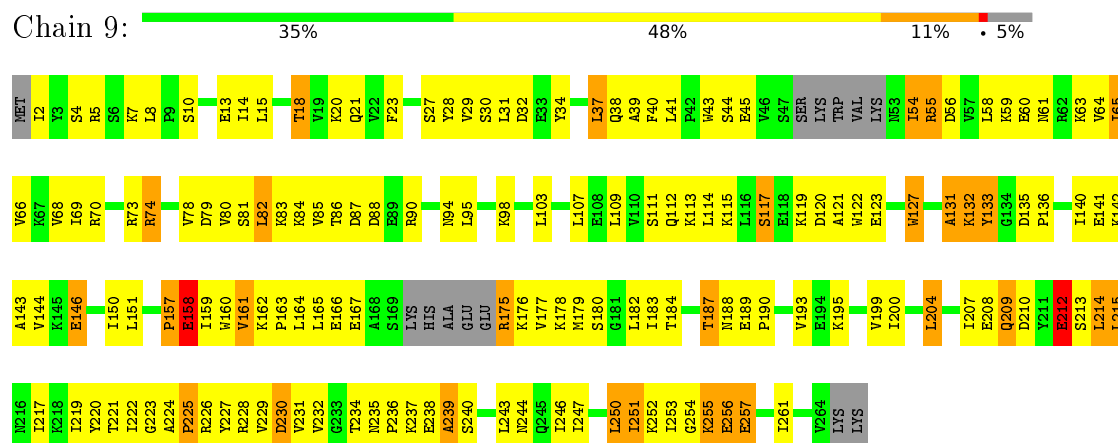
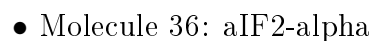
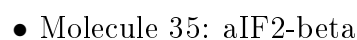
- Molecule 32: initiator Met-tRNA fMet from E. coli (A1U72 variant)



- Molecule 33: aIF1A



- Molecule 34: aIF2-gamma



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	12600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	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, GNP, H2U, MG, ZN

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	2	0.65	17/35964 (0.0%)	0.91	59/56130 (0.1%)
10	X	0.78	0/570	1.06	2/760 (0.3%)
11	Y	0.76	0/421	0.78	0/558
12	H	0.95	1/1765 (0.1%)	1.19	12/2371 (0.5%)
13	K	0.79	0/1088	0.92	3/1455 (0.2%)
14	M	0.77	0/1022	0.96	3/1375 (0.2%)
15	N	0.81	0/1156	1.07	2/1535 (0.1%)
16	Q	0.76	0/1338	0.99	5/1797 (0.3%)
17	R	0.72	0/956	0.95	2/1287 (0.2%)
18	A	0.68	0/1585	0.89	2/2124 (0.1%)
19	B	0.75	0/1654	0.98	4/2233 (0.2%)
2	Z	0.70	0/1480	0.87	2/1985 (0.1%)
20	V	0.67	0/839	1.00	3/1122 (0.3%)
21	W	0.65	0/485	0.88	0/651
22	D	0.75	2/1457 (0.1%)	0.94	5/1953 (0.3%)
23	E	0.68	0/2025	0.95	7/2732 (0.3%)
24	F	0.77	1/1745 (0.1%)	1.00	3/2350 (0.1%)
25	G	0.75	0/999	1.09	7/1337 (0.5%)
26	I	0.71	1/1049 (0.1%)	0.96	4/1408 (0.3%)
27	J	0.67	0/1013	0.92	0/1349
29	0	1.18	2/216 (0.9%)	1.11	0/279
3	3	0.86	0/951	0.90	1/1281 (0.1%)
30	5	0.42	0/434	0.72	0/675
31	1	0.39	0/636	0.50	0/843
32	4	0.41	0/1743	0.68	0/2716
33	6	0.33	0/808	0.54	0/1093
34	7	0.65	2/3227 (0.1%)	0.80	2/4367 (0.0%)
35	8	0.50	0/1046	0.81	1/1402 (0.1%)
36	9	0.52	0/2050	0.76	1/2760 (0.0%)
4	L	0.76	1/830 (0.1%)	1.08	3/1113 (0.3%)
5	O	0.82	0/1208	0.96	2/1619 (0.1%)
6	P	0.73	0/471	1.11	1/620 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	S	0.80	0/562	0.96	1/744 (0.1%)
8	T	0.84	0/942	0.91	0/1257
9	U	0.86	0/1203	0.95	3/1621 (0.2%)
All	All	0.68	27/74938 (0.0%)	0.92	140/108902 (0.1%)

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	X	0	3
12	H	4	9
13	K	0	2
15	N	0	2
16	Q	0	1
17	R	0	1
19	B	0	1
2	Z	0	1
20	V	0	3
23	E	0	1
24	F	0	2
25	G	1	7
26	I	0	1
27	J	0	3
32	4	0	1
34	7	0	3
36	9	0	1
5	O	0	1
All	All	5	43

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1019	A	O3'-P	32.77	2.00	1.61
1	2	1351	U	O3'-P	-26.03	1.29	1.61
34	7	271	PRO	C-N	21.68	1.83	1.34
29	0	3	TRP	CB-CG	-7.26	1.37	1.50
34	7	256	LEU	C-N	7.03	1.47	1.34

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	2	1019	A	P-O3'-C3'	21.19	145.13	119.70
1	2	1350	U	P-O3'-C3'	-16.16	100.30	119.70
1	2	1414	G	O5'-P-OP1	-15.24	91.99	105.70
1	2	962	G	O5'-P-OP1	-13.70	93.37	105.70
1	2	1350	U	O3'-P-O5'	11.66	126.15	104.00

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	H	85	PHE	CA
12	H	86	MET	CA
12	H	87	ARG	CA
12	H	96	LYS	CA
25	G	53	LYS	CA

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	O	124	LEU	Peptide
10	X	22	GLY	Peptide
10	X	4	ASP	Peptide
10	X	66	GLU	Peptide
2	Z	157	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32135	0	16232	1511	0
2	Z	1459	0	1549	10	0
3	3	939	0	994	5	0
4	L	822	0	870	25	0
5	O	1189	0	1248	11	0
6	P	462	0	492	6	0
7	S	556	0	604	5	0
8	T	923	0	986	7	0
9	U	1175	0	1216	20	0
10	X	568	0	600	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Y	409	0	410	3	0
12	H	1728	0	1775	127	0
13	K	1072	0	1128	16	0
14	M	1004	0	1041	15	0
15	N	1140	0	1235	47	0
16	Q	1310	0	1392	21	0
17	R	934	0	960	19	0
18	A	1559	0	1648	26	0
19	B	1623	0	1682	110	0
20	V	823	0	847	27	0
21	W	478	0	524	3	0
22	D	1434	0	1498	28	0
23	E	1976	0	2046	34	0
24	F	1716	0	1769	108	0
25	G	984	0	1044	98	0
26	I	1028	0	1065	44	0
27	J	1004	0	1088	17	0
28	C	286	0	61	3	0
29	0	213	0	250	11	0
30	5	388	0	193	30	0
31	1	632	0	668	125	0
32	4	1621	0	827	168	0
33	6	792	0	815	26	0
34	7	3171	0	3291	290	0
35	8	1033	0	1074	178	0
36	9	2025	0	2130	156	0
37	4	8	0	8	16	0
38	7	1	0	0	0	0
39	7	32	0	13	1	0
40	8	1	0	0	0	0
All	All	70653	0	55273	2703	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 22.

The worst 5 of 2703 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)
1:2:1367:C:H1'	31:1:65:ALA:CB	1.17	1.58
1:2:1367:C:C1'	31:1:65:ALA:CB	1.89	1.49
31:1:32:THR:HG21	31:1:42:ILE:CD1	1.40	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1053:A:C8	19:B:125:GLN:OE1	1.63	1.47
1:2:1053:A:N1	19:B:98:PRO:C	1.71	1.44

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	
2	Z	184/210 (88%)	167 (91%)	15 (8%)	2 (1%)	17	63
3	3	121/123 (98%)	102 (84%)	14 (12%)	5 (4%)	3	35
4	L	100/102 (98%)	90 (90%)	3 (3%)	7 (7%)	1	22
5	O	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	3	35
6	P	54/56 (96%)	43 (80%)	10 (18%)	1 (2%)	10	52
7	S	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	T	109/132 (83%)	97 (89%)	9 (8%)	3 (3%)	6	44
9	U	142/150 (95%)	129 (91%)	10 (7%)	3 (2%)	9	50
10	X	69/71 (97%)	56 (81%)	11 (16%)	2 (3%)	6	43
11	Y	48/50 (96%)	40 (83%)	8 (17%)	0	100	100
12	H	212/215 (99%)	161 (76%)	32 (15%)	19 (9%)	1	17
13	K	133/135 (98%)	117 (88%)	13 (10%)	3 (2%)	8	48
14	M	131/137 (96%)	116 (88%)	12 (9%)	3 (2%)	8	48
15	N	143/147 (97%)	119 (83%)	12 (8%)	12 (8%)	1	17
16	Q	156/158 (99%)	140 (90%)	12 (8%)	4 (3%)	7	45
17	R	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	21	66
18	A	188/198 (95%)	163 (87%)	15 (8%)	10 (5%)	2	29
19	B	200/202 (99%)	170 (85%)	28 (14%)	2 (1%)	19	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	V	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	29
21	W	61/63 (97%)	52 (85%)	8 (13%)	1 (2%)	12	56
22	D	170/180 (94%)	148 (87%)	15 (9%)	7 (4%)	3	35
23	E	239/243 (98%)	209 (87%)	21 (9%)	9 (4%)	4	37
24	F	215/236 (91%)	176 (82%)	32 (15%)	7 (3%)	5	41
25	G	123/125 (98%)	97 (79%)	15 (12%)	11 (9%)	1	17
26	I	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	12	56
27	J	125/127 (98%)	106 (85%)	13 (10%)	6 (5%)	3	31
29	0	20/22 (91%)	20 (100%)	0	0	100	100
31	1	78/102 (76%)	70 (90%)	6 (8%)	2 (3%)	7	45
33	6	95/113 (84%)	95 (100%)	0	0	100	100
34	7	407/415 (98%)	317 (78%)	68 (17%)	22 (5%)	2	29
35	8	125/139 (90%)	95 (76%)	27 (22%)	3 (2%)	7	47
36	9	247/266 (93%)	184 (74%)	46 (19%)	17 (7%)	1	22
All	All	4441/4674 (95%)	3760 (85%)	506 (11%)	175 (4%)	7	36

5 of 175 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	158	ALA
4	L	30	THR
4	L	92	GLU
10	X	4	ASP
12	H	13	HIS

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	
2	Z	145/167 (87%)	142 (98%)	3 (2%)	61	85
3	3	99/99 (100%)	93 (94%)	6 (6%)	23	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	91/91 (100%)	85 (93%)	6 (7%)	21	58
5	O	122/122 (100%)	118 (97%)	4 (3%)	45	76
6	P	46/46 (100%)	41 (89%)	5 (11%)	8	35
7	S	61/61 (100%)	58 (95%)	3 (5%)	31	67
8	T	99/114 (87%)	95 (96%)	4 (4%)	38	71
9	U	121/127 (95%)	113 (93%)	8 (7%)	21	58
10	X	60/60 (100%)	53 (88%)	7 (12%)	7	32
11	Y	41/41 (100%)	38 (93%)	3 (7%)	17	55
12	H	183/184 (100%)	167 (91%)	16 (9%)	13	46
13	K	111/111 (100%)	102 (92%)	9 (8%)	15	50
14	M	100/104 (96%)	91 (91%)	9 (9%)	12	44
15	N	118/121 (98%)	105 (89%)	13 (11%)	8	35
16	Q	143/143 (100%)	131 (92%)	12 (8%)	14	49
17	R	102/102 (100%)	99 (97%)	3 (3%)	50	78
18	A	166/171 (97%)	160 (96%)	6 (4%)	42	74
19	B	173/173 (100%)	161 (93%)	12 (7%)	19	57
20	V	89/89 (100%)	81 (91%)	8 (9%)	12	44
21	W	54/54 (100%)	52 (96%)	2 (4%)	41	74
22	D	153/160 (96%)	145 (95%)	8 (5%)	29	66
23	E	212/213 (100%)	194 (92%)	18 (8%)	13	49
24	F	181/197 (92%)	173 (96%)	8 (4%)	35	69
25	G	108/108 (100%)	93 (86%)	15 (14%)	4	27
26	I	107/108 (99%)	96 (90%)	11 (10%)	9	37
27	J	103/103 (100%)	99 (96%)	4 (4%)	39	72
29	0	21/21 (100%)	21 (100%)	0	100	100
31	1	69/91 (76%)	64 (93%)	5 (7%)	18	56
33	6	85/99 (86%)	81 (95%)	4 (5%)	32	68
34	7	352/357 (99%)	299 (85%)	53 (15%)	3	23
35	8	118/126 (94%)	104 (88%)	14 (12%)	6	32
36	9	226/239 (95%)	198 (88%)	28 (12%)	6	31
All	All	3859/4002 (96%)	3552 (92%)	307 (8%)	20	51

5 of 307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	W	14	LEU
24	F	153	ARG
36	9	56	ASP
22	D	118	MET
23	E	151	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
23	E	38	ASN
23	E	157	ASN
35	8	93	ASN
23	E	113	HIS
23	E	143	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1493/1518 (98%)	338 (22%)	112 (7%)
30	5	17/26 (65%)	12 (70%)	2 (11%)
32	4	75/76 (98%)	25 (33%)	0
All	All	1585/1620 (97%)	375 (23%)	114 (7%)

5 of 375 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	C
1	2	14	C
1	2	25	C
1	2	38	G

5 of 114 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	856	G
1	2	963	A
1	2	1453	U
1	2	891	A

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Mol	Chain	Res	Type
1	2	924	U

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

3 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$
32	H2U	4	21	32	17,21,22	3.23	4 (23%)	23,30,33	2.43	1 (4%)
32	OMC	4	33	32	14,21,23	0.90	1 (7%)	18,30,34	0.45	0
32	5MU	4	55	32	13,22,23	1.13	2 (15%)	16,32,35	4.76	3 (18%)

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
32	H2U	4	21	32	-	0/7/38/39	0/2/2/2
32	OMC	4	33	32	-	0/3/25/28	0/2/2/2
32	5MU	4	55	32	-	0/3/25/26	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	21	H2U	C6-C5	-10.78	1.34	1.52
32	4	21	H2U	C6-N1	-6.78	1.38	1.47
32	4	21	H2U	C5-C4	-2.60	1.43	1.50
32	4	55	5MU	C6-C5	-2.26	1.34	1.40
32	4	33	OMC	C6-C5	-2.11	1.33	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	55	5MU	C5-C4-N3	-11.93	115.34	125.35
32	4	55	5MU	C5M-C5-C6	2.16	123.01	118.63
32	4	21	H2U	C5-C6-N1	10.98	122.80	110.76
32	4	55	5MU	C4-N3-C2	14.53	127.28	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	4	21	H2U	1	0
32	4	55	5MU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
37	MET	4	101	-	5,7,8	0.40	0	4,7,9	0.94	0
39	GNP	7	502	38	29,34,34	2.85	11 (37%)	28,54,54	1.76	5 (17%)

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
37	MET	4	101	-	-	0/4/6/8	0/0/0/0
39	GNP	7	502	38	-	0/16/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	502	GNP	PB-O3A	-7.56	1.49	1.59
39	7	502	GNP	C5-C6	-6.33	1.41	1.53
39	7	502	GNP	C4-N9	-6.13	1.39	1.47
39	7	502	GNP	PB-O2B	-3.20	1.48	1.56
39	7	502	GNP	PG-O2G	-2.97	1.48	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	502	GNP	PA-O3A-PB	-3.35	120.55	132.71
39	7	502	GNP	C3'-C2'-C1'	2.35	106.16	101.44
39	7	502	GNP	O2B-PB-O1B	2.94	115.81	110.02
39	7	502	GNP	O6-C6-C5	4.05	127.44	119.69
39	7	502	GNP	C4-C5-N7	5.47	111.20	102.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	4	101	MET	16	0
39	7	502	GNP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	4

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Mol	Chain	Number of breaks
34	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1342:C	O3'	1343:C	P	3.20
1	2	1060:G	O3'	1061:A	P	2.56
1	2	1019:A	O3'	1020:G	P	2.00
1	7	271:PRO	C	272:ILE	N	1.83
1	2	1351:U	O3'	1352:G	P	1.29