



wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 03:56 PM EDT

PDB ID : 5LMU
EMDB ID: : EMD-4080
Title : Structure of bacterial 30S-IF3-mRNA-tRNA translation pre-initiation complex, closed form (state-4)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 4.00 Å(reported)

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) : rb-20027939

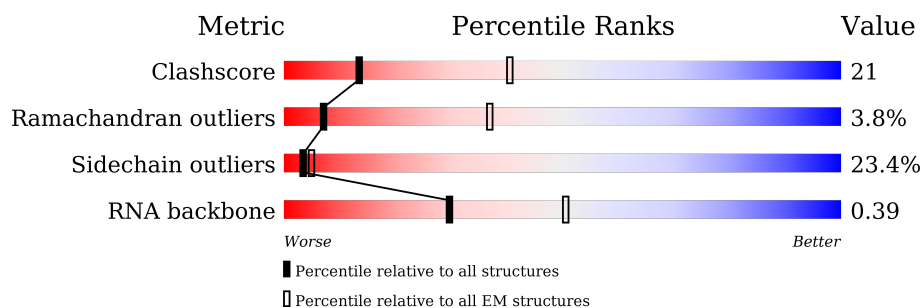
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.










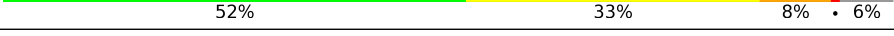

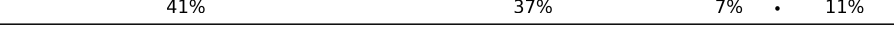
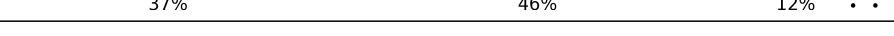
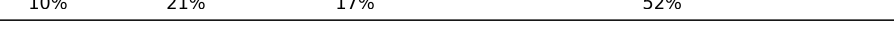
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	1522	22% 55% 22% .
2	B	256	45% 34% 11% . 9%
3	C	239	49% 31% 6% 14%
4	D	209	49% 39% 11%
5	E	162	58% 23% 12% 7%
6	F	101	51% 39% 8% .
7	G	156	69% 30% ..
8	H	138	63% 29% 7% .

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Mol	Chain	Length	Quality of chain
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	X	171	
23	Y	42	
24	Z	77	

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
26	ZN	D	300	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 55195 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	A	1515	Total	C	N	O	P	0	0
			32548	14490	6022	10523	1513		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	118	Total	C	N	O	S	0	0
			937	579	193	163	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			655	419	120	114	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	164	Total	C	N	O	S	0	0
			1336	841	245	241	9		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 24 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	77	Total	C	N	O	P	S	0	0
			1646	735	297	536	77	1		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	Z	1	Total	Mg	0
			1	1	
25	A	78	Total	Mg	0
			78	78	
25	L	1	Total	Mg	0
			1	1	

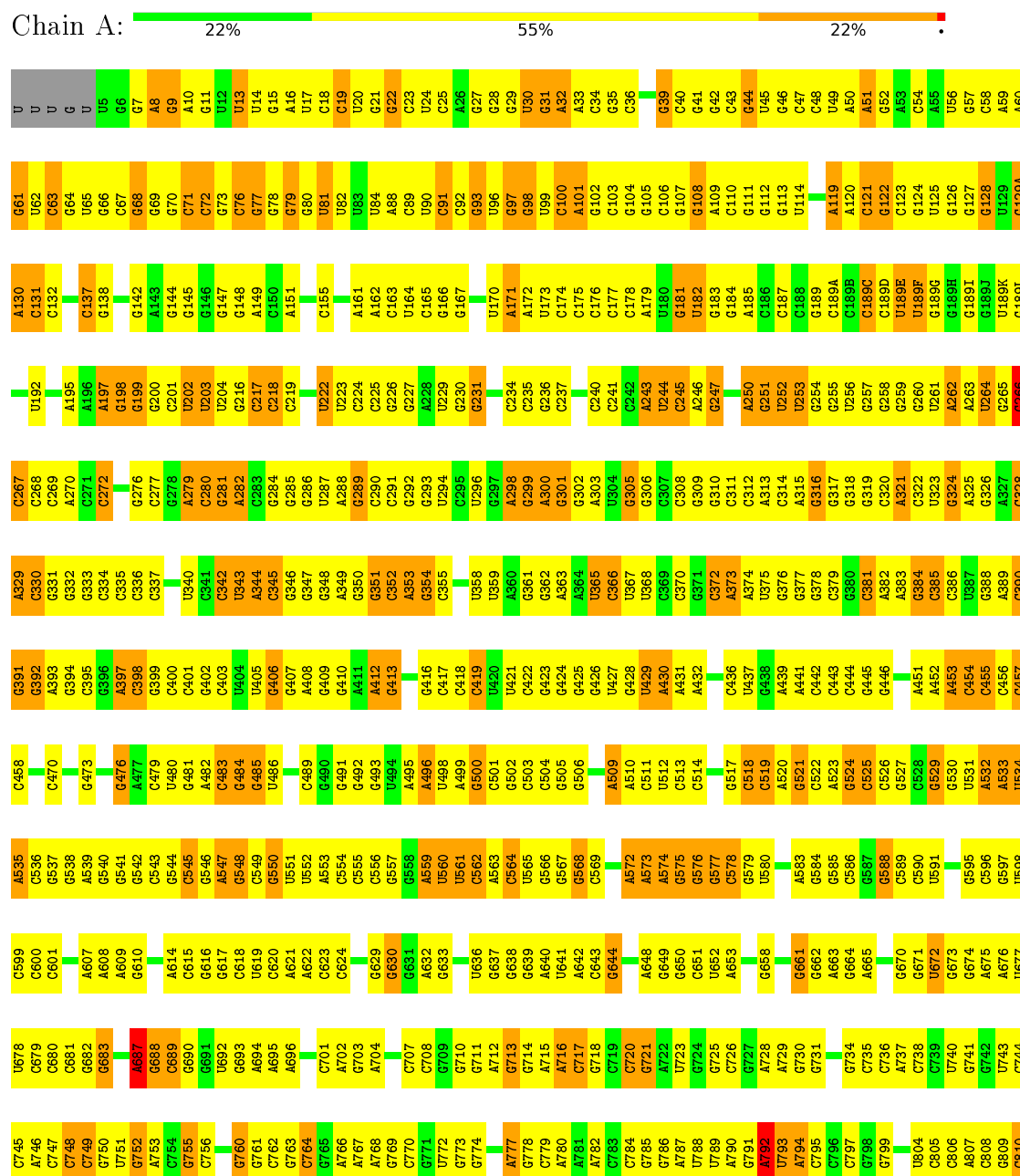
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	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: 16S ribosomal RNA



V239
Q240
GLU
ALA
GLU
ALA
ALA
THR
GLU
THR
PRO
GLU
GLY
GLY
SER
GLU
VAL
GLU
ALA

• Molecule 3: 30S ribosomal protein S3

Chain C: 49% 31% 6% 14%

YET G2 R3 H6 P7 T8 G9 T14 T15 T16 D17 S20 R21 V22 K26 K27 K28 Y29 L32 L33 L34 E35 I39 L42 L43 E44 K45 G51 L52 V55 D56 I57 E58 E59 A65 V66 T67 V68 V69 V70 A71 I77 T78 R79 G80 G81 E82 R83 I84 R85 V86 L87 R88 E89 E90 L91 L94 T95 T96 N98 L101 Q104 E105 V106 Q107 N108 L111 S112 A113 P114 R119 Q123 I124 E125 R131 V138 Q139 R140 G148 A149 I150 V151 E152 V153 S154 G155 R156 I157 E161 R164 T165 E166 W167 R172 L175 H176 T177 L178 R179 L188 A189 R190 T191 T192 Y193 L196 Y201 L204 E205 E206 V207 ILE GLY GLN GLN LYS LYS LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU ARG PRO ARG ARG ARG ARG PRO VAL VAL LYS GLU

• Molecule 4: 30S ribosomal protein S4

Chain D: 49% 39% 11%

YET G2 R3 Y4 I5 G6 P7 V8 C9 R10 L11 L12 R13 R14 E15 Y20 L21 K22 K23 K24 E24 C26 Y27 C31 A32 R33 R34 R35 R36 P37 T38 P39 P40 P41 G44 Q45 Q46 R47 R48 A48 R49 E50 P51 S52 D53 V56 R57 L58 R59 E60 G61 Q62 K63 L64 R65 R66 L67 Y68 G69 S70 S71 E72 F75 L78 F79 L97 R100 D102 V104 V105 L108 G109 F110 A111 V112 R115 R118 Q119 R120 V121 R122 H125 R131 R132 V133 D134 L135 P136 A137 X138 R139 V140 R141 D144 R145 I146 E150 L155 E156 L157 L158 L162 E163 A164 M165 K166 G167 R168 W173 L174 L175 L176 D177 V178 M181 K182 G183 L186 R187 L188 E192 D193 L196 P197 V198 N199 E200 Q201 L202 V203 L204 E205 F206 V207 S208 R209

• Molecule 5: 30S ribosomal protein S5

Chain E: 58% 23% 12% 7%

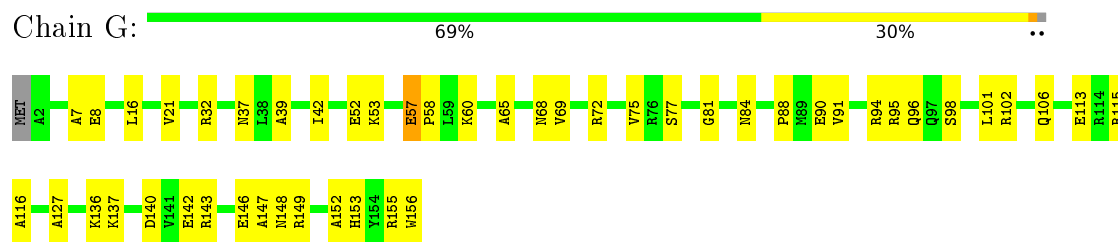
YET PRO THR D5 T11 T12 T13 R14 R15 T16 Q20 A21 R24 R25 F26 R27 F28 V32 V33 V34 Q38 Q39 R40 V41 K47 E50 V51 P52 V55 Q56 R57 A58 Q59 V60 V61 A62 R63 E68 V69 V70 L71 E79 I80 E81 V82 V90 L91 R92 P93 V100 I101 A102 V105 P106 R107 L110 A113 G114 V115 T116 D117 I118 E122 L123 R126 N127 P128 I131 L139 L142 R143 V148 E152 K153 G154 GLU ALA HIS ALA GLN ALA GLN GLY Q56 R57 A58 Q59 V60 V61 A62 R63 E68 V69 V70 L71 E79 I80 E81 V82 V90 L91 R92 P93 V100 I101 A102 V105 P106 R107 L110 A113 G114 V115 T116 D117 I118 E122 L123 R126 N127 P128 I131 L139 L142 R143 V148 E152 K153 G154 GLU ALA HIS ALA GLN ALA GLN GLY

• Molecule 6: 30S ribosomal protein S6

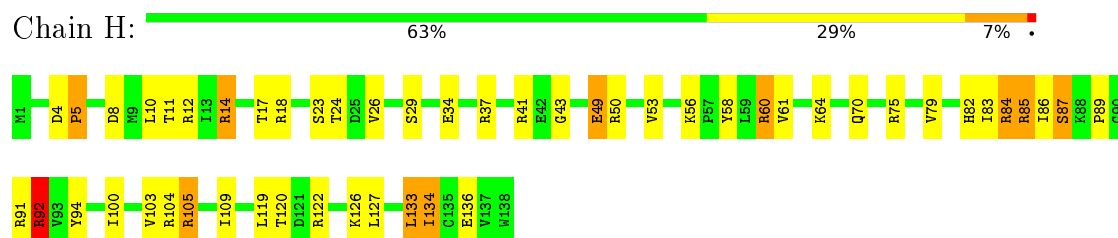
Chain F: 51% 39% 8%

H1 R2 R3 Y4 E5 V6 I7 I8 V9 L10 D15 L19 A20 L21 E24 A35 R36 V37 E38 K39 V40 E41 E42 L43 G44 L45 R46 R47 I52 A53 Y59 F60 L61 W62 Y63 Q64 Q65 E66 M67 E68 E69 V72 L73 A76 R77 E78 L79 R80 I81 R86 R87 R88 R89 V90 Y91 R92 S93 Q94 E95 P96 A101

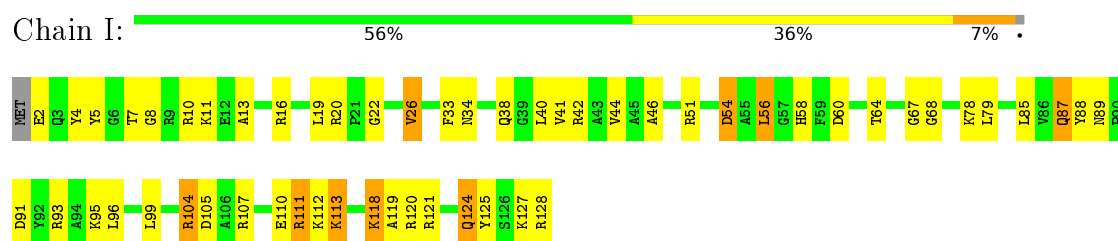
• Molecule 7: 30S ribosomal protein S7



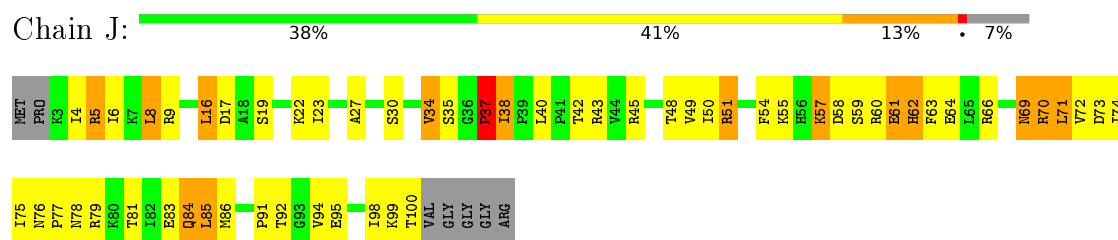
- Molecule 8: 30S ribosomal protein S8



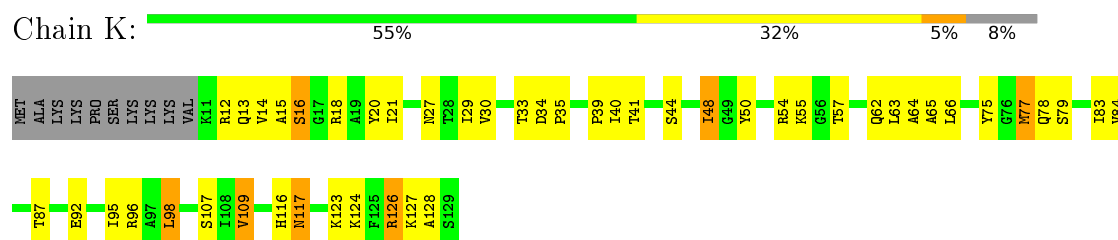
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

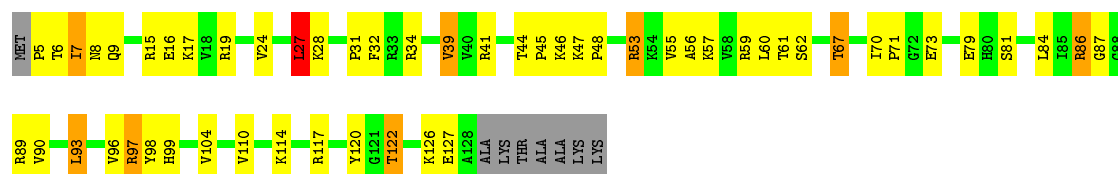


- Molecule 11: 30S ribosomal protein S11



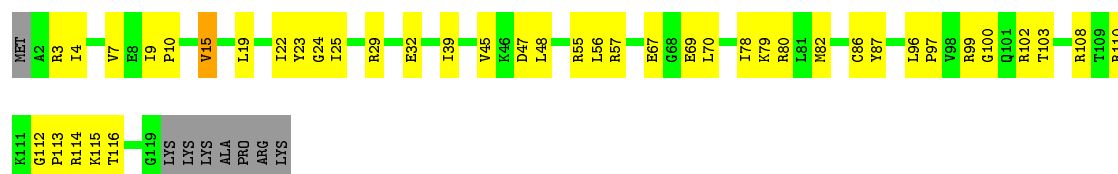
- Molecule 12: 30S ribosomal protein S12





- Molecule 13: 30S ribosomal protein S13

Chain M: 60% 33% 6%



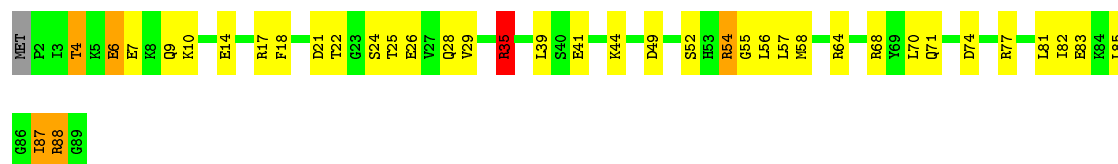
- Molecule 14: 30S ribosomal protein S14 type Z

Chain N: 54% 36% 8%



- Molecule 15: 30S ribosomal protein S15

Chain O: 56% 36% 6%



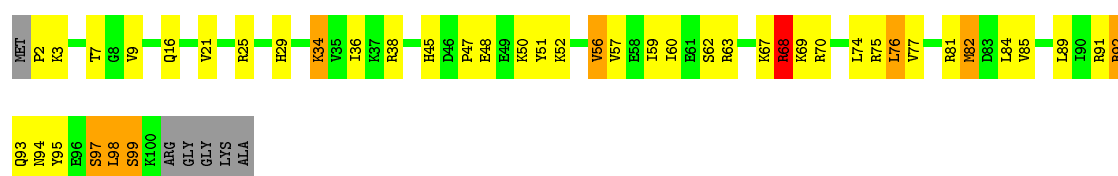
- Molecule 16: 30S ribosomal protein S16

Chain P: 65% 22% 8%

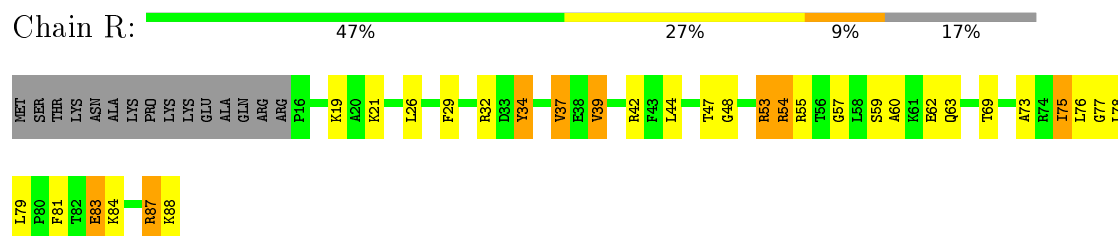


- Molecule 17: 30S ribosomal protein S17

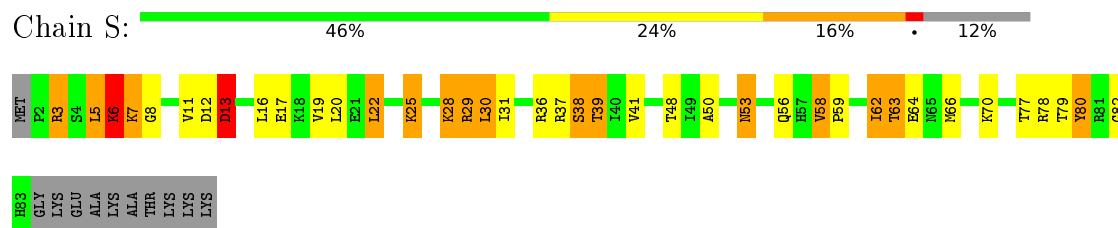
Chain Q: 52% 33% 8%



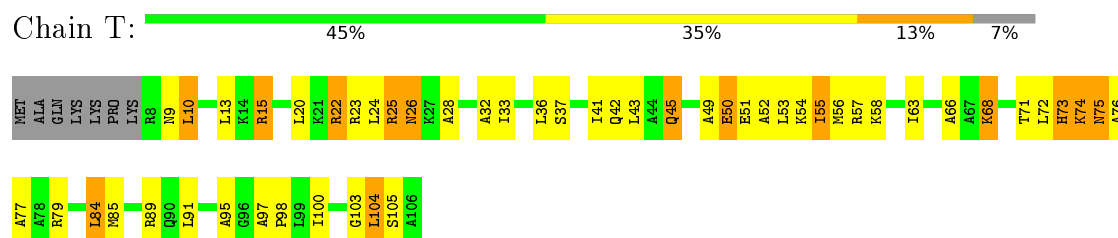
- Molecule 18: 30S ribosomal protein S18



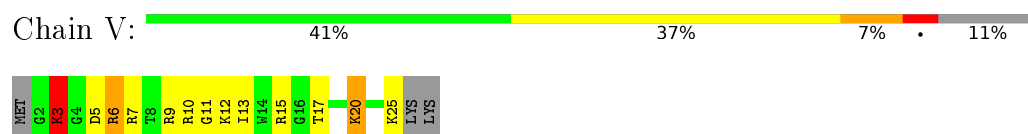
- Molecule 19: 30S ribosomal protein S19



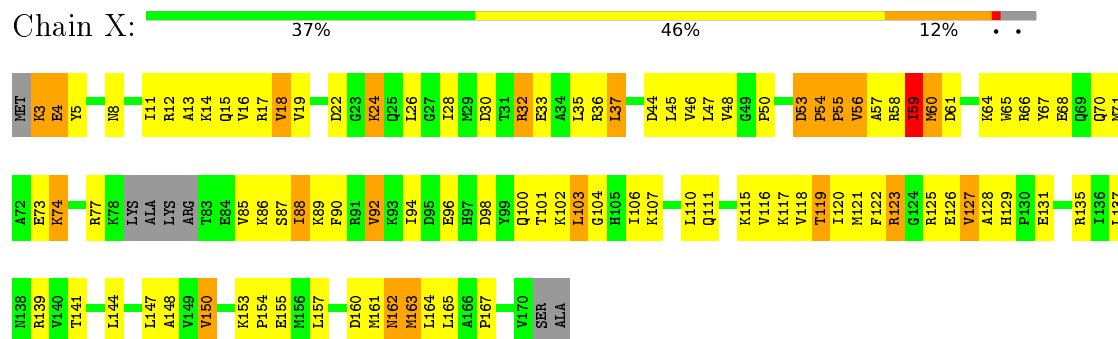
- Molecule 20: 30S ribosomal protein S20



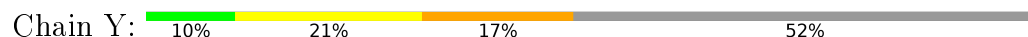
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: Translation initiation factor IF-3

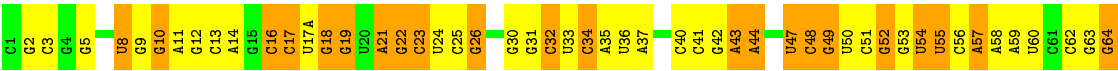
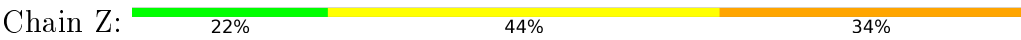


- Molecule 23: mRNA





● Molecule 24: tRNAi



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	26949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	78000	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, ZN, G7M, MG, 4SU, 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	A	0.32	1/36426 (0.0%)	0.75	13/56837 (0.0%)
10	J	0.43	0/805	0.78	1/1082 (0.1%)
11	K	0.45	0/900	0.78	0/1213
12	L	0.37	0/986	0.82	0/1320
13	M	0.43	0/947	0.80	0/1270
14	N	0.41	0/501	0.83	1/664 (0.2%)
15	O	0.46	0/745	0.93	1/992 (0.1%)
16	P	0.44	0/716	0.79	0/963
17	Q	0.40	0/836	0.80	0/1117
18	R	0.44	0/604	0.83	0/801
19	S	0.43	0/670	0.81	0/903
2	B	0.52	0/1935	0.92	4/2609 (0.2%)
20	T	0.43	0/765	0.92	1/1007 (0.1%)
21	V	0.42	0/212	0.83	0/277
22	X	0.57	0/1354	1.00	6/1813 (0.3%)
23	Y	0.34	0/493	0.74	0/766
24	Z	0.42	0/1721	0.79	1/2682 (0.0%)
3	C	0.47	0/1636	0.82	1/2205 (0.0%)
4	D	0.41	0/1733	0.84	0/2318
5	E	0.43	0/1162	0.83	0/1564
6	F	0.43	0/856	0.86	2/1154 (0.2%)
7	G	0.43	0/1276	0.81	0/1709
8	H	0.42	0/1136	0.81	0/1527
9	I	0.44	0/1029	0.77	0/1379
All	All	0.37	1/59444 (0.0%)	0.78	31/88172 (0.0%)

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
1	A	0	2
19	S	0	1
22	X	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	C	O3'-P	-5.67	1.54	1.61

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	4	GLU	N-CA-CB	-14.85	83.86	110.60
1	A	266	G	C2'-C3'-O3'	7.90	126.87	109.50
1	A	1145	C	C2'-C3'-O3'	7.31	125.58	109.50
1	A	1498	U	C2'-C3'-O3'	7.03	124.96	109.50
22	X	35	LEU	CA-CB-CG	6.98	131.34	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1445	C	Sidechain
1	A	218	C	Sidechain
19	S	3	ARG	Peptide
22	X	3	LYS	Peptide
22	X	53	ASP	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	A	32548	0	16440	1268	0
2	B	1900	0	1951	72	0
3	C	1612	0	1675	61	0
4	D	1703	0	1767	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1146	0	1207	46	0
6	F	843	0	857	25	0
7	G	1257	0	1296	14	0
8	H	1116	0	1177	20	0
9	I	1010	0	1037	30	0
10	J	792	0	834	99	0
11	K	885	0	904	16	0
12	L	970	0	1057	31	0
13	M	937	0	995	18	0
14	N	492	0	531	15	0
15	O	734	0	771	14	0
16	P	700	0	720	17	0
17	Q	823	0	891	24	0
18	R	598	0	670	17	0
19	S	655	0	672	26	0
20	T	763	0	861	46	0
21	V	208	0	221	9	0
22	X	1336	0	1388	85	0
23	Y	439	0	219	18	0
24	Z	1646	0	843	57	0
25	A	78	0	0	3	0
25	L	1	0	0	0	0
25	Z	1	0	0	0	0
26	D	1	0	0	2	0
26	N	1	0	0	1	0
All	All	55195	0	38984	1968	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 21.

The worst 5 of 1968 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)
10:J:38:ILE:HG23	10:J:71:LEU:CB	1.24	1.66
10:J:38:ILE:CG2	10:J:71:LEU:HB3	1.04	1.50
1:A:412:A:N3	4:D:35:ARG:NH1	1.66	1.44
1:A:1358:U:H3	1:A:1363(A):A:N6	1.13	1.43
1:A:1061:G:C5'	10:J:59:SER:OG	1.68	1.39

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	232/256 (91%)	184 (79%)	33 (14%)	15 (6%)	1	26
3	C	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	9	54
4	D	206/209 (99%)	176 (85%)	26 (13%)	4 (2%)	10	54
5	E	148/162 (91%)	125 (84%)	19 (13%)	4 (3%)	6	47
6	F	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	2	31
7	G	153/156 (98%)	132 (86%)	18 (12%)	3 (2%)	9	54
8	H	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	13	58
9	I	125/128 (98%)	104 (83%)	14 (11%)	7 (6%)	2	29
10	J	96/105 (91%)	79 (82%)	12 (12%)	5 (5%)	2	31
11	K	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	2	31
12	L	122/132 (92%)	95 (78%)	24 (20%)	3 (2%)	7	49
13	M	116/126 (92%)	100 (86%)	13 (11%)	3 (3%)	7	48
14	N	58/61 (95%)	44 (76%)	9 (16%)	5 (9%)	1	17
15	O	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	8	51
16	P	81/88 (92%)	71 (88%)	8 (10%)	2 (2%)	7	49
17	Q	97/105 (92%)	82 (84%)	10 (10%)	5 (5%)	2	31
18	R	71/88 (81%)	62 (87%)	8 (11%)	1 (1%)	14	59
19	S	80/93 (86%)	63 (79%)	12 (15%)	5 (6%)	2	27
20	T	97/106 (92%)	81 (84%)	11 (11%)	5 (5%)	2	31
21	V	22/27 (82%)	19 (86%)	1 (4%)	2 (9%)	1	16
22	X	160/171 (94%)	137 (86%)	17 (11%)	6 (4%)	4	39
All	All	2506/2709 (92%)	2111 (84%)	301 (12%)	94 (4%)	7	39

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
2	B	229	VAL
4	D	37	PRO
5	E	21	ALA

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	B	202/220 (92%)	154 (76%)	48 (24%)	1	8
3	C	160/188 (85%)	121 (76%)	39 (24%)	1	7
4	D	180/181 (99%)	132 (73%)	48 (27%)	0	5
5	E	115/123 (94%)	83 (72%)	32 (28%)	0	4
6	F	90/90 (100%)	72 (80%)	18 (20%)	1	13
7	G	126/127 (99%)	103 (82%)	23 (18%)	2	16
8	H	119/119 (100%)	86 (72%)	33 (28%)	0	4
9	I	98/99 (99%)	76 (78%)	22 (22%)	1	10
10	J	87/92 (95%)	69 (79%)	18 (21%)	1	11
11	K	90/99 (91%)	67 (74%)	23 (26%)	0	6
12	L	104/109 (95%)	82 (79%)	22 (21%)	1	11
13	M	94/101 (93%)	79 (84%)	15 (16%)	3	23
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	4
15	O	79/80 (99%)	53 (67%)	26 (33%)	0	3
16	P	72/74 (97%)	57 (79%)	15 (21%)	1	11
17	Q	94/97 (97%)	78 (83%)	16 (17%)	2	20
18	R	64/77 (83%)	47 (73%)	17 (27%)	0	5
19	S	71/80 (89%)	50 (70%)	21 (30%)	0	4
20	T	76/82 (93%)	56 (74%)	20 (26%)	0	6
21	V	19/22 (86%)	13 (68%)	6 (32%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	X	145/150 (97%)	121 (83%)	24 (17%)	3 21
All	All	2134/2260 (94%)	1634 (77%)	500 (23%)	3 8

5 of 500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	84	ARG
10	J	85	LEU
20	T	50	GLU
8	H	105	ARG
9	I	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	68	ASN
10	J	78	ASN
22	X	129	HIS
9	I	87	GLN
9	I	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1522 (99%)	452 (29%)	109 (7%)
23	Y	18/42 (42%)	9 (50%)	1 (5%)
24	Z	76/77 (98%)	37 (48%)	5 (6%)
All	All	1603/1641 (97%)	498 (31%)	115 (7%)

5 of 498 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	19	C
1	A	22	G

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	850	U
1	A	993	G
1	A	1503	A
1	A	864	A
1	A	960	U

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

5 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$
24	OMC	Z	32	24	15,22,23	0.77	1 (6%)	20,31,34	1.50	3 (15%)
24	G7M	Z	46	24	18,26,27	2.81	3 (16%)	21,39,42	2.84	7 (33%)
24	5MU	Z	54	24	13,22,23	0.82	0	16,32,35	3.32	4 (25%)
24	PSU	Z	55	24	15,21,22	0.88	0	16,30,33	2.56	5 (31%)
24	4SU	Z	8	24	12,21,22	1.01	1 (8%)	15,30,33	1.80	3 (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
24	OMC	Z	32	24	-	0/5/27/28	0/2/2/2
24	G7M	Z	46	24	-	0/3/25/26	0/3/3/3
24	5MU	Z	54	24	-	0/3/25/26	0/2/2/2
24	PSU	Z	55	24	-	0/7/25/26	0/2/2/2
24	4SU	Z	8	24	-	0/3/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	32	OMC	O4'-C1'	2.04	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	8	4SU	O4'-C1'	2.56	1.44	1.41
24	Z	46	G7M	C6-C5	3.90	1.49	1.41
24	Z	46	G7M	C8-N7	7.30	1.46	1.33
24	Z	46	G7M	C8-N9	8.01	1.48	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	54	5MU	C5-C4-N3	-8.42	118.28	125.35
24	Z	46	G7M	N7-C8-N9	-8.24	96.51	108.67
24	Z	46	G7M	C5-C6-N1	-5.39	116.47	123.52
24	Z	8	4SU	C5-C4-N3	-4.44	118.85	123.56
24	Z	55	PSU	C5-C1'-C2'	-4.29	108.15	115.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	32	OMC	1	0
24	Z	54	5MU	2	0
24	Z	55	PSU	2	0
24	Z	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 82 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
23	Y	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1442(A):G	O3'	1442(B):A	P	5.11
1	A	84:U	O3'	88:A	P	5.07
1	A	93:G	O3'	96:U	P	4.99
1	A	204:U	O3'	216:G	P	4.97
1	A	841:U	O3'	848:C	P	4.05