



wwPDB EM Validation Summary Report ⓘ

Feb 19, 2025 – 12:17 pm GMT

PDB ID : 8P6P
EMDB ID : EMD-17133
Title : Mycoplasma pneumoniae small ribosomal subunit in chloramphenicol-treated cells
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-05-27
Resolution : 3.20 Å (reported)
Based on initial models : 7OOC, 7OOD

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

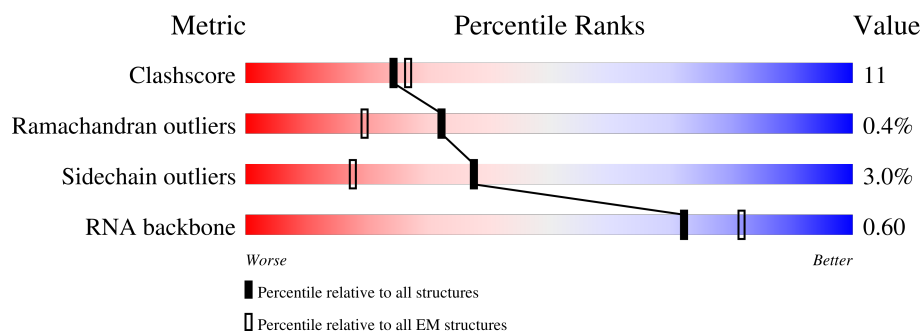
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.




















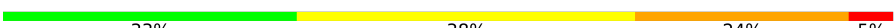

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	3	2907	99%
2	5	1520	52% 41% 6%
3	7	75	20% 17% 60%
4	8	76	20% 18% 61%
5	A	294	58% 31% 10%
6	B	273	67% 17% 15%
7	C	205	62% 36%

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Mol	Chain	Length	Quality of chain
8	D	219	
9	E	215	
10	F	155	
11	G	142	
12	H	132	
13	I	108	
14	J	121	
15	K	139	
16	L	124	
17	M	61	
18	N	86	
19	O	94	
20	P	85	
21	Q	104	
22	R	87	
23	S	87	
24	T	60	
25	Y	21	
26	x	97	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 55465 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	24	Total	C	N	O	P	0	0
			512	229	93	166	24		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	1507	Total	C	N	O	P	0	0
			32258	14420	5847	10484	1507		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 3 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	30	Total	C	N	O	P	0	0
			640	285	112	213	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 4 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	30	Total	C	N	O	P	0	0
			639	286	114	209	30		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	266	Total	C	N	O	S	0	0
			2138	1359	376	394	9		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	232	Total	C	N	O	S	0	0
			1835	1158	343	329	5		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	155	Total	C	N	O	S	0	0
			1191	753	228	207	3		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	184	Total	C	N	O	S	0	0
			1509	950	270	287	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1254	790	240	217	7		

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	129	Total	C	N	O	S	0	0
			1040	661	195	183	1		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	104	Total	C	N	O	S	0	0
			832	536	147	148	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	135	Total	C	N	O	S	0	0
			1071	677	212	180	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	123	Total	C	N	O	0	0
			991	618	200	173		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	60	Total	C	N	O	0	0
			474	302	96	72	4	

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	N	85	Total	C	N	O	0	0
			689	436	130	123		

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	87	Total	C	N	O	S	0	0
			705	453	130	118	4		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	85	Total	C	N	O	S	0	0
			693	436	138	118	1		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	71	Total	C	N	O	S	0	0
			590	378	115	93	4		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	86	Total	C	N	O	S	0	0
			700	444	132	122	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	79	Total	C	N	O		0	0
			643	391	138	114			

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	59	Total	C	N	O	S	0	0
			519	326	111	80	2		

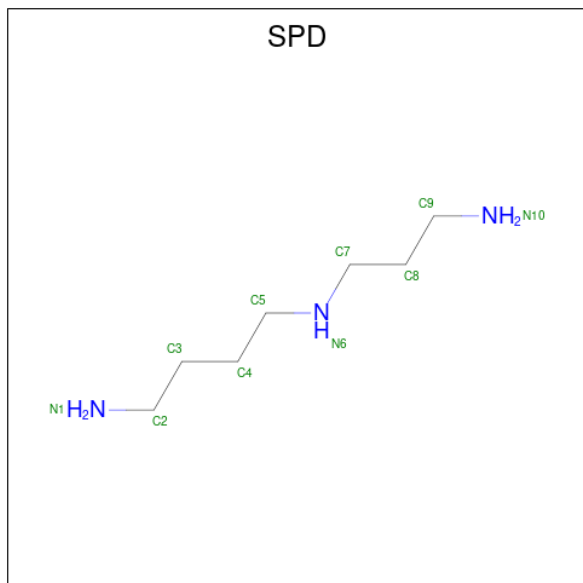
- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	21	Total	C	N	O	P	0	0
			446	200	79	146	21		

- Molecule 26 is a protein called 50S ribosomal protein L31.

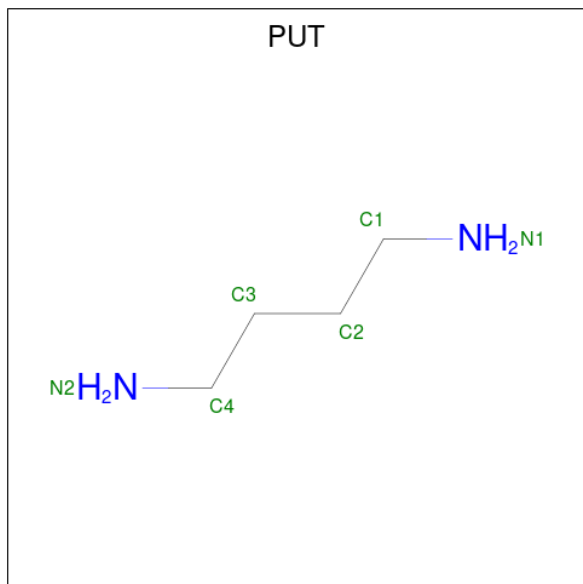
Mol	Chain	Residues	Atoms				AltConf	Trace
26	x	43	Total	C	N	O	0	0
			342	214	65	63		

- Molecule 27 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



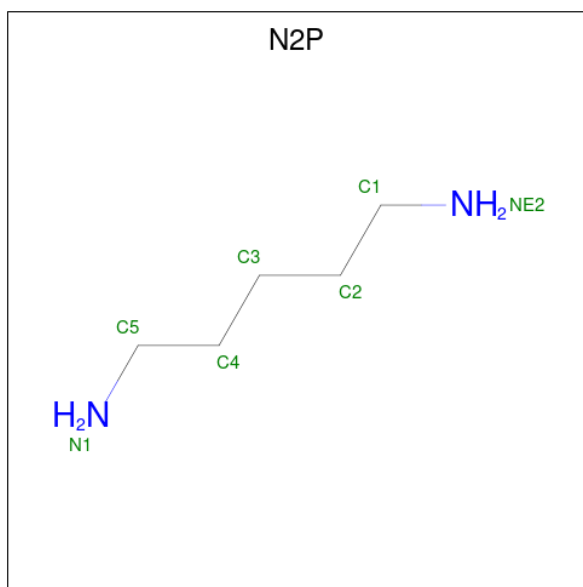
Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	N	0
			10	7	3	
27	5	1	Total	C	N	0
			10	7	3	

- Molecule 28 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	N	0
			6	4	2	
28	5	1	Total	C	N	0
			6	4	2	

- Molecule 29 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: C₅H₁₄N₂).



Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	N	0
			7	5	2	

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	5	96	Total	Mg	0
			96	96	
30	7	1	Total	Mg	0
			1	1	
30	8	1	Total	Mg	0
			1	1	
30	H	1	Total	Mg	0
			1	1	
30	K	1	Total	Mg	0
			1	1	
30	L	1	Total	Mg	0
			1	1	
30	P	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
30	Y	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	M	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	

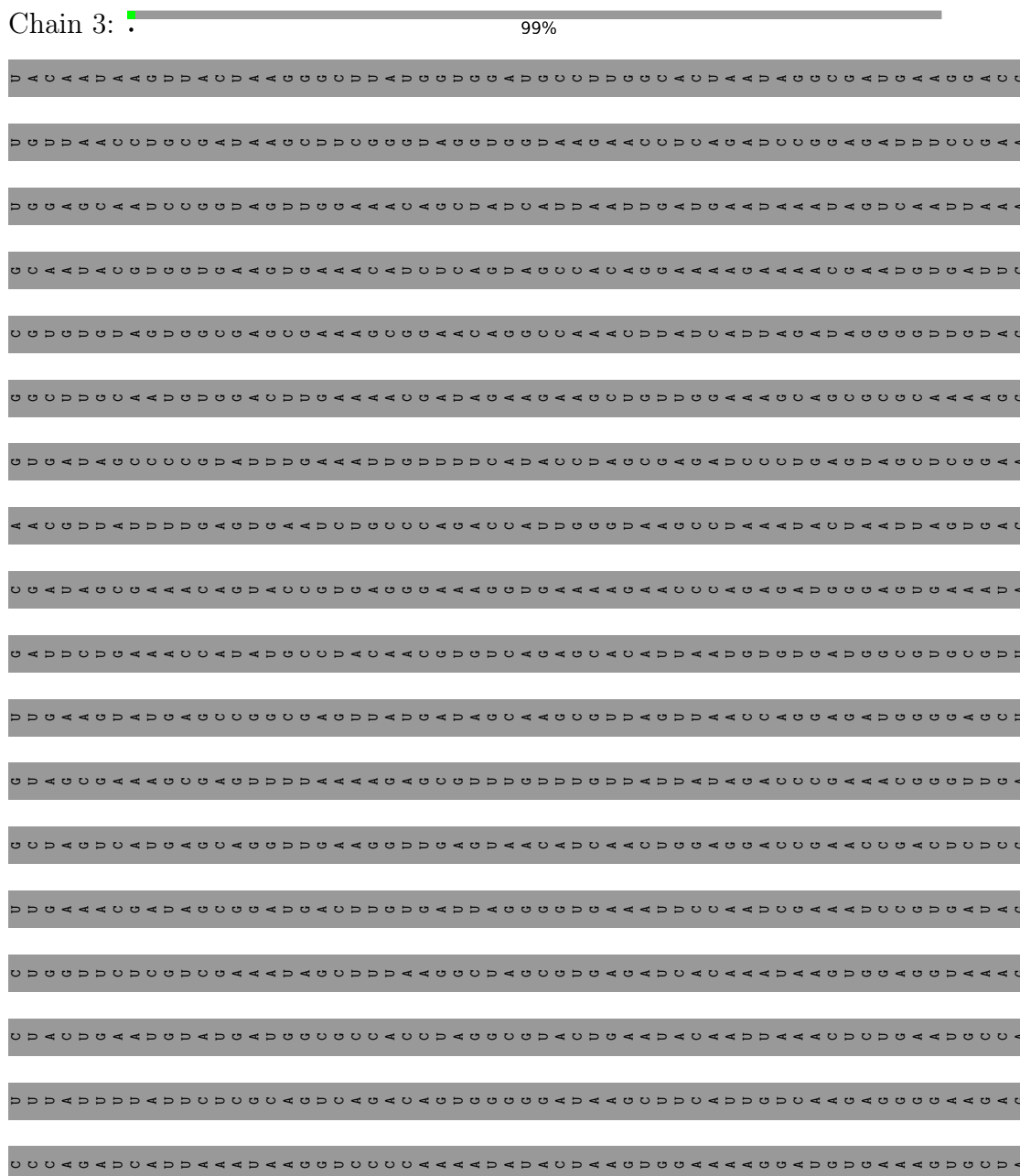
- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	5	1	Total	O	0
			1	1	
32	A	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

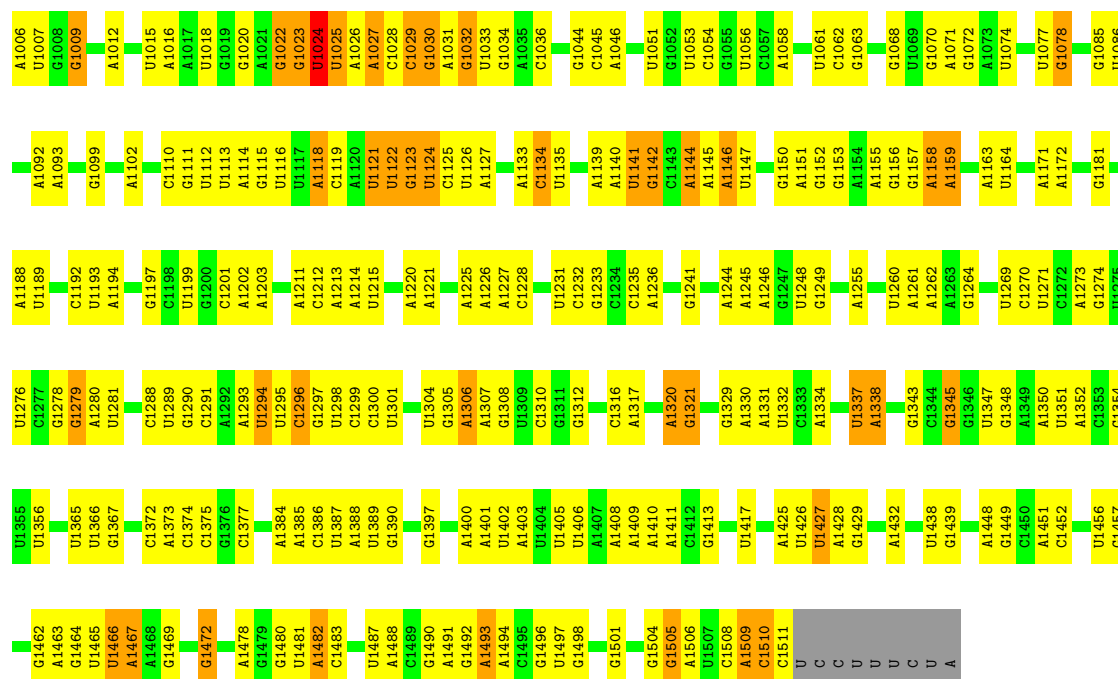
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 23S ribosomal RNA



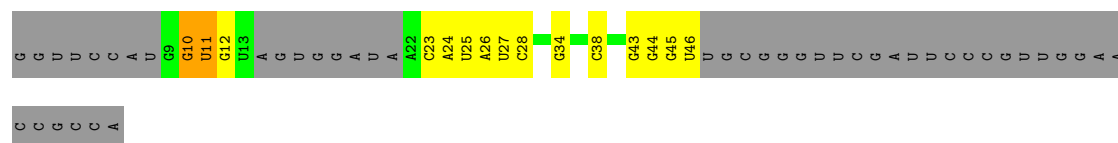
A A A C A G C A A G G A U G U U U G G C C U U A A G A A G C A U C C G U U U A A A G A G U G C G U A A C A G C C A C U
U G U C G A G U G U U U U G G C C G A A A G A U G U A A C G G G C U A A G U U A C C G A A U U U A U G G A U
A A G A U U A U C A A U U G U G G G U A G A C G U U G A U U U G A A G U U C A A G C G U A C A C U
U G G U G G A U C A A A A G G U G A G A C G A A G C C G U U G A U U U G A A G U U C A A A G C G U A C C
C A A A C C G A A U U G A C U A A A G G U U U C C U G G A C C G A G G U C C U U C C A G G G U U A G U C C U
A A G C U G A G G C U U A A A G C G U U G G G A C C A A C C A G G U U A A U U C U U A C A G U U
A G A C U U G G A A A G A A A G G U U U U C C A C C C C A U A A U U G A A U U U G G G G A A A U C C A
U A A G G U G G U A A C A U A G G C A A A A U G U C C A U A A A G U G A A U C C G A U U C G A A U
G A G U G A A A G A A G C A A G G A A A A G G U U U A A A U C A A A A A A A A A A A A A A A A
U C U A G C U G U G U A A C C A A G U A G U C A A C G G A A A A C A C A G G U U U A
G C G A G U G A A C U A A G C C A A G G A A A C U C U G G C C A A A U U U A A G U U A G C C G U
G C U U A A A A A G U A A G C C G G C A A G A A A A C G A A G G A A A C A A C A A C
U C U A U C C A A A A C C G U A A A G C G U G A A U A A A G G U G A A C C A C C C U U A A A G G U U A
A A G A A A A A A A A G C A A G C C U U U U U U A A C C U U G C C C A A G G U U U A
G U A G A A A A A A A G C A A G C C G G G U A A A A U U C C G U C C G U G U A A A A A A A
C U G U C C G G C U U A A G A C C A A G U G A A A A U C C A A G G U A A A A A A A A A A A
C G G G A A C G G A A A C C C G U G A A A A G C C U U G A A A A A A A A A A A A A A A U
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G A A U A C C U A C C G U G U G U G U G C C U U C C U A A A C U U A A C C U U A A C C A A G
U G U U A G G G A A G U U G A C U U G G A A G G U C C A A A A A A A A A A A A A A A A
G G U A C C U C A G U C G G A
U G A A A C A A A C G C A A A A G G A
G A A U G C C U C C A
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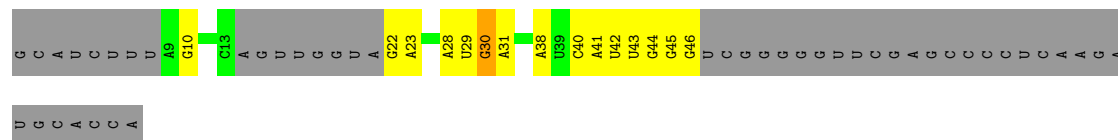
• Molecule 3: tRNA-Asp (P-site)

Chain 7: 20% 17% 60%



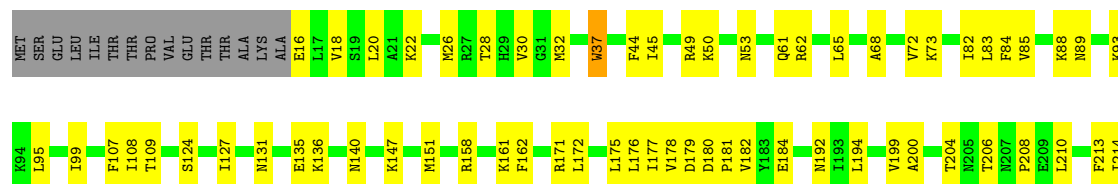
• Molecule 4: tRNA-Lys (A-site)

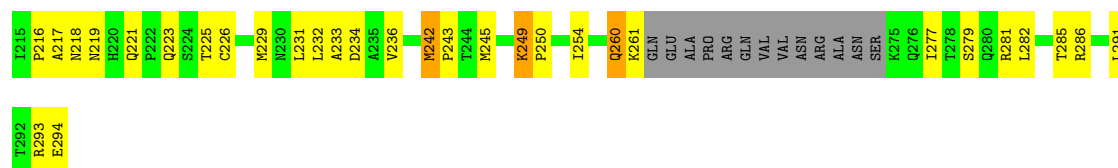
Chain 8: 20% 18% 61%



• Molecule 5: 30S ribosomal protein S2

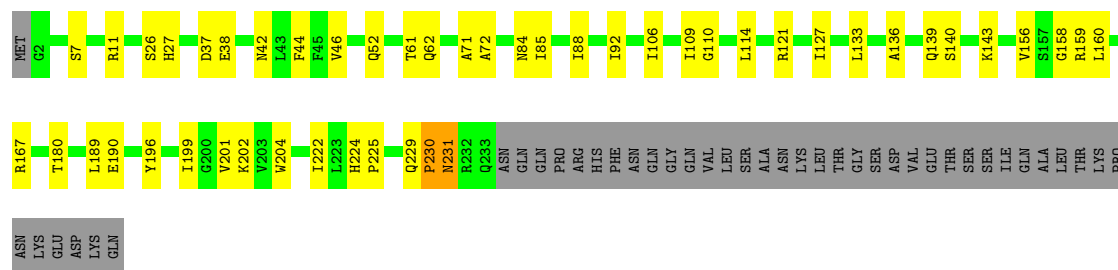
Chain A: 58% 31% 10%





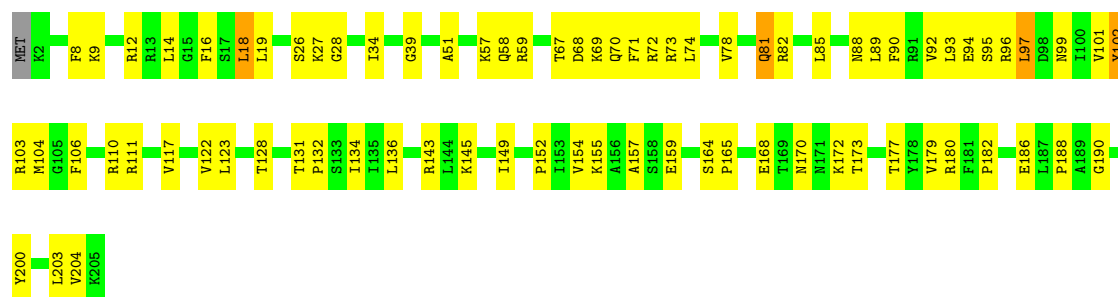
• Molecule 6: 30S ribosomal protein S3

Chain B: 67% 17% 15%



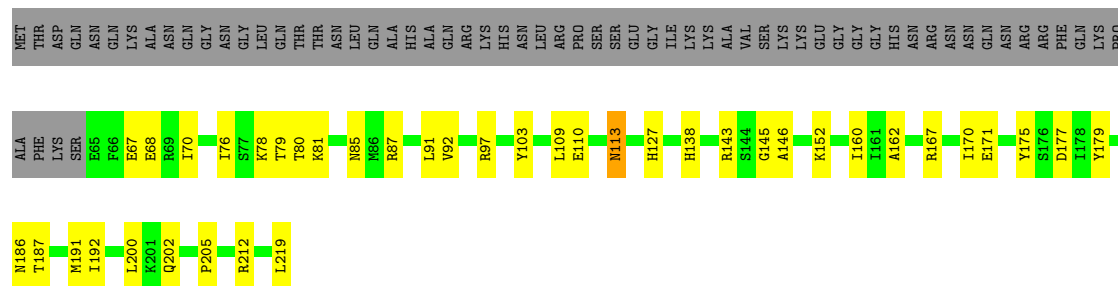
• Molecule 7: 30S ribosomal protein S4

Chain C: 62% 36% 2%



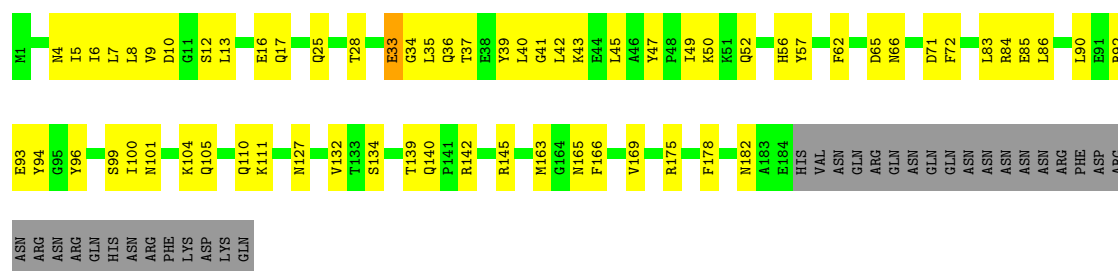
• Molecule 8: 30S ribosomal protein S5

Chain D: 53% 18% 29%



• Molecule 9: 30S ribosomal protein S6

Chain E: 55% 30% 14%



MT	ALA	LYS	LYS	LYS	LYS	ILE	N8	I14	H15	V16	S17	C18	S19	N22	T23	I24	V25	S26	A27	S28	D29	F30	N33	V34	L35	C36	M43	S48	A56	K76	F93	L98	E102	P108	R121
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- [illegible]

- [illegible]

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|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ME1 | A2 | K7 | V8 | K9 | Q10 | T11 | R12 | R19 | A20 | Y21 | T22 | R23 | R26 | L34 | S35 | G38 | V39 | C40 | R41 | L42 | C43 | K58 | A59 | S60 | W61 |
|-----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

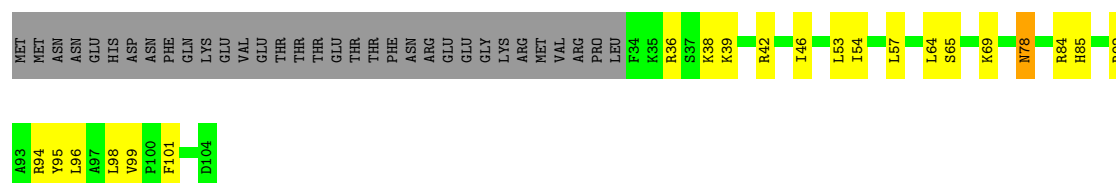
- | MET | Q2 | I3 | D4 | K5 | N6 | | I9 | K10 | | L13 | L14 | H15 | | D18 | V19 | G20 | S21 | | V26 | S27 | L28 | L29 | | Q32 | I33 | K34 | Q35 | L36 | T37 | D38 | | K59 | | K68 | | Y75 | R76 | N77 | L78 | | T81 | | G86 |
|-----|----|----|----|----|----|--|----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|-----|-----|-----|--|-----|--|-----|
|-----|----|----|----|----|----|--|----|-----|--|-----|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|-----|-----|-----|--|-----|--|-----|

- | | |
|-----|-----|
| K86 | M1 |
| K87 | R5 |
| LYS | L6 |
| PRO | W7 |
| VAL | R3 |
| ALA | M9 |
| LYS | G10 |
| SER | R11 |
| LYS | T16 |
| | Y17 |
| | R18 |
| | I19 |
| | D23 |
| | S24 |
| | R25 |
| | V26 |
| | K27 |
| | R28 |
| | A34 |
| | L35 |
| | I36 |
| | L39 |
| | N40 |
| | P41 |
| | A42 |
| | L43 |
| | K44 |
| | E45 |
| | N46 |
| | K47 |
| | C48 |
| | D51 |
| | E52 |
| | A55 |
| | W68 |
| | L59 |
| | K64 |
| | P65 |
| | T66 |
| | D67 |
| | T68 |
| | V69 |
| | R70 |
| | S71 |
| | L72 |
| | L78 |
| | W79 |
| | K90 |
| | K81 |

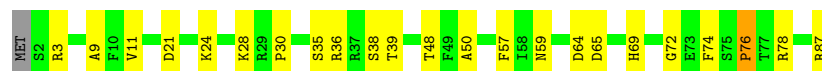
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M1	K2	V8	L9	N18	A19	E27	S28	K31	H36	R41	H42	K43	K44	Y45	N49	E52	V53	L54	A55	K56	D57	G58	V61	V64	S70	K73	R74	F75	R76	I80	R83	A84	G85
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- Chain Q:  48% 19% . 32%

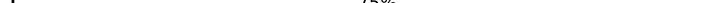


- Chain R:  72% 25% ..



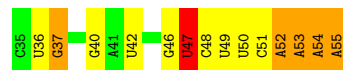
- Chain S:  66% 25% 9%



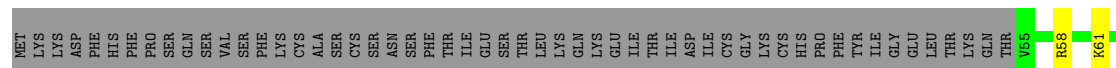
- Chain T:  75% 23%



- Chain Y: 33% 38% 24% 5%



- Chain x: 42% . 56%



1100

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PUT, ZN, SPD, MA6, B8T, 5MC, MG, G7M, N2P

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 > 5$	RMSZ	# $ Z > 5$
1	3	0.24	0/572	0.76	0/889
2	5	0.30	0/35992	0.77	4/56111 (0.0%)
3	7	0.25	0/713	0.77	0/1107
4	8	0.20	0/713	0.77	0/1106
5	A	0.26	0/2172	0.51	0/2934
6	B	0.28	0/1863	0.56	0/2516
7	C	0.37	1/1700 (0.1%)	0.69	3/2278 (0.1%)
8	D	0.27	0/1206	0.55	1/1616 (0.1%)
9	E	0.27	0/1536	0.54	0/2072
10	F	0.26	0/1274	0.55	0/1710
11	G	0.27	0/1126	0.52	0/1517
12	H	0.28	0/1056	0.61	0/1409
13	I	0.27	0/843	0.55	0/1132
14	J	0.31	0/844	0.66	2/1136 (0.2%)
15	K	0.26	0/1089	0.58	0/1461
16	L	0.26	0/1002	0.61	0/1340
17	M	0.30	0/483	0.58	0/643
18	N	0.25	0/695	0.54	0/926
19	O	0.34	0/718	0.74	2/962 (0.2%)
20	P	0.24	0/702	0.56	0/934
21	Q	0.26	0/601	0.57	0/801
22	R	0.30	0/716	0.62	1/958 (0.1%)
23	S	0.27	0/645	0.54	0/857
24	T	0.28	0/524	0.58	0/685
25	Y	0.27	0/498	0.87	1/773 (0.1%)
26	x	0.25	0/347	0.53	0/457
All	All	0.29	1/59630 (0.0%)	0.71	14/88330 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	152	PRO	CG-CD	-10.24	1.16	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	152	PRO	N-CD-CG	-13.35	83.17	103.20
14	J	108	PRO	CA-N-CD	-12.03	94.65	111.50
22	R	76	PRO	CA-N-CD	-9.30	98.48	111.50
19	O	41	PRO	CA-N-CD	-8.45	99.67	111.50
19	O	41	PRO	N-CD-CG	-6.60	93.30	103.20

There are no chirality outliers.

There are no planarity outliers.

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	3	512	0	260	1	0
2	5	32258	0	16204	502	0
3	7	640	0	324	15	0
4	8	639	0	324	9	0
5	A	2138	0	2204	59	0
6	B	1835	0	1909	36	0
7	C	1669	0	1729	58	0
8	D	1191	0	1284	27	0
9	E	1509	0	1520	48	0
10	F	1254	0	1320	32	0
11	G	1110	0	1226	30	0
12	H	1040	0	1107	25	0
13	I	832	0	918	26	0
14	J	829	0	855	16	0
15	K	1071	0	1165	27	0
16	L	991	0	1061	39	0
17	M	474	0	505	16	0
18	N	689	0	746	13	0
19	O	705	0	755	30	0
20	P	693	0	753	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	590	0	625	23	0
22	R	700	0	709	15	0
23	S	643	0	694	18	0
24	T	519	0	578	8	0
25	Y	446	0	226	11	0
26	x	342	0	354	0	0
27	5	20	0	38	2	0
28	5	12	0	24	0	0
29	5	7	0	14	0	0
30	5	96	0	0	0	0
30	7	1	0	0	0	0
30	8	1	0	0	0	0
30	H	1	0	0	0	0
30	K	1	0	0	0	0
30	L	1	0	0	0	0
30	P	1	0	0	0	0
30	Y	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
32	5	1	0	0	0	0
32	A	1	0	0	0	0
All	All	55465	0	39431	976	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 11.

The worst 5 of 976 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)
3:7:34:G:H1	25:Y:42:U:H3	1.16	0.92
2:5:169:G:N2	2:5:219:A:O2'	2.13	0.81
2:5:983:G:H21	2:5:1012:A:H8	1.28	0.81
18:N:26:VAL:HG11	18:N:78:LEU:HD21	1.62	0.81
2:5:452:A:OP1	19:O:70:ARG:NH2	2.14	0.80

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	
5	A	262/294 (89%)	240 (92%)	22 (8%)	0	100	100
6	B	230/273 (84%)	215 (94%)	13 (6%)	2 (1%)	14	49
7	C	202/205 (98%)	171 (85%)	30 (15%)	1 (0%)	25	60
8	D	153/219 (70%)	148 (97%)	5 (3%)	0	100	100
9	E	182/215 (85%)	161 (88%)	20 (11%)	1 (0%)	25	60
10	F	153/155 (99%)	139 (91%)	13 (8%)	1 (1%)	19	54
11	G	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
12	H	127/132 (96%)	114 (90%)	12 (9%)	1 (1%)	16	51
13	I	102/108 (94%)	90 (88%)	12 (12%)	0	100	100
14	J	112/121 (93%)	104 (93%)	8 (7%)	0	100	100
15	K	133/139 (96%)	122 (92%)	9 (7%)	2 (2%)	8	38
16	L	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
17	M	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
18	N	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
19	O	85/94 (90%)	82 (96%)	2 (2%)	1 (1%)	11	43
20	P	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	11	43
21	Q	69/104 (66%)	64 (93%)	5 (7%)	0	100	100
22	R	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
23	S	77/87 (88%)	75 (97%)	2 (3%)	0	100	100
24	T	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	x	41/97 (42%)	30 (73%)	10 (24%)	1 (2%)	5	29
All	All	2553/2888 (88%)	2345 (92%)	197 (8%)	11 (0%)	32	64

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	230	PRO
20	P	54	LEU
15	K	56	LYS
7	C	81	GLN
6	B	231	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	
5	A	238/262 (91%)	228 (96%)	10 (4%)	25	58
6	B	195/232 (84%)	195 (100%)	0	100	100
7	C	182/183 (100%)	174 (96%)	8 (4%)	24	57
8	D	125/178 (70%)	123 (98%)	2 (2%)	58	79
9	E	165/196 (84%)	160 (97%)	5 (3%)	36	66
10	F	132/132 (100%)	125 (95%)	7 (5%)	19	52
11	G	123/124 (99%)	122 (99%)	1 (1%)	79	90
12	H	112/115 (97%)	111 (99%)	1 (1%)	75	89
13	I	97/99 (98%)	95 (98%)	2 (2%)	48	74
14	J	91/97 (94%)	88 (97%)	3 (3%)	33	64
15	K	117/120 (98%)	111 (95%)	6 (5%)	20	53
16	L	104/105 (99%)	98 (94%)	6 (6%)	17	49
17	M	47/48 (98%)	46 (98%)	1 (2%)	48	74
18	N	77/78 (99%)	73 (95%)	4 (5%)	19	52
19	O	76/82 (93%)	73 (96%)	3 (4%)	27	60
20	P	75/75 (100%)	73 (97%)	2 (3%)	40	69
21	Q	62/94 (66%)	61 (98%)	1 (2%)	58	79
22	R	76/77 (99%)	74 (97%)	2 (3%)	41	70
23	S	71/77 (92%)	71 (100%)	0	100	100
24	T	55/56 (98%)	52 (94%)	3 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	x	35/86 (41%)	34 (97%)	1 (3%)	37 67
All	All	2255/2516 (90%)	2187 (97%)	68 (3%)	37 66

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	O	48	CYS
20	P	49	ASN
24	T	19	LYS
9	E	178	PHE
9	E	175	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
16	L	100	GLN
26	x	98	ASN
8	D	193	HIS
9	E	17	GLN
9	E	25	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	23/2907 (0%)	1 (4%)	0
2	5	1503/1520 (98%)	234 (15%)	6 (0%)
25	Y	20/21 (95%)	11 (55%)	1 (5%)
3	7	28/75 (37%)	2 (7%)	1 (3%)
4	8	28/76 (36%)	4 (14%)	0
All	All	1602/4599 (34%)	252 (15%)	8 (0%)

5 of 252 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	1920	A
2	5	6	C
2	5	10	G
2	5	40	G
2	5	48	C

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	Y	51	C
3	7	10	G
2	5	1123	G
2	5	1024	U
2	5	1158	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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
2	G7M	5	525	2	20,26,27	4.04	10 (50%)	17,39,42	1.02	1 (5%)
2	5MC	5	1375	2	18,22,23	4.02	7 (38%)	26,32,35	1.03	2 (7%)
2	B8T	5	1377	2	19,22,23	3.24	8 (42%)	26,31,34	0.84	1 (3%)
2	MA6	5	1494	2	18,26,27	1.08	2 (11%)	19,38,41	3.41	3 (15%)
2	MA6	5	1493	2	18,26,27	1.06	2 (11%)	19,38,41	3.40	3 (15%)

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
2	G7M	5	525	2	-	2/3/25/26	0/3/3/3
2	5MC	5	1375	2	-	2/7/25/26	0/2/2/2
2	B8T	5	1377	2	-	2/7/27/28	0/2/2/2
2	MA6	5	1494	2	-	2/7/29/30	0/3/3/3
2	MA6	5	1493	2	-	0/7/29/30	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	525	G7M	C8-N7	10.07	1.51	1.33
2	5	1375	5MC	C6-C5	9.87	1.50	1.34
2	5	525	G7M	C8-N9	9.85	1.51	1.33
2	5	1375	5MC	C4-N3	7.42	1.46	1.34
2	5	1377	B8T	C4-N3	7.11	1.45	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1493	MA6	N1-C6-N6	-12.42	103.98	117.06
2	5	1494	MA6	N1-C6-N6	-12.35	104.06	117.06
2	5	1494	MA6	N3-C2-N1	-5.58	119.96	128.68
2	5	1494	MA6	C1'-N9-C4	5.50	136.30	126.64
2	5	1493	MA6	C1'-N9-C4	5.44	136.19	126.64

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	525	G7M	O4'-C4'-C5'-O5'
2	5	525	G7M	C3'-C4'-C5'-O5'
2	5	1494	MA6	O4'-C4'-C5'-O5'
2	5	1377	B8T	O4'-C4'-C5'-O5'
2	5	1494	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	525	G7M	1	0
2	5	1493	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 105 are monoatomic - leaving 5 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	$\# Z > 2$
27	SPD	5	1604	-	9,9,9	0.32	0	8,8,8	0.88	0
28	PUT	5	1605	-	5,5,5	0.24	0	4,4,4	0.52	0
29	N2P	5	1603	-	6,6,6	0.24	0	5,5,5	0.64	0
27	SPD	5	1601	-	9,9,9	0.32	0	8,8,8	0.91	0
28	PUT	5	1602	-	5,5,5	0.24	0	4,4,4	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SPD	5	1604	-	-	0/7/7/7	-
28	PUT	5	1605	-	-	0/3/3/3	-
29	N2P	5	1603	-	-	0/4/4/4	-
27	SPD	5	1601	-	-	1/7/7/7	-
28	PUT	5	1602	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	5	1601	SPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	5	1604	SPD	1	0
27	5	1601	SPD	1	0

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.