



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 24, 2017 – 05:58 AM EDT

PDB ID : 5LZE  
EMDB ID: : EMD-4125  
Title : Structure of the 70S ribosome with Sec-tRNA<sup>Sec</sup> in the classical pre-translocation state (C)  
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.  
Deposited on : unknown  
Resolution : 3.50 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](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

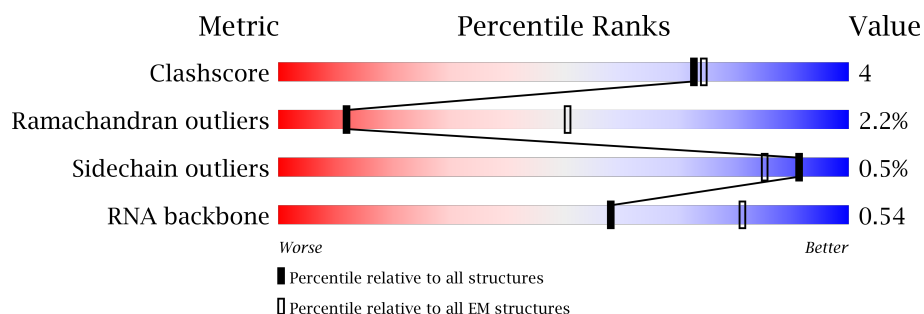
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.





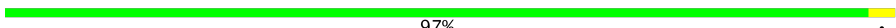










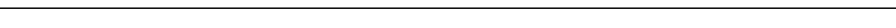











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	1539	69% 28% .
2	b	218	97% .
3	c	206	99% .
4	d	205	99% .
5	e	157	94% . .
6	f	100	93% 5% .
7	g	151	98% .
8	h	129	98% .

























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Mol	Chain	Length	Quality of chain
9	i	127	 94% 5% .
10	j	98	 94% 5% .
11	k	116	 97% .
12	l	123	 95% . .
13	m	114	 93% 6% .
14	n	100	 96% .
15	o	88	 92% 7% .
16	p	82	 94% . .
17	q	80	 96% . .
18	r	65	 94% 6%
19	s	79	 96% . .
20	t	85	 100%
21	u	65	 86% 12% .
22	v	77	 65% 31% .
23	x	48	 33% 46% 21%
24	y	95	 72% 26% .
25	A	2903	 62% 29% 8% .
26	B	120	 64% 26% 9% .
27	C	271	 78% 21%
28	D	209	 90% 10%
29	E	201	 88% 11%
30	F	177	 84% 16%
31	G	176	 86% 14% .
32	I	141	 83% 16% .
33	H	149	 81% 16% .

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Mol	Chain	Length	Quality of chain
34	J	142	 89% 11% .
35	K	122	 81% 17% .
36	L	143	 81% 17% ..
37	M	136	 90% 9% .
38	N	120	 88% 12%
39	O	116	 89% 11%
40	P	114	 82% 18%
41	Q	117	 90% 9% .
42	R	103	 82% 17% .
43	S	110	 86% 14%
44	T	93	 84% 16%
45	U	102	 84% 13% .
46	V	94	 82% 18%
47	W	75	 85% 13% .
48	X	77	 82% 18%
49	Y	63	 94% 6%
50	Z	58	 91% 9%
51	0	56	 89% 9% .
52	1	50	 88% 8% .
53	2	46	 83% 17%
54	3	64	 84% 16%
55	4	38	 55% 42% .
56	6	66	 64% 30% 6%
57	w	3	 100%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
25	G7M	A	2069	X	-	-	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148018 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	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- 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
			1625	1028	305	289	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- 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
			787	493	150	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- 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
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called tRNA<sup>f</sup>Met.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called fMetSec-tRNA<sup>Sec</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2900	Total	C	N	O	P	0	0
			62274	27787	11459	20128	2900		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 57 is a RNA chain called CCA 3' end of E-site tRNA<sup>Sec</sup> (low occupancy).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

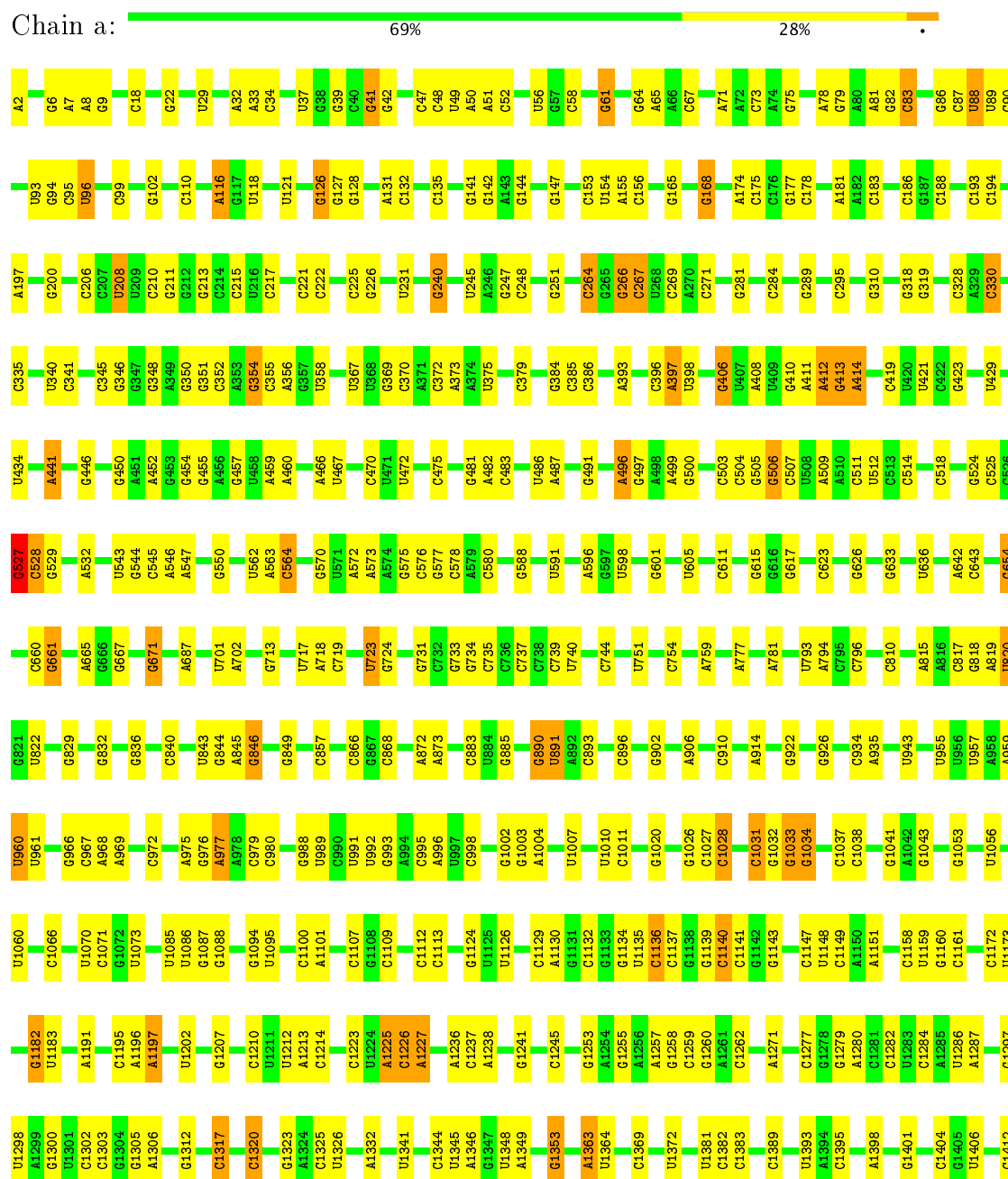
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

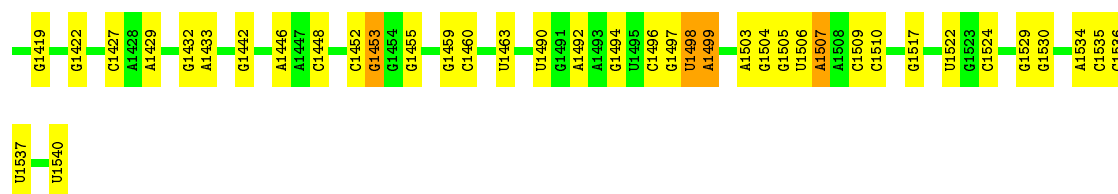
Mol	Chain	Residues	Atoms		AltConf
58	4	1	Total	Zn	0
			1	1	
58	6	1	Total	Zn	0
			1	1	

### 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 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: 16S ribosomal RNA





- Molecule 2: 30S ribosomal protein S2

Chain b: 97%



- Molecule 3: 30S ribosomal protein S3

Chain c: 99%



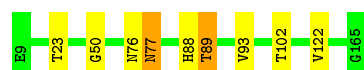
- Molecule 4: 30S ribosomal protein S4

Chain d: 99%



- Molecule 5: 30S ribosomal protein S5

Chain e: 94%



- Molecule 6: 30S ribosomal protein S6

Chain f: 93% 5%



- Molecule 7: 30S ribosomal protein S7

Chain g: 98%



- Molecule 8: 30S ribosomal protein S8



Chain h:  98% .



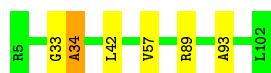
- Molecule 9: 30S ribosomal protein S9

Chain i:  94% 5% .



- Molecule 10: 30S ribosomal protein S10

Chain j:  94% 5% .



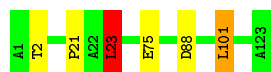
- Molecule 11: 30S ribosomal protein S11

Chain k:  97% .



- Molecule 12: 30S ribosomal protein S12

Chain l:  95% . .



- Molecule 13: 30S ribosomal protein S13

Chain m:  93% 6% .



- Molecule 14: 30S ribosomal protein S14

Chain n:  96% .



- Molecule 15: 30S ribosomal protein S15

Chain o:  92% 7% .



- Molecule 16: 30S ribosomal protein S16

Chain p: 94% ..



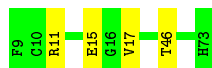
- Molecule 17: 30S ribosomal protein S17

Chain q: 96% ..



- Molecule 18: 30S ribosomal protein S18

Chain r: 94% 6%



- Molecule 19: 30S ribosomal protein S19

Chain s: 96% ..



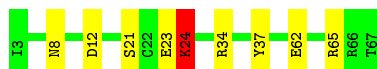
- Molecule 20: 30S ribosomal protein S20

Chain t: 100%

There are no outlier residues recorded for this chain.

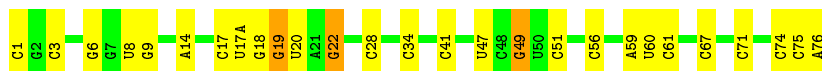
- Molecule 21: 30S ribosomal protein S21

Chain u: 86% 12% .



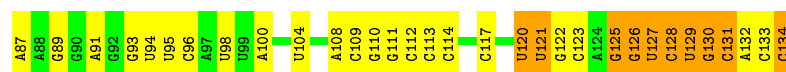
- Molecule 22: tRNA<sup>fMet</sup>

Chain v: 65% 31% .



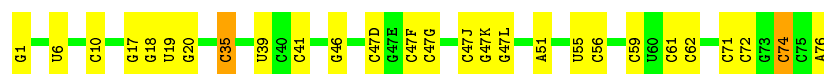
- Molecule 23: SECIS mRNA

Chain x:  33% 46% 21%



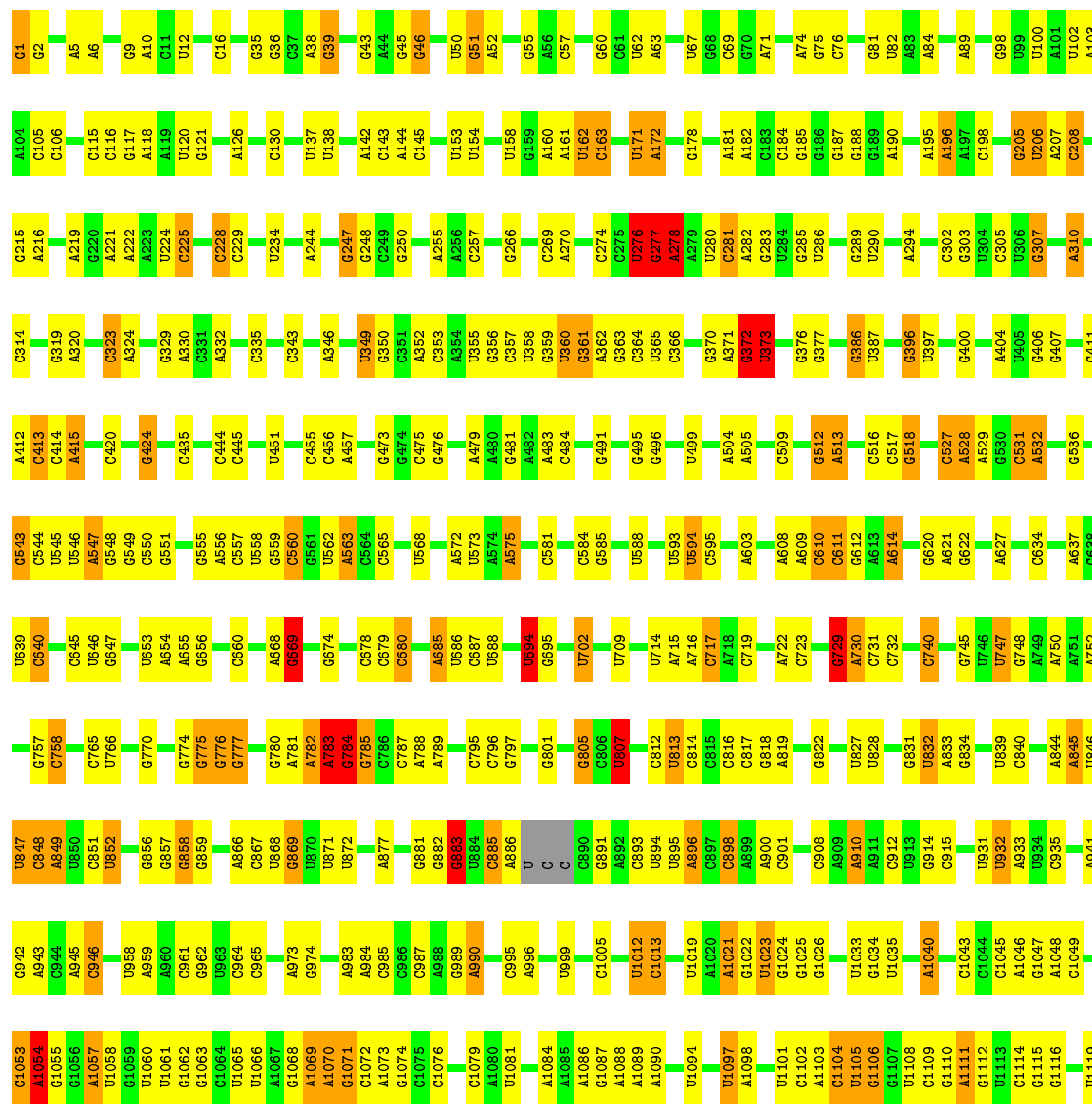
• Molecule 24: fMetSec-tRNA<sup>Sec</sup>

Chain y:  72% 26% .



• Molecule 25: 23S ribosomal RNA

Chain A:  62% 29% 8% .

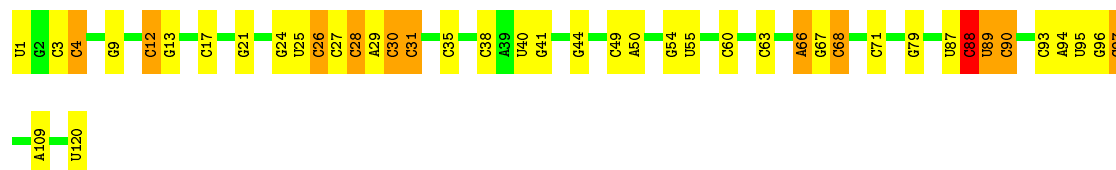






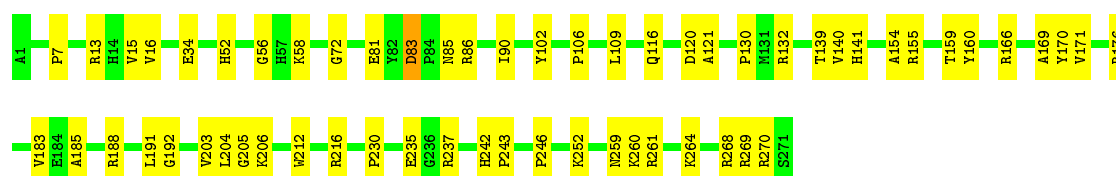

- Molecule 26: 5S ribosomal RNA

Chain B: 64% 26% 9%



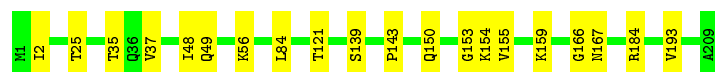
- Molecule 27: 50S ribosomal protein L2

Chain C: 78% 21%



- Molecule 28: 50S ribosomal protein L3

Chain D: 90% 10%



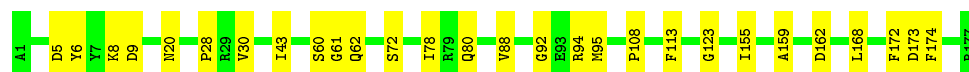
- Molecule 29: 50S ribosomal protein L4

Chain E: 88% 11%



- Molecule 30: 50S ribosomal protein L5

Chain F: 84% 16%

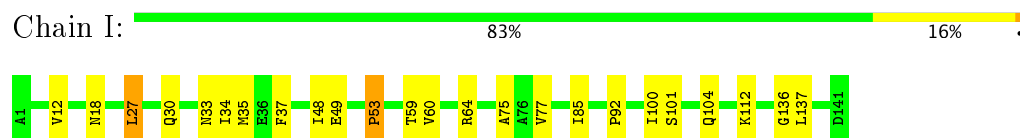


- Molecule 31: 50S ribosomal protein L6

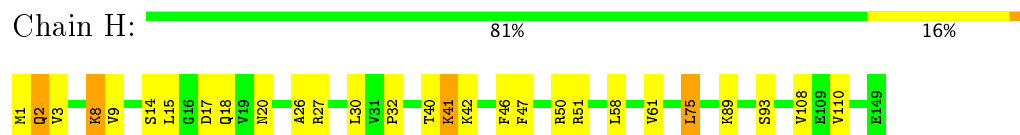
Chain G: 86% 14%



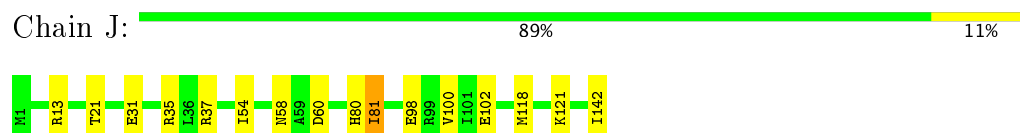
- Molecule 32: 50S ribosomal protein L11



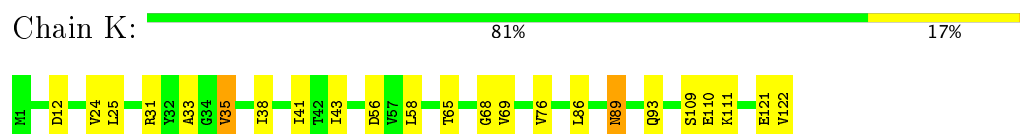
- Molecule 33: 50S ribosomal protein L9



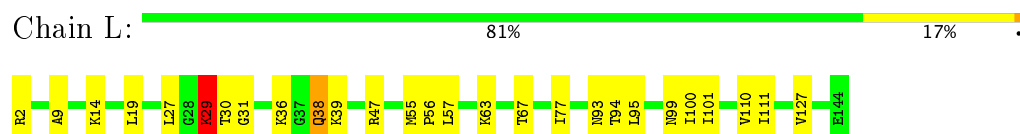
- Molecule 34: 50S ribosomal protein L13



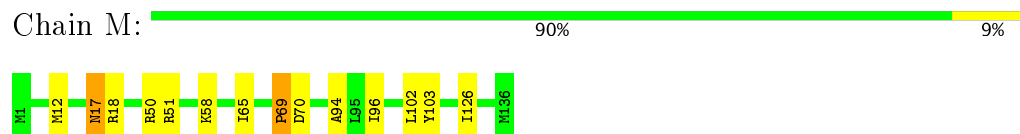
- Molecule 35: 50S ribosomal protein L14



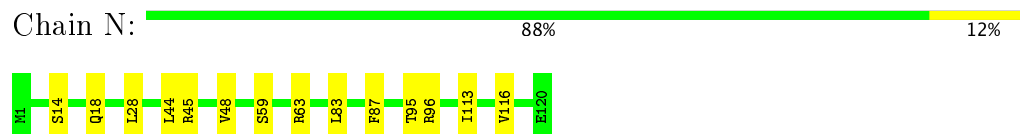
- Molecule 36: 50S ribosomal protein L15




- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17




- Molecule 39: 50S ribosomal protein L18

Chain O:  89% 11%



- Molecule 40: 50S ribosomal protein L19

Chain P:  82% 18%




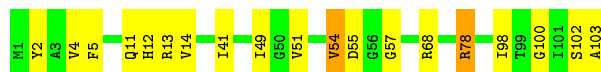
- Molecule 41: 50S ribosomal protein L20

Chain Q:  90% 9%




- Molecule 42: 50S ribosomal protein L21

Chain R:  82% 17%




- Molecule 43: 50S ribosomal protein L22

Chain S:  86% 14%




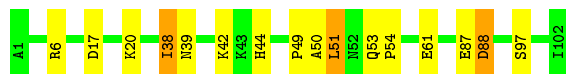
- Molecule 44: 50S ribosomal protein L23

Chain T:  84% 16%




- Molecule 45: 50S ribosomal protein L24

Chain U:  84% 13%



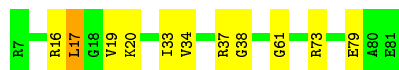
- Molecule 46: 50S ribosomal protein L25

Chain V:  82% 18%



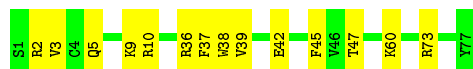
- Molecule 47: 50S ribosomal protein L27

Chain W: 85% 13%



- Molecule 48: 50S ribosomal protein L28

Chain X: 82% 18%



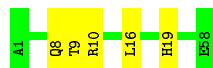
- Molecule 49: 50S ribosomal protein L29

Chain Y: 94% 6%



- Molecule 50: 50S ribosomal protein L30

Chain Z: 91% 9%



- Molecule 51: 50S ribosomal protein L32

Chain 0: 89% 9%



- Molecule 52: 50S ribosomal protein L33

Chain 1: 88% 8%



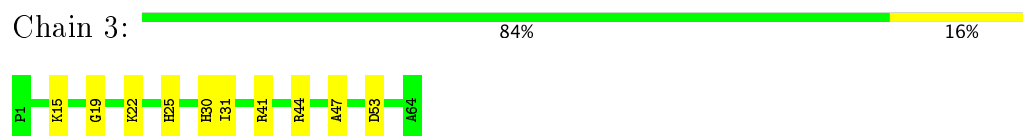
- Molecule 53: 50S ribosomal protein L34

Chain 2: 83% 17%

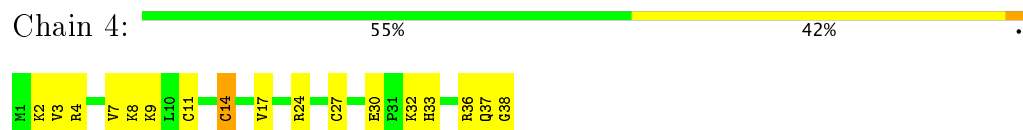




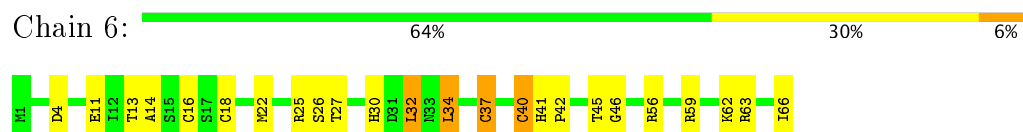
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L31



- Molecule 57: CCA 3' end of E-site tRNA<sup>Sec</sup> (low occupancy)



There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	130705	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	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, 3TD, ZN, 6IA, OMG, 5MC, MA6, G7M, OMC, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 1MG, 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	0.84	6/36701 (0.0%)	1.37	537/57246 (0.9%)
10	j	0.44	0/797	0.78	0/1077
11	k	0.46	0/886	0.71	1/1195 (0.1%)
12	l	0.43	0/969	0.77	1/1300 (0.1%)
13	m	0.46	0/893	0.82	3/1193 (0.3%)
14	n	0.51	0/806	0.68	0/1074
15	o	0.45	0/722	0.73	2/964 (0.2%)
16	p	0.53	0/659	0.84	1/884 (0.1%)
17	q	0.49	0/658	0.78	1/881 (0.1%)
18	r	0.46	0/512	0.74	1/689 (0.1%)
19	s	0.50	0/653	0.87	3/877 (0.3%)
2	b	0.44	0/1736	0.69	1/2338 (0.0%)
20	t	0.44	0/671	0.64	0/888
21	u	0.53	0/501	0.98	2/668 (0.3%)
22	v	0.79	1/1747 (0.1%)	1.48	44/2721 (1.6%)
23	x	0.91	3/1145 (0.3%)	1.67	32/1781 (1.8%)
24	y	0.67	1/2162 (0.0%)	1.42	33/3351 (1.0%)
25	A	0.93	12/69171 (0.0%)	1.32	778/107904 (0.7%)
26	B	0.76	1/2873 (0.0%)	1.41	53/4478 (1.2%)
27	C	0.54	0/2122	0.74	2/2852 (0.1%)
28	D	0.48	0/1586	0.70	0/2134
29	E	0.49	0/1571	0.67	2/2113 (0.1%)
3	c	0.44	0/1652	0.63	0/2225
30	F	0.48	0/1435	0.74	1/1926 (0.1%)
31	G	0.45	0/1343	0.66	2/1816 (0.1%)
32	I	0.43	0/1046	0.71	1/1410 (0.1%)
33	H	0.40	0/1122	0.70	1/1515 (0.1%)
34	J	0.50	0/1152	0.64	0/1551
35	K	0.53	0/948	0.74	1/1268 (0.1%)
36	L	0.50	0/1054	0.78	1/1403 (0.1%)
37	M	0.47	0/1093	0.68	1/1460 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	N	0.49	0/974	0.68	0/1301
39	O	0.45	0/902	0.61	0/1209
4	d	0.42	0/1665	0.64	0/2227
40	P	0.50	0/929	0.70	1/1242 (0.1%)
41	Q	0.59	0/960	0.68	1/1278 (0.1%)
42	R	0.47	0/829	0.72	2/1107 (0.2%)
43	S	0.47	0/864	0.66	1/1156 (0.1%)
44	T	0.44	0/745	0.60	0/994
45	U	0.49	0/788	0.82	4/1051 (0.4%)
46	V	0.44	0/766	0.62	1/1025 (0.1%)
47	W	0.49	0/582	0.64	0/769
48	X	0.49	0/635	0.59	0/848
49	Y	0.42	0/510	0.61	0/677
5	e	0.49	0/1170	0.74	2/1573 (0.1%)
50	Z	0.39	0/453	0.65	0/605
51	0	0.51	0/450	0.75	0/599
52	1	0.47	0/417	0.78	1/554 (0.2%)
53	2	0.49	0/380	0.65	0/498
54	3	0.49	0/513	0.65	0/676
55	4	0.79	1/303 (0.3%)	1.05	1/397 (0.3%)
56	6	0.60	1/532 (0.2%)	1.09	4/709 (0.6%)
57	w	0.28	0/68	1.00	0/103
6	f	0.51	0/836	0.85	3/1128 (0.3%)
7	g	0.42	0/1196	0.62	0/1602
8	h	0.47	0/989	0.69	0/1326
9	i	0.49	1/1034 (0.1%)	0.78	1/1375 (0.1%)
All	All	0.79	27/159876 (0.0%)	1.22	1527/239211 (0.6%)

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	2	0
10	j	0	3
12	l	0	2
13	m	0	2
15	o	0	1
16	p	0	1
17	q	0	1
19	s	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
21	u	0	2
25	A	2	0
27	C	0	1
28	D	0	1
29	E	0	1
30	F	0	1
33	H	0	3
35	K	0	1
36	L	0	1
45	U	0	2
5	e	0	3
51	0	0	1
52	1	0	1
54	3	0	1
6	f	0	2
9	i	0	2
All	All	4	35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	1	G	OP3-P	-10.82	1.48	1.61
25	A	1	G	OP3-P	-10.72	1.48	1.61
22	v	1	C	OP3-P	-10.66	1.48	1.61
26	B	1	U	OP3-P	-10.62	1.48	1.61
1	a	2	A	OP3-P	-10.55	1.48	1.61

The worst 5 of 1527 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	529	G	C5-C6-O6	-14.39	119.96	128.60
24	y	35	C	C5-C6-N1	13.59	127.79	121.00
1	a	1027	C	C5-C6-N1	13.56	127.78	121.00
25	A	1313	U	N3-C2-O2	-12.91	113.16	122.20
24	y	35	C	C6-N1-C2	-12.72	115.21	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'
25	A	2069	G7M	C4',C3'

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	72	LYS	Peptide
5	e	76	ASN	Mainchain,Peptide
5	e	88	HIS	Peptide
6	f	52	ASN	Mainchain
6	f	97	THR	Mainchain

## 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	33029	0	16644	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1157	0	1199	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1644	0	840	0	0
23	x	1025	0	518	0	0
24	y	2031	0	1046	0	0
25	A	62274	0	31342	279	0
26	B	2570	0	1301	8	0
27	C	2083	0	2157	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	1565	0	1616	11	0
29	E	1552	0	1619	17	0
30	F	1411	0	1447	16	0
31	G	1323	0	1374	13	0
32	I	1032	0	1088	10	0
33	H	1111	0	1148	14	0
34	J	1129	0	1162	12	0
35	K	939	0	1012	11	0
36	L	1045	0	1117	18	0
37	M	1074	0	1157	10	0
38	N	961	0	1000	8	0
39	O	892	0	923	7	0
40	P	917	0	965	12	0
41	Q	947	0	1022	9	0
42	R	816	0	839	11	0
43	S	857	0	922	9	0
44	T	739	0	807	8	0
45	U	780	0	834	5	0
46	V	753	0	780	8	0
47	W	575	0	592	8	0
48	X	625	0	655	11	0
49	Y	509	0	543	2	0
50	Z	449	0	491	3	0
51	0	444	0	461	3	0
52	1	410	0	440	3	0
53	2	377	0	418	6	0
54	3	504	0	574	6	0
55	4	302	0	340	11	0
56	6	523	0	521	9	0
57	w	62	0	34	0	0
58	4	1	0	0	0	0
58	6	1	0	0	0	0
All	All	148018	0	99207	514	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 4.

The worst 5 of 514 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)
25:A:2164:C:H41	25:A:2171:A:H61	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:1171:G:H1	25:A:1177:G:H1	1.26	0.82
25:A:1171:G:N2	25:A:1178:C:O2	2.18	0.77
55:4:2:LYS:HD2	55:4:4:ARG:HH12	1.50	0.76
25:A:585:G:N7	41:Q:5:ARG:NH1	2.32	0.76

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	b	216/218 (99%)	190 (88%)	23 (11%)	3 (1%)	13	53
3	c	204/206 (99%)	191 (94%)	10 (5%)	3 (2%)	12	52
4	d	203/205 (99%)	181 (89%)	19 (9%)	3 (2%)	12	52
5	e	155/157 (99%)	139 (90%)	9 (6%)	7 (4%)	3	27
6	f	98/100 (98%)	83 (85%)	10 (10%)	5 (5%)	2	23
7	g	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	9	46
8	h	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	11	50
9	i	125/127 (98%)	105 (84%)	14 (11%)	6 (5%)	2	25
10	j	96/98 (98%)	83 (86%)	8 (8%)	5 (5%)	2	23
11	k	114/116 (98%)	102 (90%)	10 (9%)	2 (2%)	10	48
12	l	121/123 (98%)	101 (84%)	14 (12%)	6 (5%)	2	24
13	m	112/114 (98%)	100 (89%)	8 (7%)	4 (4%)	4	33
14	n	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	3	29
15	o	86/88 (98%)	73 (85%)	9 (10%)	4 (5%)	3	26
16	p	80/82 (98%)	69 (86%)	7 (9%)	4 (5%)	2	24
17	q	78/80 (98%)	65 (83%)	11 (14%)	2 (3%)	6	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	63/65 (97%)	53 (84%)	7 (11%)	3 (5%)	2	25
19	s	77/79 (98%)	71 (92%)	5 (6%)	1 (1%)	14	55
20	t	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
21	u	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	12
27	C	269/271 (99%)	245 (91%)	19 (7%)	5 (2%)	9	47
28	D	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	13	53
29	E	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	12	52
30	F	175/177 (99%)	160 (91%)	13 (7%)	2 (1%)	17	59
31	G	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	11	49
32	I	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	5	38
33	H	147/149 (99%)	125 (85%)	17 (12%)	5 (3%)	4	35
34	J	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	13	53
35	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	35
36	L	141/143 (99%)	127 (90%)	10 (7%)	4 (3%)	6	39
37	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	12	52
38	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
39	O	114/116 (98%)	104 (91%)	9 (8%)	1 (1%)	20	63
40	P	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
41	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
42	R	101/103 (98%)	89 (88%)	9 (9%)	3 (3%)	5	37
43	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
44	T	91/93 (98%)	78 (86%)	11 (12%)	2 (2%)	8	44
45	U	100/102 (98%)	87 (87%)	7 (7%)	6 (6%)	2	19
46	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
47	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	13	53
48	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
49	Y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	11	50
50	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
51	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	9	47
52	1	48/50 (96%)	47 (98%)	0	1 (2%)	8	45
53	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	11	50
55	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
56	6	64/66 (97%)	58 (91%)	5 (8%)	1 (2%)	11	50
All	All	5717/5817 (98%)	5151 (90%)	439 (8%)	127 (2%)	12	44

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	73	ARG
5	e	77	ASN
5	e	89	THR
5	e	93	VAL
6	f	53	LYS

### 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	180/180 (100%)	178 (99%)	2 (1%)	78	91
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	103 (100%)	0	100	100
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	o	76/76 (100%)	75 (99%)	1 (1%)	73	90
16	p	65/65 (100%)	64 (98%)	1 (2%)	70	88
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	41 (93%)	3 (7%)	18	56
27	C	216/216 (100%)	215 (100%)	1 (0%)	91	96
28	D	164/164 (100%)	164 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/148 (100%)	148 (100%)	0	100	100
31	G	137/137 (100%)	137 (100%)	0	100	100
32	I	109/109 (100%)	105 (96%)	4 (4%)	39	73
33	H	114/114 (100%)	114 (100%)	0	100	100
34	J	116/116 (100%)	116 (100%)	0	100	100
35	K	103/103 (100%)	103 (100%)	0	100	100
36	L	102/102 (100%)	101 (99%)	1 (1%)	80	91
37	M	109/109 (100%)	108 (99%)	1 (1%)	82	93
38	N	100/100 (100%)	100 (100%)	0	100	100
39	O	86/86 (100%)	86 (100%)	0	100	100
40	P	99/99 (100%)	99 (100%)	0	100	100
41	Q	89/89 (100%)	89 (100%)	0	100	100
42	R	84/84 (100%)	84 (100%)	0	100	100
43	S	93/93 (100%)	93 (100%)	0	100	100
44	T	80/80 (100%)	80 (100%)	0	100	100
45	U	83/83 (100%)	82 (99%)	1 (1%)	75	90
46	V	78/78 (100%)	77 (99%)	1 (1%)	73	90
47	W	57/57 (100%)	57 (100%)	0	100	100
48	X	67/67 (100%)	67 (100%)	0	100	100
49	Y	55/55 (100%)	55 (100%)	0	100	100
50	Z	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	0	47/47 (100%)	46 (98%)	1 (2%)	59 84
52	1	45/45 (100%)	44 (98%)	1 (2%)	57 83
53	2	38/38 (100%)	38 (100%)	0	100 100
54	3	51/51 (100%)	51 (100%)	0	100 100
55	4	34/34 (100%)	34 (100%)	0	100 100
56	6	59/59 (100%)	51 (86%)	8 (14%)	4 23
All	All	4728/4751 (100%)	4702 (100%)	26 (0%)	91 96

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	I	37	PHE
45	U	39	ASN
56	6	45	THR
36	L	38	GLN
37	M	17	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
29	E	41	GLN
31	G	127	GLN
46	V	78	GLN
27	C	52	HIS
27	C	116	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	247 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	22 (46%)	0
24	y	87/95 (91%)	12 (13%)	0
25	A	2894/2903 (99%)	513 (17%)	34 (1%)
26	B	119/120 (99%)	19 (15%)	3 (2%)
57	w	2/3 (66%)	0	0
All	All	4760/4785 (99%)	828 (17%)	37 (0%)

5 of 828 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	7	A
1	a	8	A
1	a	9	G
1	a	22	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1432	G
25	A	1900	A
26	B	24	G
25	A	1458	U
25	A	1567	G

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

43 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	$\# Z  > 2$
25	6MZ	A	1618	25	18,25,26	1.10	1 (5%)	16,36,39	3.02	4 (25%)
25	2MG	A	1835	25	19,26,27	0.96	2 (10%)	20,38,41	2.25	7 (35%)
25	PSU	A	1911	25	16,21,22	1.55	4 (25%)	20,30,33	3.38	6 (30%)
25	3TD	A	1915	25	16,22,23	3.01	5 (31%)	19,32,35	1.97	5 (26%)
25	PSU	A	1917	25	16,21,22	1.54	4 (25%)	20,30,33	3.29	6 (30%)
25	5MU	A	1939	25	14,22,23	1.04	1 (7%)	16,32,35	2.01	3 (18%)
25	5MC	A	1962	25	15,22,23	1.22	1 (6%)	17,32,35	1.49	3 (17%)
25	6MZ	A	2030	25	18,25,26	1.15	2 (11%)	16,36,39	3.31	4 (25%)
25	G7M	A	2069	25	19,26,27	1.33	3 (15%)	19,39,42	2.43	7 (36%)
25	OMG	A	2251	25,22	18,26,27	1.10	2 (11%)	22,38,41	2.07	6 (27%)
25	2MG	A	2445	25	19,26,27	1.06	2 (10%)	20,38,41	2.23	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	H2U	A	2449	25	17,21,22	1.44	4 (23%)	21,30,33	2.18	3 (14%)
25	PSU	A	2457	25	16,21,22	2.12	4 (25%)	20,30,33	3.30	7 (35%)
25	OMC	A	2498	25	15,22,23	1.13	3 (20%)	19,31,34	0.84	0
25	2MA	A	2503	25	18,25,26	1.48	3 (16%)	17,37,40	2.23	2 (11%)
25	PSU	A	2504	25	16,21,22	1.71	5 (31%)	20,30,33	3.47	6 (30%)
25	OMU	A	2552	25	14,22,23	0.91	2 (14%)	18,31,34	1.94	1 (5%)
25	PSU	A	2580	25	16,21,22	1.73	5 (31%)	20,30,33	3.44	6 (30%)
25	PSU	A	2604	25	16,21,22	1.59	3 (18%)	20,30,33	3.87	6 (30%)
25	PSU	A	2605	25	16,21,22	1.45	4 (25%)	20,30,33	3.16	5 (25%)
25	1MG	A	745	25	18,26,27	1.53	2 (11%)	18,39,42	1.75	3 (16%)
25	PSU	A	746	25	16,21,22	1.77	5 (31%)	20,30,33	3.55	6 (30%)
25	5MU	A	747	25	14,22,23	0.93	2 (14%)	16,32,35	2.35	3 (18%)
25	PSU	A	955	25	16,21,22	1.62	5 (31%)	20,30,33	3.47	6 (30%)
1	2MG	a	1207	1	19,26,27	1.24	3 (15%)	20,38,41	2.20	8 (40%)
1	4OC	a	1402	1	16,23,24	0.99	2 (12%)	19,32,35	1.27	1 (5%)
1	5MC	a	1407	1	15,22,23	1.28	1 (6%)	17,32,35	1.11	1 (5%)
1	UR3	a	1498	1	14,22,23	1.06	1 (7%)	16,32,35	0.96	1 (6%)
1	2MG	a	1516	1	19,26,27	1.19	2 (10%)	20,38,41	2.32	6 (30%)
1	MA6	a	1518	1	16,26,27	1.08	1 (6%)	18,38,41	2.48	7 (38%)
1	MA6	a	1519	1	16,26,27	0.87	1 (6%)	18,38,41	2.56	7 (38%)
1	PSU	a	516	1	16,21,22	1.49	3 (18%)	20,30,33	3.57	6 (30%)
1	G7M	a	527	1	19,26,27	1.22	2 (10%)	19,39,42	2.61	8 (42%)
1	2MG	a	966	1	19,26,27	1.21	2 (10%)	20,38,41	2.42	8 (40%)
1	5MC	a	967	1	15,22,23	1.40	2 (13%)	17,32,35	1.14	2 (11%)
22	H2U	v	20	22	17,21,22	1.07	2 (11%)	21,30,33	1.76	3 (14%)
22	5MU	v	54	22	14,22,23	0.73	1 (7%)	16,32,35	2.50	2 (12%)
22	PSU	v	55	22	16,21,22	1.32	2 (12%)	20,30,33	3.49	8 (40%)
22	4SU	v	8	22	14,21,22	1.42	1 (7%)	15,30,33	1.30	2 (13%)
24	H2U	y	19	24	17,21,22	1.11	2 (11%)	21,30,33	1.24	3 (14%)
24	6IA	y	37	24	21,29,30	1.06	2 (9%)	21,41,44	2.28	4 (19%)
24	5MU	y	54	24	14,22,23	0.73	0	16,32,35	2.55	2 (12%)
24	PSU	y	55	24	16,21,22	1.61	3 (18%)	20,30,33	3.65	7 (35%)

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
25	6MZ	A	1618	25	-	0/5/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
25	PSU	A	1917	25	-	0/7/25/26	0/2/2/2
25	5MU	A	1939	25	-	0/3/25/26	0/2/2/2
25	5MC	A	1962	25	-	0/3/25/26	0/2/2/2
25	6MZ	A	2030	25	-	0/5/27/28	0/3/3/3
25	G7M	A	2069	25	2/2/5/5	0/3/25/26	0/3/3/3
25	OMG	A	2251	25,22	-	0/5/27/28	0/3/3/3
25	2MG	A	2445	25	-	0/5/27/28	0/3/3/3
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2498	25	-	0/5/27/28	0/2/2/2
25	2MA	A	2503	25	-	0/3/25/26	0/3/3/3
25	PSU	A	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	A	2552	25	-	0/5/27/28	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	1MG	A	745	25	-	0/3/25/26	0/3/3/3
25	PSU	A	746	25	-	0/7/25/26	0/2/2/2
25	5MU	A	747	25	-	0/3/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2
24	H2U	y	19	24	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	6IA	y	37	24	-	0/9/31/32	0/3/3/3
24	5MU	y	54	24	-	0/3/25/26	0/2/2/2
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2457	PSU	C5-C1'	-6.71	1.46	1.52
25	A	746	PSU	C5-C1'	-5.23	1.47	1.52
25	A	2504	PSU	C5-C1'	-5.16	1.47	1.52
24	y	55	PSU	C5-C1'	-4.93	1.48	1.52
25	A	2604	PSU	C5-C1'	-4.62	1.48	1.52

The worst 5 of 197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	955	PSU	N1-C2-N3	-10.07	121.16	128.40
25	A	2604	PSU	N1-C2-N3	-9.59	121.50	128.40
25	A	746	PSU	N1-C2-N3	-9.39	121.64	128.40
1	a	516	PSU	N1-C2-N3	-9.36	121.67	128.40
25	A	2605	PSU	N1-C2-N3	-9.31	121.70	128.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
25	A	2069	G7M	C4'
25	A	2069	G7M	C3'

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1915	3TD	1	0
25	A	2030	6MZ	1	0
25	A	2251	OMG	1	0
25	A	2445	2MG	1	0
25	A	745	1MG	1	0
25	A	747	5MU	1	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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
24	y	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	5(A):A	O3'	6:U	P	3.00
1	y	47(Q):G	O3'	48:G	P	3.00
1	y	67(A):U	O3'	68:C	P	3.00
1	y	5:G	O3'	5(A):A	P	2.99
1	y	67:A	O3'	67(A):U	P	2.99