



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 6, 2017 – 04:30 AM EDT

PDB ID : 5L3P
EMDB ID: : EMD-4001
Title : Cryo-EM structure of stringent response factor RelA bound to ErmCL-stalled ribosome complex
Authors : Arenz, S.; Wilson, D.N.
Deposited on : unknown
Resolution : 3.70 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (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

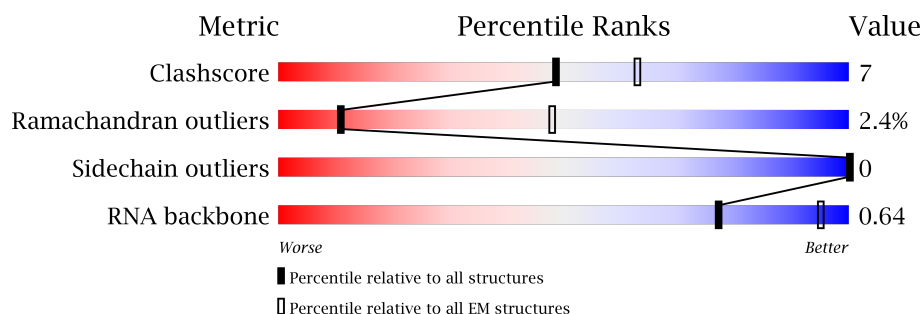
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.
















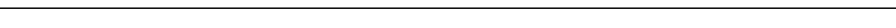











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 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	2903	63% 32% 5%
2	B	120	69% 26% 5%
3	D	273	73% 26% .
4	E	209	78% 22%
5	F	201	76% 24%
6	G	179	75% 24% .
7	H	177	83% 16% .
8	I	149	79% 19% .


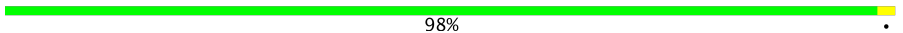



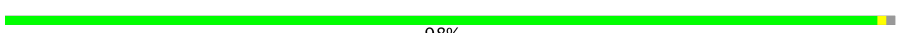










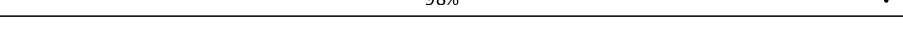

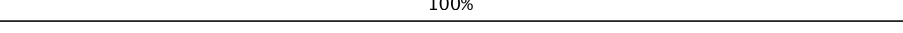



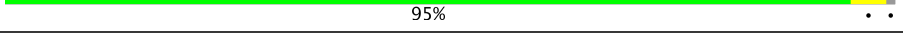


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Mol	Chain	Length	Quality of chain
9	N	142	
10	O	123	
11	P	144	
12	Q	136	
13	R	127	
14	S	117	
15	T	115	
16	U	118	
17	V	103	
18	W	110	
19	X	100	
20	Y	104	
21	Z	94	
22	0	85	
23	1	78	
24	2	63	
25	3	59	
26	4	70	
27	5	57	
28	6	55	
29	7	46	
30	8	65	
31	9	38	
32	a	1539	
33	b	240	

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Mol	Chain	Length	Quality of chain
34	c	233	
35	d	206	
36	e	167	
37	f	135	
38	g	179	
39	h	130	
40	i	130	
41	j	103	
42	k	129	
43	l	124	
44	m	118	
45	o	89	
46	p	82	
47	q	84	
48	r	75	
49	t	87	
50	u	71	
51	v	6	
52	x	77	
53	J	165	
54	K	142	
55	n	102	
56	s	92	
57	z	819	
58	y	73	

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
1	2MG	A	1835	X	-	-	-
1	PSU	A	1911	X	-	-	-
1	3TD	A	1915	X	-	-	-
1	PSU	A	1917	X	-	-	-
1	5MU	A	1939	X	-	-	-
1	7MG	A	2069	X	-	-	-
1	OMG	A	2251	X	-	-	-
1	2MG	A	2445	X	-	-	-
1	H2U	A	2449	X	-	-	-
1	PSU	A	2457	X	-	-	-
1	OMC	A	2498	X	-	-	-
1	2MA	A	2503	X	-	-	-
1	PSU	A	2504	X	-	-	-
1	OMU	A	2552	X	-	-	-
1	PSU	A	2580	X	-	-	-
1	PSU	A	2604	X	-	-	-
1	PSU	A	2605	X	-	-	-
1	PSU	A	746	X	-	-	-
1	PSU	A	955	X	-	-	-
32	2MG	a	1207	X	-	-	-
32	4OC	a	1402	X	-	-	-
32	UR3	a	1498	X	-	-	-
32	2MG	a	1516	X	-	-	-
32	MA6	a	1518	X	-	-	-
32	MA6	a	1519	X	-	-	-
32	PSU	a	516	X	-	-	-
32	7MG	a	527	X	-	-	-
32	2MG	a	966	X	-	-	-
52	H2U	x	20	X	-	-	-
52	5MU	x	54	X	-	-	-
52	PSU	x	55	X	-	-	-
52	4SU	x	8	X	-	-	-
58	H2U	y	16	X	-	-	-
58	H2U	y	17	X	-	-	-
58	H2U	y	20	X	-	-	-
58	7MG	y	46	X	-	-	-
58	5MU	y	54	X	-	-	-
58	PSU	y	55	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 149606 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	A	2890	Total	C	N	O	P	0	0
			62057	27688	11422	20057	2890		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 999944586

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 49 is a protein called 30S ribosomal protein S20.

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 52 is a RNA chain called P-site tRNA.

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

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 54 is a protein called 50S ribosomal protein L11.

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

- Molecule 55 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 57 is a protein called GTP pyrophosphokinase,GTP pyrophosphokinase,GTP pyrophosphokinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	545	Total	C	N	O		0	0
			2255	1165	545	545			

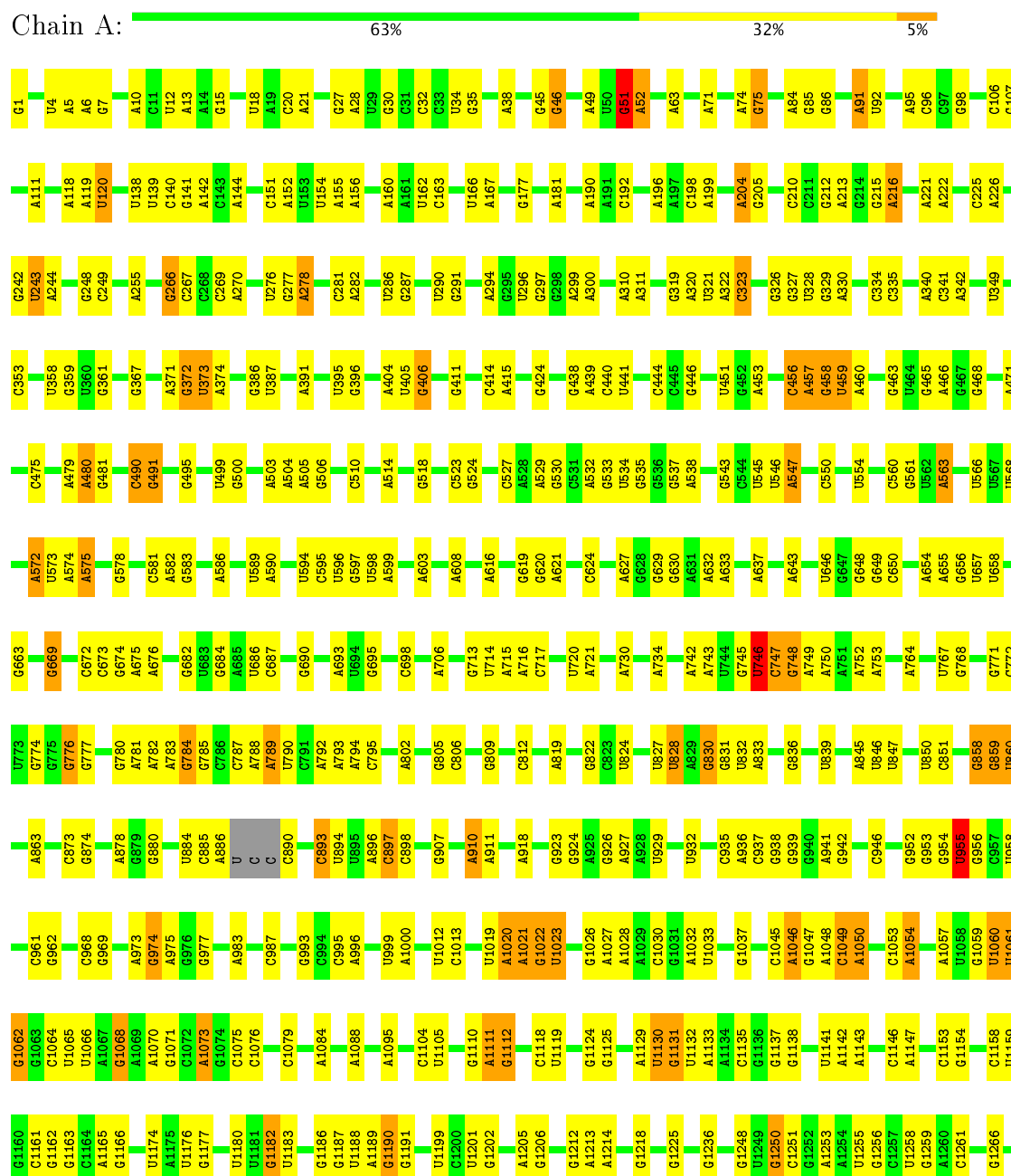
- Molecule 58 is a RNA chain called deacylated A/R-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	73	Total	C	N	O	P	0	0
			1581	709	280	519	73		

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: 23S ribosomal RNA





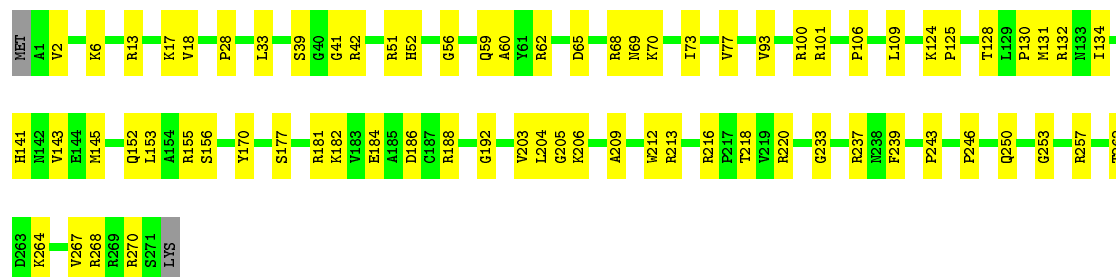

- Molecule 2: 5S ribosomal RNA

Chain B: 




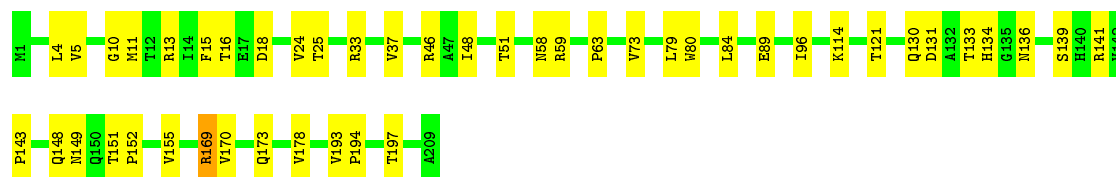
- Molecule 3: 50S ribosomal protein L2

Chain D: 




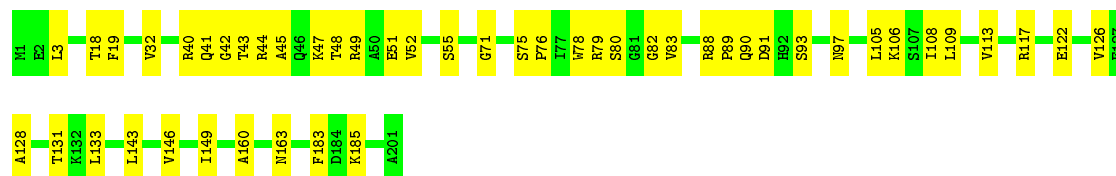
- Molecule 4: 50S ribosomal protein L3

Chain E: 



- Molecule 5: 50S ribosomal protein L4

Chain F: 




- Molecule 6: 50S ribosomal protein L5

Chain G: 




- Molecule 7: 50S ribosomal protein L6

Chain H:  83% 16%



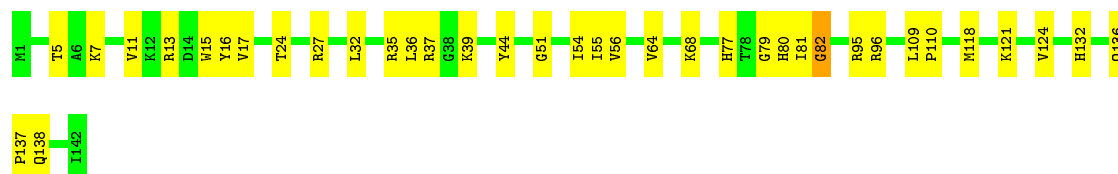
- Molecule 8: 50S ribosomal protein L9

Chain I:  79% 19%



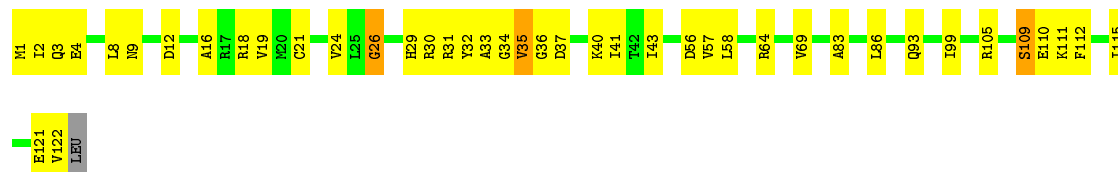
- Molecule 9: 50S ribosomal protein L13

Chain N:  74% 25%



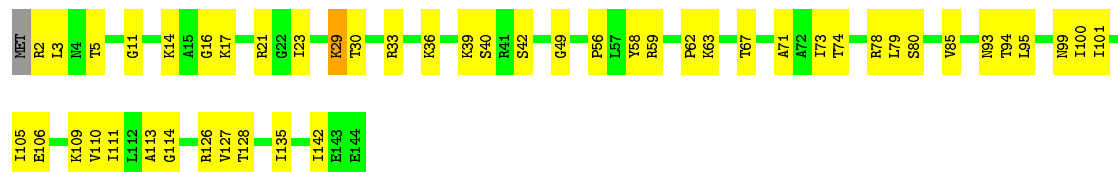
- Molecule 10: 50S ribosomal protein L14

Chain O:  65% 32%




- Molecule 11: 50S ribosomal protein L15

Chain P:  66% 33%

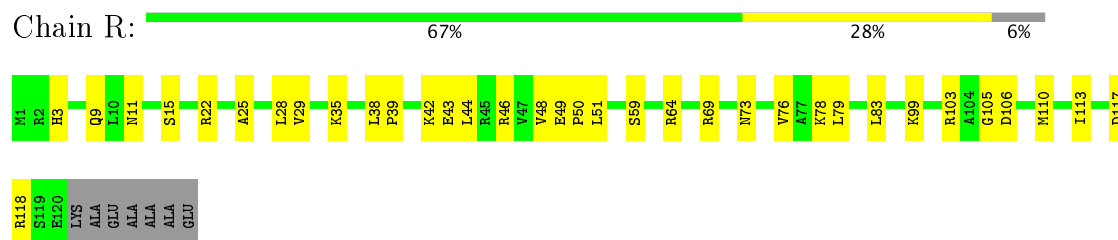


- Molecule 12: 50S ribosomal protein L16

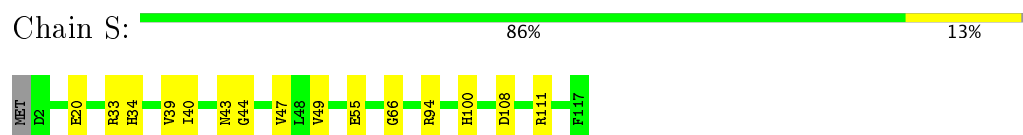
Chain Q:  81% 18%



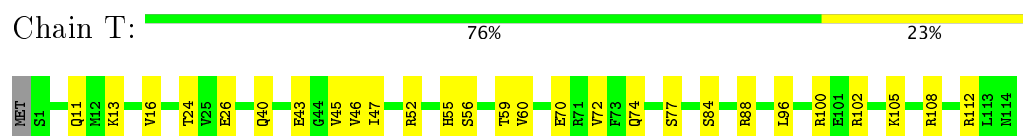
- Molecule 13: 50S ribosomal protein L17



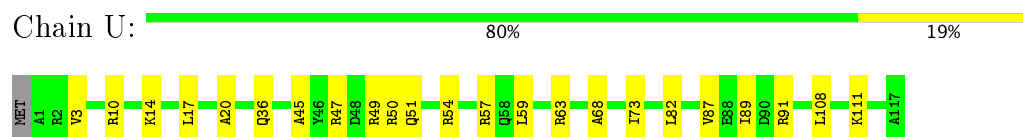
- Molecule 14: 50S ribosomal protein L18



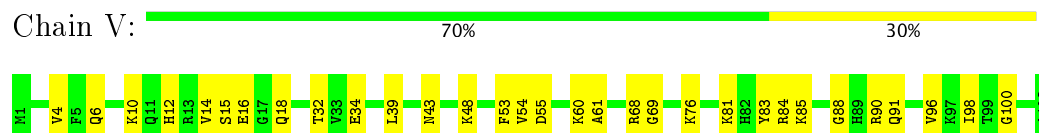
- Molecule 15: 50S ribosomal protein L19



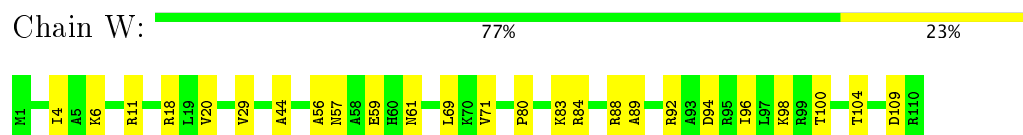
- Molecule 16: 50S ribosomal protein L20



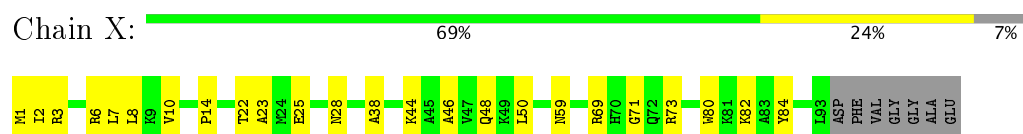
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

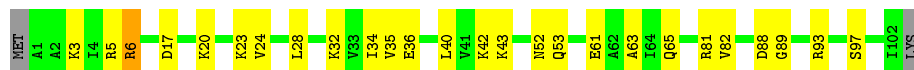


- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

Chain Y:  73% 24% ..



- Molecule 21: 50S ribosomal protein L25

Chain Z:  74% 26%




- Molecule 22: 50S ribosomal protein L27

Chain 0:  65% 22% 12%



- Molecule 23: 50S ribosomal protein L28

Chain 1:  81% 18%



- Molecule 24: 50S ribosomal protein L29

Chain 2:  76% 24%




- Molecule 25: 50S ribosomal protein L30

Chain 3:  69% 29%




- Molecule 26: 50S ribosomal protein L31

Chain 4:  80% 13% 6%



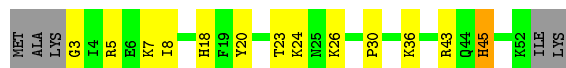
- Molecule 27: 50S ribosomal protein L32

Chain 5:  79% 19%



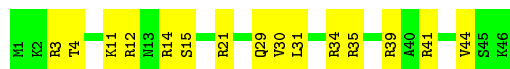
- Molecule 28: 50S ribosomal protein L33

Chain 6: 67% 22% 9%



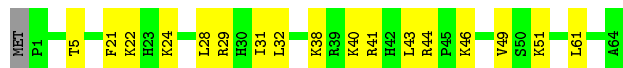
- Molecule 29: 50S ribosomal protein L34

Chain 7: 67% 33%



- Molecule 30: 50S ribosomal protein L35

Chain 8: 72% 26%



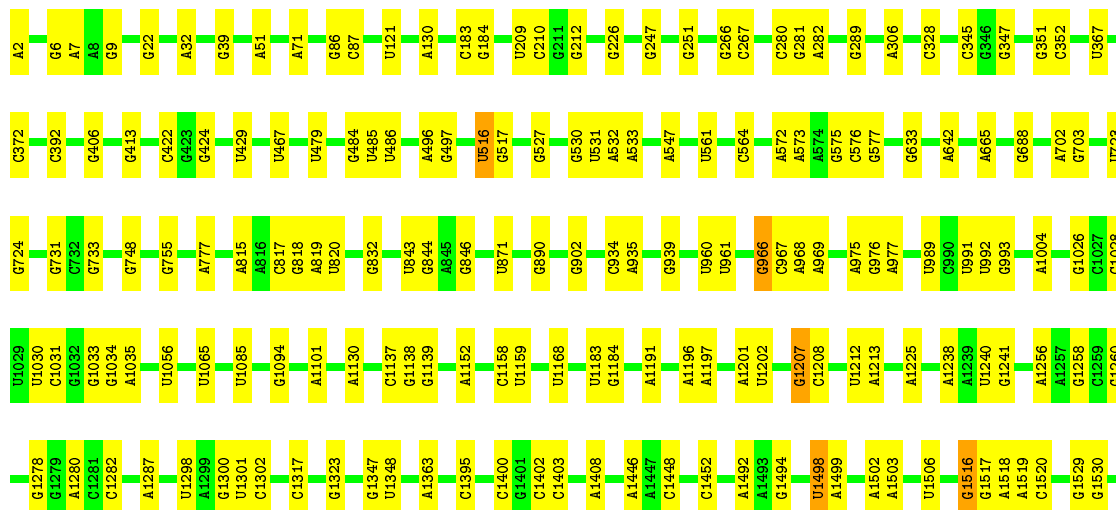
- Molecule 31: 50S ribosomal protein L36

Chain 9: 79% 21%



- Molecule 32: 16S ribosomal RNA

Chain a: 88% 11%





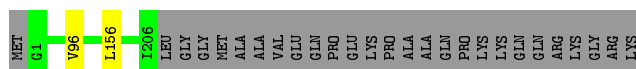
- Molecule 33: 30S ribosomal protein S2

Chain b: 89% 9%



- Molecule 34: 30S ribosomal protein S3

Chain c: 88% 12%



- Molecule 35: 30S ribosomal protein S4

Chain d: 98%



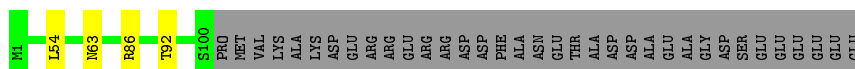
- Molecule 36: 30S ribosomal protein S5

Chain e: 90% 6%



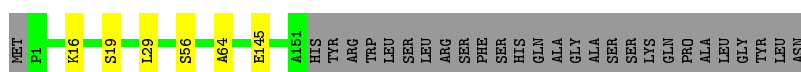
- Molecule 37: 30S ribosomal protein S6

Chain f: 71% 26%



- Molecule 38: 30S ribosomal protein S7

Chain g: 81% 16%



- Molecule 39: 30S ribosomal protein S8

Chain h: 98%




- Molecule 40: 30S ribosomal protein S9

Chain i:  94% . .



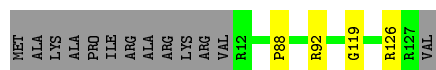
- Molecule 41: 30S ribosomal protein S10

Chain j:  89% 6% 5%



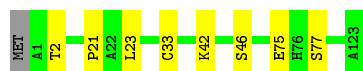
- Molecule 42: 30S ribosomal protein S11

Chain k:  87% 10%



- Molecule 43: 30S ribosomal protein S12

Chain l:  93% 6% .



- Molecule 44: 30S ribosomal protein S13

Chain m:  95% . .



- Molecule 45: 30S ribosomal protein S15

Chain o:  93% 6% .




- Molecule 46: 30S ribosomal protein S16

Chain p:  98% .




- Molecule 47: 30S ribosomal protein S17

Chain q:  90% 5% 5%



- Molecule 48: 30S ribosomal protein S18

Chain r:  83% 13%




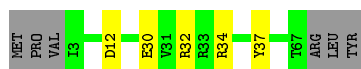
- Molecule 49: 30S ribosomal protein S20

Chain t:  98%



- Molecule 50: 30S ribosomal protein S21

Chain u:  85% 7% 8%




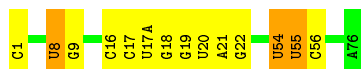
- Molecule 51: mRNA

Chain v:  100%

There are no outlier residues recorded for this chain.

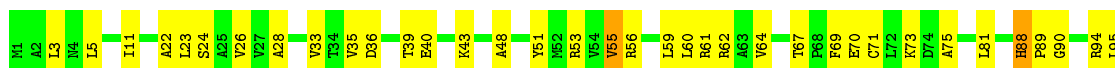
- Molecule 52: P-site tRNA

Chain x:  82% 14%



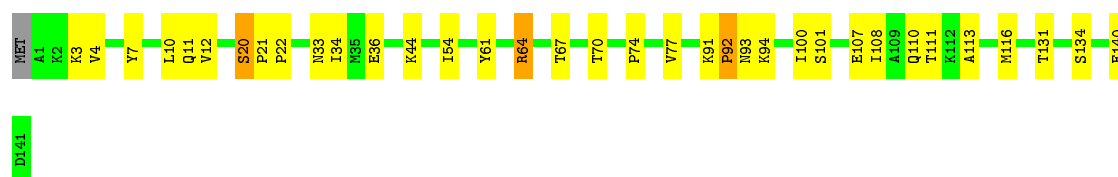
- Molecule 53: 50S ribosomal protein L10

Chain J:  50% 27% 21%



- Molecule 54: 50S ribosomal protein L11

Chain K:  75% 23%




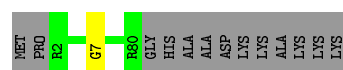
- Molecule 55: 30S ribosomal protein S14

Chain n: 95% .



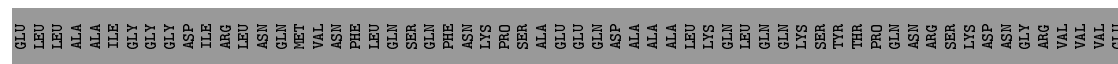
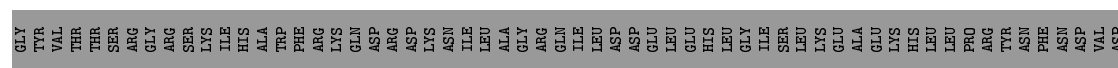
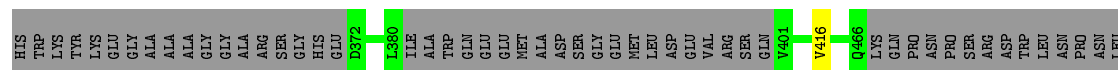
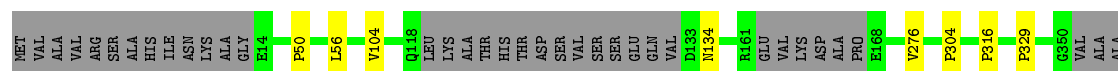
- Molecule 56: 30S ribosomal protein S19

Chain s:  85% • 14%



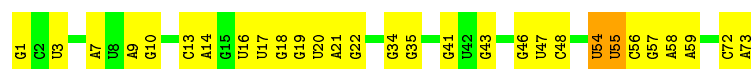
- Molecule 57: GTP pyrophosphokinase, GTP pyrophosphokinase, GTP pyrophosphokinase

Chain z:  65% . 33%



- Molecule 58: deacylated A/R-tRNA

Chain v:  60% 37%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	24749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	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: 3TD, OMC, OMG, OMU, MA6, H2U, YG, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, 5MU, 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	0.12	1/68920 (0.0%)	0.67	20/107498 (0.0%)
10	O	0.20	0/947	0.40	0/1268
11	P	0.20	0/1054	0.39	0/1403
12	Q	0.21	0/1093	0.41	0/1460
13	R	0.21	0/973	0.39	0/1301
14	S	0.20	0/902	0.35	0/1209
15	T	0.20	0/929	0.41	0/1242
16	U	0.21	0/960	0.35	0/1278
17	V	0.21	0/829	0.38	0/1107
18	W	0.19	0/864	0.39	0/1156
19	X	0.20	0/744	0.39	0/994
2	B	0.23	1/2876 (0.0%)	0.65	0/4483
20	Y	0.21	0/787	0.37	0/1051
21	Z	0.20	0/766	0.36	0/1025
22	0	0.20	0/582	0.35	0/769
23	1	0.19	0/635	0.36	0/848
24	2	0.21	0/510	0.36	0/677
25	3	0.21	0/453	0.41	0/605
26	4	0.21	0/531	0.40	0/709
27	5	0.19	0/450	0.36	0/599
28	6	0.21	0/416	0.41	0/554
29	7	0.20	0/380	0.36	0/498
3	D	0.20	0/2121	0.39	0/2852
30	8	0.21	0/513	0.42	0/676
31	9	0.19	0/303	0.38	0/397
32	a	0.13	1/36701 (0.0%)	0.66	5/57246 (0.0%)
33	b	0.21	0/1735	0.39	0/2338
34	c	0.21	0/1651	0.41	0/2225
35	d	0.21	0/1665	0.38	0/2227
36	e	0.22	0/1154	0.41	0/1554
37	f	0.21	0/835	0.39	0/1128

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	g	0.20	0/1195	0.39	0/1602
39	h	0.21	0/989	0.40	0/1326
4	E	0.21	0/1586	0.38	0/2134
40	i	0.21	0/1034	0.40	0/1375
41	j	0.21	0/796	0.42	0/1077
42	k	0.20	0/885	0.39	0/1195
43	l	0.21	0/969	0.42	0/1300
44	m	0.20	0/892	0.41	0/1193
45	o	0.20	0/722	0.35	0/964
46	p	0.20	0/659	0.35	0/884
47	q	0.22	0/657	0.43	0/881
48	r	0.20	0/511	0.40	0/689
49	t	0.20	0/671	0.34	0/888
5	F	0.20	0/1571	0.37	0/2113
50	u	0.21	0/500	0.38	0/668
51	v	0.10	0/144	0.64	0/222
52	x	0.27	1/1747 (0.1%)	0.64	0/2721
53	J	0.22	0/1001	0.43	0/1350
54	K	0.21	0/1046	0.41	0/1410
55	n	0.20	0/811	0.37	0/1081
56	s	0.20	0/652	0.37	0/877
57	z	0.16	0/1874	0.32	0/2332
58	y	0.29	1/1585 (0.1%)	0.66	0/2469
6	G	0.21	0/1434	0.40	0/1926
7	H	0.20	0/1343	0.37	0/1816
8	I	0.21	0/1122	0.38	0/1515
9	N	0.21	0/1152	0.39	0/1551
All	All	0.16	5/160827 (0.0%)	0.60	25/239936 (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	35	0
32	a	17	0
52	x	9	0
58	y	9	0
All	All	70	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.62	1.48	1.61
58	y	1	G	OP3-P	-10.62	1.48	1.61
52	x	1	C	OP3-P	-10.58	1.48	1.61
32	a	2	A	OP3-P	-10.57	1.48	1.61
1	A	1	G	OP3-P	-10.54	1.48	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1049	C	C2-N3-C4	18.01	128.91	119.90
1	A	1050	A	N1-C2-N3	16.54	137.57	129.30
1	A	1073	A	N1-C2-N3	16.48	137.54	129.30
1	A	1050	A	C2-N3-C4	12.07	116.63	110.60
1	A	1073	A	C2-N3-C4	11.70	116.45	110.60

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	746	PSU	C4',C2'
1	A	955	PSU	C4',C2'
1	A	1835	2MG	C2',C3'
1	A	1911	PSU	C4',C2'
1	A	1915	3TD	C4'

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62057	0	31229	577	0
2	B	2572	0	1302	20	0
3	D	2082	0	2157	57	0
4	E	1565	0	1616	36	0
5	F	1552	0	1619	34	0
6	G	1410	0	1447	27	0
7	H	1323	0	1374	17	0
8	I	1111	0	1148	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	1129	0	1162	28	0
10	O	938	0	1012	26	0
11	P	1045	0	1117	32	0
12	Q	1074	0	1157	18	0
13	R	960	0	1000	25	0
14	S	892	0	923	10	0
15	T	917	0	965	20	0
16	U	947	0	1022	18	0
17	V	816	0	839	20	0
18	W	857	0	922	19	0
19	X	738	0	807	15	0
20	Y	779	0	834	16	0
21	Z	753	0	780	17	0
22	0	575	0	592	16	0
23	1	625	0	655	10	0
24	2	509	0	543	11	0
25	3	449	0	491	13	0
26	4	522	0	522	9	0
27	5	444	0	461	6	0
28	6	409	0	440	10	0
29	7	377	0	418	16	0
30	8	504	0	574	11	0
31	9	302	0	343	6	0
32	a	33029	0	16645	0	0
33	b	1704	0	1732	0	0
34	c	1624	0	1699	0	0
35	d	1643	0	1710	0	0
36	e	1141	0	1170	0	0
37	f	817	0	808	0	0
38	g	1181	0	1240	0	0
39	h	979	0	1034	0	0
40	i	1022	0	1070	0	0
41	j	786	0	828	0	0
42	k	869	0	878	0	0
43	l	955	0	1019	0	0
44	m	883	0	944	0	0
45	o	714	0	737	0	0
46	p	649	0	666	0	0
47	q	648	0	691	0	0
48	r	504	0	502	0	0
49	t	665	0	714	0	0
50	u	495	0	486	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	v	129	0	65	0	0
52	x	1644	0	840	0	0
53	J	988	0	1025	26	0
54	K	1032	0	1088	19	0
55	n	799	0	841	0	0
56	s	637	0	665	0	0
57	z	2255	0	592	0	0
58	y	1581	0	813	0	0
All	All	149606	0	99973	1011	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 7.

The worst 5 of 1011 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)
6:G:140:ILE:HG22	6:G:142:TYR:H	1.46	0.80
21:Z:9:ARG:HD3	21:Z:39:ALA:HB1	1.65	0.77
1:A:2279:G:HO2'	1:A:2327:A:HO2'	1.31	0.77
17:V:98:ILE:HG22	17:V:100:GLY:H	1.50	0.77
7:H:94:ARG:HB2	7:H:105:SER:HB2	1.68	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	
3	D	269/273 (98%)	243 (90%)	25 (9%)	1 (0%)	38	77
4	E	207/209 (99%)	187 (90%)	17 (8%)	3 (1%)	13	55
5	F	199/201 (99%)	184 (92%)	11 (6%)	4 (2%)	9	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	175/179 (98%)	154 (88%)	18 (10%)	3 (2%)	11	53
7	H	174/177 (98%)	149 (86%)	23 (13%)	2 (1%)	17	61
8	I	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	6	43
9	N	140/142 (99%)	130 (93%)	8 (6%)	2 (1%)	13	55
10	O	120/123 (98%)	108 (90%)	7 (6%)	5 (4%)	3	32
11	P	141/144 (98%)	122 (86%)	13 (9%)	6 (4%)	3	32
12	Q	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	48
13	R	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	6	45
14	S	114/117 (97%)	106 (93%)	6 (5%)	2 (2%)	10	52
15	T	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
16	U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
17	V	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	3	34
18	W	108/110 (98%)	94 (87%)	14 (13%)	0	100	100
19	X	91/100 (91%)	81 (89%)	8 (9%)	2 (2%)	8	48
20	Y	100/104 (96%)	87 (87%)	11 (11%)	2 (2%)	9	50
21	Z	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
22	0	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	13	55
23	1	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
24	2	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
25	3	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
26	4	64/70 (91%)	56 (88%)	7 (11%)	1 (2%)	11	54
27	5	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	9	51
28	6	48/55 (87%)	43 (90%)	4 (8%)	1 (2%)	8	49
29	7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
30	8	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	11	54
31	9	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	43
33	b	216/240 (90%)	187 (87%)	25 (12%)	4 (2%)	9	51
34	c	204/233 (88%)	188 (92%)	14 (7%)	2 (1%)	18	62
35	d	203/206 (98%)	180 (89%)	19 (9%)	4 (2%)	9	50
36	e	155/167 (93%)	132 (85%)	17 (11%)	6 (4%)	3	34
37	f	98/135 (73%)	85 (87%)	9 (9%)	4 (4%)	3	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	g	149/179 (83%)	130 (87%)	13 (9%)	6 (4%)	3	34
39	h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	22	66
40	i	125/130 (96%)	107 (86%)	13 (10%)	5 (4%)	3	34
41	j	96/103 (93%)	79 (82%)	11 (12%)	6 (6%)	1	23
42	k	114/129 (88%)	99 (87%)	11 (10%)	4 (4%)	4	38
43	l	121/124 (98%)	104 (86%)	9 (7%)	8 (7%)	1	22
44	m	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	10	52
45	o	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	2	24
46	p	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	6	45
47	q	78/84 (93%)	65 (83%)	9 (12%)	4 (5%)	2	28
48	r	63/75 (84%)	56 (89%)	4 (6%)	3 (5%)	2	29
49	t	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
50	u	63/71 (89%)	48 (76%)	10 (16%)	5 (8%)	1	16
53	J	129/165 (78%)	102 (79%)	21 (16%)	6 (5%)	3	30
54	K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	2	28
55	n	99/102 (97%)	87 (88%)	8 (8%)	4 (4%)	3	34
56	s	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	14	57
57	z	458/819 (56%)	423 (92%)	24 (5%)	11 (2%)	7	46
All	All	6305/7039 (90%)	5637 (89%)	516 (8%)	152 (2%)	11	46

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	81	ILE
11	P	128	THR
34	c	96	VAL
34	c	156	LEU
36	e	122	VAL

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	
3	D	216/218 (99%)	216 (100%)	0	100	100
4	E	164/164 (100%)	164 (100%)	0	100	100
5	F	165/165 (100%)	165 (100%)	0	100	100
6	G	148/150 (99%)	148 (100%)	0	100	100
7	H	137/138 (99%)	137 (100%)	0	100	100
8	I	114/114 (100%)	114 (100%)	0	100	100
9	N	116/116 (100%)	116 (100%)	0	100	100
10	O	103/104 (99%)	103 (100%)	0	100	100
11	P	102/103 (99%)	102 (100%)	0	100	100
12	Q	109/109 (100%)	109 (100%)	0	100	100
13	R	100/103 (97%)	100 (100%)	0	100	100
14	S	86/87 (99%)	86 (100%)	0	100	100
15	T	99/100 (99%)	99 (100%)	0	100	100
16	U	89/90 (99%)	89 (100%)	0	100	100
17	V	84/84 (100%)	84 (100%)	0	100	100
18	W	93/93 (100%)	93 (100%)	0	100	100
19	X	80/84 (95%)	80 (100%)	0	100	100
20	Y	83/85 (98%)	83 (100%)	0	100	100
21	Z	78/78 (100%)	78 (100%)	0	100	100
22	0	57/63 (90%)	57 (100%)	0	100	100
23	1	67/68 (98%)	67 (100%)	0	100	100
24	2	55/55 (100%)	55 (100%)	0	100	100
25	3	48/49 (98%)	48 (100%)	0	100	100
26	4	59/62 (95%)	59 (100%)	0	100	100
27	5	47/48 (98%)	47 (100%)	0	100	100
28	6	45/49 (92%)	45 (100%)	0	100	100
29	7	38/38 (100%)	38 (100%)	0	100	100
30	8	51/52 (98%)	51 (100%)	0	100	100
31	9	34/34 (100%)	34 (100%)	0	100	100
33	b	180/198 (91%)	180 (100%)	0	100	100
34	c	170/190 (90%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	d	172/173 (99%)	172 (100%)	0	100	100
36	e	114/126 (90%)	114 (100%)	0	100	100
37	f	87/116 (75%)	87 (100%)	0	100	100
38	g	124/147 (84%)	124 (100%)	0	100	100
39	h	104/105 (99%)	104 (100%)	0	100	100
40	i	105/107 (98%)	105 (100%)	0	100	100
41	j	86/90 (96%)	86 (100%)	0	100	100
42	k	89/99 (90%)	89 (100%)	0	100	100
43	l	103/104 (99%)	103 (100%)	0	100	100
44	m	92/96 (96%)	92 (100%)	0	100	100
45	o	76/77 (99%)	76 (100%)	0	100	100
46	p	65/65 (100%)	65 (100%)	0	100	100
47	q	74/78 (95%)	74 (100%)	0	100	100
48	r	48/65 (74%)	48 (100%)	0	100	100
49	t	65/66 (98%)	65 (100%)	0	100	100
50	u	44/61 (72%)	44 (100%)	0	100	100
53	J	100/123 (81%)	100 (100%)	0	100	100
54	K	109/110 (99%)	109 (100%)	0	100	100
55	n	79/84 (94%)	79 (100%)	0	100	100
56	s	70/79 (89%)	70 (100%)	0	100	100
All	All	4823/5062 (95%)	4823 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
25	3	19	HIS
35	d	119	HIS
49	t	74	HIS
28	6	18	HIS
31	9	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2881/2903 (99%)	415 (14%)	43 (1%)
2	B	119/120 (99%)	13 (10%)	2 (1%)
32	a	1535/1539 (99%)	176 (11%)	0
51	v	5/6 (83%)	0	0
52	x	76/77 (98%)	13 (17%)	0
58	y	72/73 (98%)	28 (38%)	0
All	All	4688/4718 (99%)	645 (13%)	45 (0%)

5 of 645 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	27	G
1	A	34	U
1	A	35	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1300	G
1	A	1939	5MU
1	A	2756	U
1	A	1835	2MG
1	A	1940	U

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

46 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
1	6MZ	A	1618	1	18,25,26	0.80	1 (5%)	16,36,39	3.13	4 (25%)
1	2MG	A	1835	1	19,26,27	3.42	2 (10%)	20,38,41	2.49	9 (45%)
1	PSU	A	1911	1	16,21,22	1.37	3 (18%)	20,30,33	3.07	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	3TD	A	1915	1	16,22,23	2.17	4 (25%)	19,32,35	1.46	4 (21%)
1	PSU	A	1917	1	16,21,22	1.47	3 (18%)	20,30,33	3.13	5 (25%)
1	5MU	A	1939	1	14,22,23	1.40	1 (7%)	16,32,35	2.77	4 (25%)
1	5MC	A	1962	1	15,22,23	1.31	2 (13%)	17,32,35	1.14	2 (11%)
1	6MZ	A	2030	1	18,25,26	0.79	1 (5%)	16,36,39	3.15	4 (25%)
1	7MG	A	2069	1	20,26,27	2.77	6 (30%)	22,39,42	2.26	6 (27%)
1	OMG	A	2251	1,52	18,26,27	2.41	2 (11%)	22,38,41	1.81	6 (27%)
1	2MG	A	2445	1	19,26,27	3.42	2 (10%)	20,38,41	2.37	9 (45%)
1	H2U	A	2449	1	17,21,22	3.65	5 (29%)	21,30,33	2.71	5 (23%)
1	PSU	A	2457	1	16,21,22	1.40	3 (18%)	20,30,33	3.06	5 (25%)
1	OMC	A	2498	1	15,22,23	1.07	2 (13%)	19,31,34	0.87	1 (5%)
1	2MA	A	2503	1	18,25,26	1.73	1 (5%)	17,37,40	1.88	2 (11%)
1	PSU	A	2504	1	16,21,22	1.36	2 (12%)	20,30,33	3.08	5 (25%)
1	OMU	A	2552	1	14,22,23	2.12	3 (21%)	18,31,34	2.05	1 (5%)
1	PSU	A	2580	1	16,21,22	1.49	3 (18%)	20,30,33	3.16	6 (30%)
1	PSU	A	2604	1	16,21,22	1.34	2 (12%)	20,30,33	3.10	6 (30%)
1	PSU	A	2605	1	16,21,22	1.47	3 (18%)	20,30,33	3.09	5 (25%)
1	1MG	A	745	1	18,26,27	2.41	3 (16%)	18,39,42	1.78	3 (16%)
1	PSU	A	746	1	16,21,22	1.30	2 (12%)	20,30,33	3.17	6 (30%)
1	5MC	A	747	1	15,22,23	1.31	2 (13%)	17,32,35	1.15	2 (11%)
1	PSU	A	955	1	16,21,22	1.42	3 (18%)	20,30,33	3.08	5 (25%)
32	2MG	a	1207	32	19,26,27	3.43	2 (10%)	20,38,41	2.38	9 (45%)
32	4OC	a	1402	32	16,23,24	1.25	2 (12%)	19,32,35	1.30	2 (10%)
32	5MC	a	1407	32	15,22,23	1.32	2 (13%)	17,32,35	1.13	2 (11%)
32	UR3	a	1498	32	14,22,23	1.63	2 (14%)	16,32,35	0.64	0
32	2MG	a	1516	32	19,26,27	3.44	2 (10%)	20,38,41	2.36	9 (45%)
32	MA6	a	1518	32	16,26,27	0.60	0	18,38,41	1.85	4 (22%)
32	MA6	a	1519	32	16,26,27	0.53	0	18,38,41	2.00	4 (22%)
32	PSU	a	516	32	16,21,22	1.38	3 (18%)	20,30,33	3.09	5 (25%)
32	7MG	a	527	32	20,26,27	2.74	5 (25%)	22,39,42	2.07	4 (18%)
32	2MG	a	966	32	19,26,27	3.41	2 (10%)	20,38,41	2.43	9 (45%)
32	5MC	a	967	32	15,22,23	1.37	2 (13%)	17,32,35	1.20	2 (11%)
52	H2U	x	20	52	17,21,22	3.65	5 (29%)	21,30,33	2.69	5 (23%)
52	5MU	x	54	52	14,22,23	1.38	1 (7%)	16,32,35	2.75	4 (25%)
52	PSU	x	55	52	16,21,22	1.45	4 (25%)	20,30,33	3.18	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	4SU	x	8	52	14,21,22	1.74	3 (21%)	15,30,33	1.38	2 (13%)
58	H2U	y	16	58	17,21,22	3.68	5 (29%)	21,30,33	2.67	5 (23%)
58	H2U	y	17	58	17,21,22	3.65	5 (29%)	21,30,33	2.75	5 (23%)
58	H2U	y	20	58	17,21,22	3.64	5 (29%)	21,30,33	2.69	4 (19%)
58	YG	y	37	1,58	29,42,43	1.46	2 (6%)	29,62,65	1.87	8 (27%)
58	7MG	y	46	58	20,26,27	2.74	5 (25%)	22,39,42	1.89	5 (22%)
58	5MU	y	54	58	14,22,23	1.38	1 (7%)	16,32,35	2.83	4 (25%)
58	PSU	y	55	58	16,21,22	1.48	3 (18%)	20,30,33	3.22	6 (30%)

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
1	6MZ	A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	A	1835	1	2/2/5/6	0/5/27/28	0/3/3/3
1	PSU	A	1911	1	2/2/5/5	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	1/1/5/5	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	2/2/5/5	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	3/3/5/5	0/3/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	A	2030	1	-	0/5/27/28	0/3/3/3
1	7MG	A	2069	1	1/1/7/7	0/7/37/38	0/3/3/3
1	OMG	A	2251	1,52	2/2/5/5	0/5/27/28	0/3/3/3
1	2MG	A	2445	1	2/2/5/6	0/5/27/28	0/3/3/3
1	H2U	A	2449	1	1/1/8/9	0/7/38/39	0/2/2/2
1	PSU	A	2457	1	2/2/5/5	0/7/25/26	0/2/2/2
1	OMC	A	2498	1	2/2/5/5	0/5/27/28	0/2/2/2
1	2MA	A	2503	1	2/2/5/5	0/3/25/26	0/3/3/3
1	PSU	A	2504	1	2/2/5/5	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	1/1/5/5	0/5/27/28	0/2/2/2
1	PSU	A	2580	1	2/2/5/5	0/7/25/26	0/2/2/2
1	PSU	A	2604	1	2/2/5/5	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	2/2/5/5	0/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	746	1	2/2/5/5	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	A	955	1	2/2/5/5	0/7/25/26	0/2/2/2
32	2MG	a	1207	32	2/2/5/6	0/5/27/28	0/3/3/3
32	4OC	a	1402	32	2/2/5/6	0/7/29/30	0/2/2/2
32	5MC	a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	a	1498	32	2/2/5/5	0/3/25/26	0/2/2/2
32	2MG	a	1516	32	2/2/5/6	0/5/27/28	0/3/3/3
32	MA6	a	1518	32	2/2/6/6	0/7/29/30	0/3/3/3
32	MA6	a	1519	32	2/2/6/6	0/7/29/30	0/3/3/3
32	PSU	a	516	32	2/2/5/5	0/7/25/26	0/2/2/2
32	7MG	a	527	32	1/1/7/7	0/7/37/38	0/3/3/3
32	2MG	a	966	32	2/2/5/6	0/5/27/28	0/3/3/3
32	5MC	a	967	32	-	0/3/25/26	0/2/2/2
52	H2U	x	20	52	1/1/8/9	0/7/38/39	0/2/2/2
52	5MU	x	54	52	3/3/5/5	0/3/25/26	0/2/2/2
52	PSU	x	55	52	2/2/5/5	0/7/25/26	0/2/2/2
52	4SU	x	8	52	3/3/5/5	0/3/25/26	0/2/2/2
58	H2U	y	16	58	1/1/8/9	0/7/38/39	0/2/2/2
58	H2U	y	17	58	1/1/8/9	0/7/38/39	0/2/2/2
58	H2U	y	20	58	1/1/8/9	0/7/38/39	0/2/2/2
58	YG	y	37	1,58	-	0/20/42/43	0/4/4/4
58	7MG	y	46	58	1/1/7/7	0/7/37/38	0/3/3/3
58	5MU	y	54	58	3/3/5/5	0/3/25/26	0/2/2/2
58	PSU	y	55	58	2/2/5/5	0/7/25/26	0/2/2/2

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	16	H2U	C6-N1	-9.40	1.35	1.47
1	A	2449	H2U	C6-N1	-9.25	1.35	1.47
52	x	20	H2U	C6-N1	-9.21	1.35	1.47
58	y	17	H2U	C6-N1	-9.21	1.35	1.47
58	y	20	H2U	C6-N1	-9.18	1.35	1.47

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1618	6MZ	N3-C2-N1	-9.08	120.95	128.86
1	A	2030	6MZ	N3-C2-N1	-9.02	121.00	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	x	55	PSU	N1-C2-N3	-8.58	122.23	128.40
58	y	55	PSU	N1-C2-N3	-8.50	122.29	128.40
1	A	2580	PSU	N1-C2-N3	-8.41	122.35	128.40

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	x	8	4SU	C4'
52	x	8	4SU	C2'
52	x	8	4SU	C3'
32	a	1498	UR3	C2'
32	a	1498	UR3	C3'

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1915	3TD	3	0
1	A	1962	5MC	1	0
1	A	2030	6MZ	1	0
1	A	2069	7MG	3	0
1	A	2251	OMG	1	0
1	A	2503	2MA	2	0
1	A	2504	PSU	1	0
1	A	2552	OMU	1	0
1	A	2580	PSU	2	0
1	A	745	1MG	2	0
1	A	746	PSU	2	0
1	A	747	5MC	3	0
1	A	955	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
57	z	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	517:UNK	C	518:UNK	N	39.33
1	z	561:UNK	C	663:ALA	N	37.34
1	z	493:UNK	C	494:UNK	N	34.24
1	z	547:UNK	C	548:UNK	N	30.19
1	z	526:UNK	C	527:UNK	N	18.32