



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:37 pm GMT

PDB ID : 8QK7  
EMDB ID : EMD-18458  
Title : E167K RF2 on E. coli 70S release complex with UAA  
Authors : Pundir, S.; Larsson, D.S.D.; Selmer, M.; Sanyal, S.  
Deposited on : 2023-09-14  
Resolution : 2.77 Å (reported)  
Based on initial models : 8B0X, 5MDV, 7K00, 1GQE

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

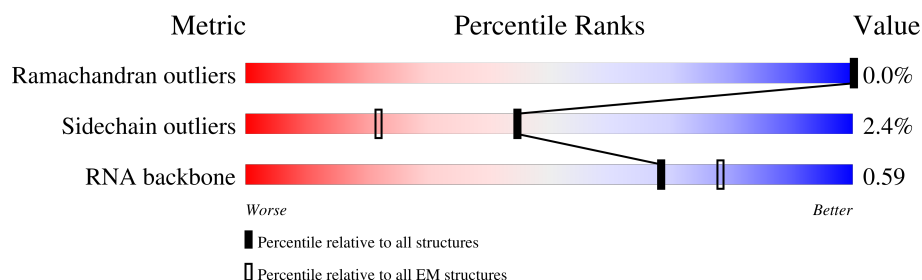
EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.77 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	2	1542	
2	g	241	
3	h	233	
4	i	206	
5	j	167	
6	k	135	
7	l	179	
8	m	130	
9	n	130	


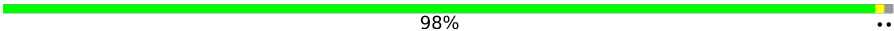
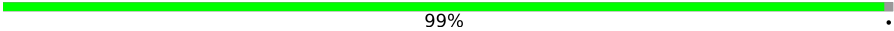
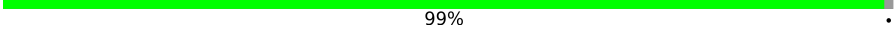
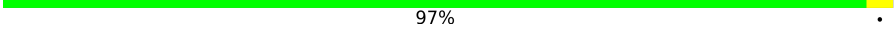
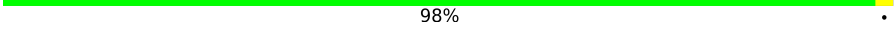

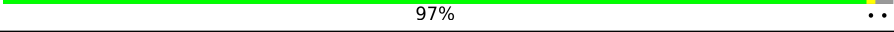
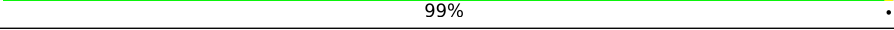

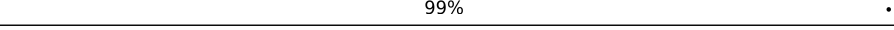
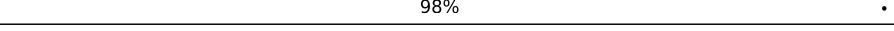
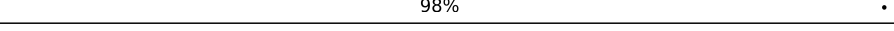
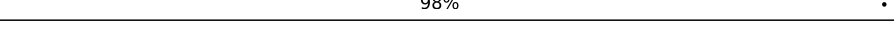

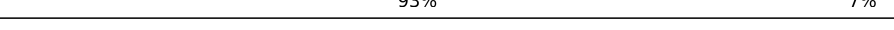
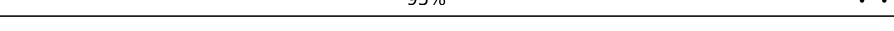
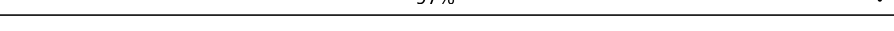

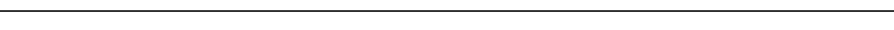

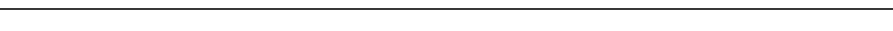
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Mol	Chain	Length	Quality of chain
10	o	103	91% 5%
11	p	129	89% 9%
12	q	124	98% ..
13	r	118	95% ..
14	s	101	99% .
15	t	89	96% ..
16	u	82	98% ..
17	v	84	92% 6%
18	w	75	88% 12%
19	x	92	91% 9%
20	y	87	95% ..
21	z	71	92% 7%
22	4	49	35% 18% 47%
23	5	76	63% 37%
24	1	2904	84% 15%
25	3	120	88% 11% .
26	B	273	99% ..
27	C	209	98% .
28	D	201	99% .
29	E	179	97% ..
30	F	177	97% ..
31	J	142	98% .
32	K	123	98% .
33	L	144	98% .
34	M	136	97% .

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Mol	Chain	Length	Quality of chain
35	N	127	 92% . 7%
36	O	117	 98% ..
37	P	115	 99% .
38	Q	118	 99% .
39	R	103	 97% .
40	S	110	 98% .
41	T	100	 91% . 7%
42	U	104	 97% ..
43	V	94	 99% .
44	W	85	 89% 11%
45	X	78	 99% .
46	Y	63	 98% .
47	Z	59	 98% .
48	b	57	 98% .
49	c	55	 91% . 7%
50	d	46	 93% 7%
51	e	65	 95% ..
52	f	38	 97% .
53	a	70	 83% . 14%
54	I	142	 46% . 52%
55	6	365	 95% ..
56	G	149	 95% 5%

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 148642 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1536	Total	C	N	O	P	0	0
			32966	14711	6044	10675	1536		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	g	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	210	Total	C	N	O	S	0	0
			1648	1043	309	292	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	p	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	r	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	u	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	26	Total	C	N	O	P	0	0
			560	251	104	179	26		

- Molecule 23 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	76	Total	C	N	O	P	2	0
			1665	742	302	543	78		

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	82	MS6	MET	variant	UNP P0ADY7

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	c	51	Total	C	N	O	S	0	0
			417	269	76	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	a	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 54 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	I	68	Total	C	N	O	S	0	0
			484	298	89	94	3		

- Molecule 55 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	361	Total	C	N	O	S	0	0
			2855	1757	501	587	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	167	LYS	GLU	engineered mutation	UNP P07012

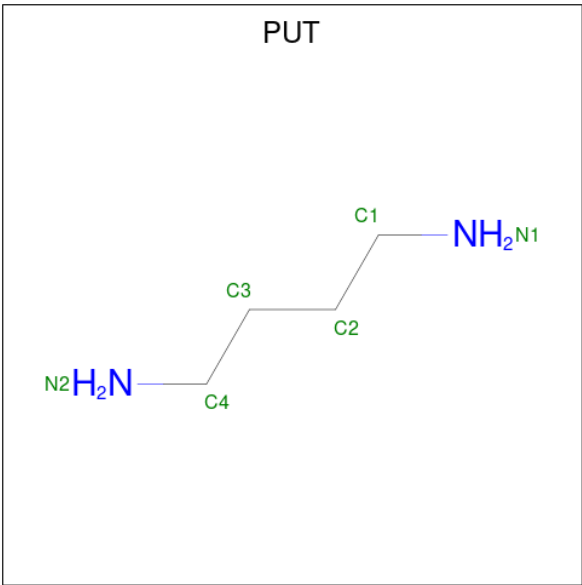
- Molecule 56 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	2	90	Total	Mg	0
			90	90	
57	5	2	Total	Mg	0
			2	2	
57	1	232	Total	Mg	0
			232	232	
57	3	5	Total	Mg	0
			5	5	
57	C	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	b	1	Total	Mg	0
			1	1	

- Molecule 58 is 1,4-DIAMINO BUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	

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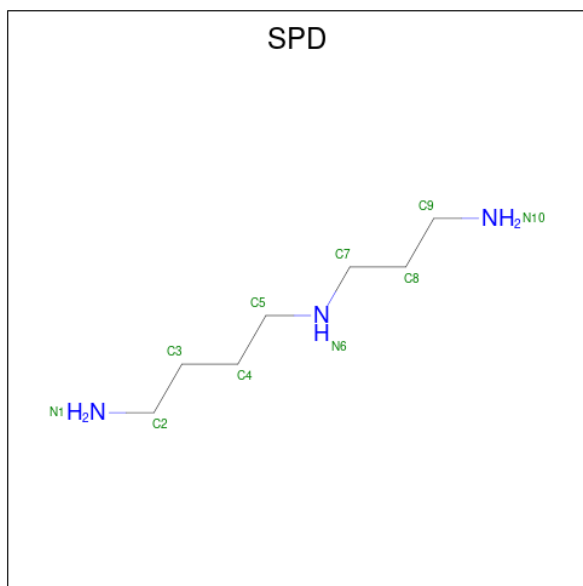
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Mol	Chain	Residues	Atoms			AltConf
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	C	1	Total	C	N	0
			6	4	2	

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

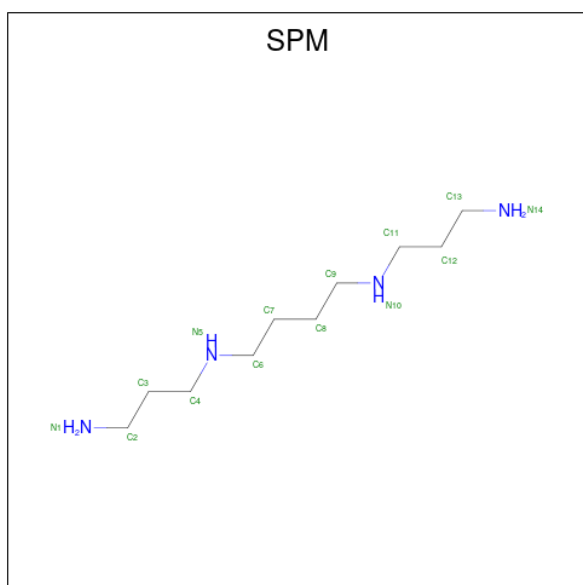
Mol	Chain	Residues	Atoms		AltConf
59	2	34	Total	K	0
			34	34	
59	1	92	Total	K	0
			92	92	

- Molecule 60 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	

- Molecule 61 is SPERMINE (three-letter code: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
61	1	1	Total	C	N	0
			14	10	4	
61	1	1	Total	C	N	0
			14	10	4	

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	f	1	Total 1	Zn 1	0
62	a	1	Total 1	Zn 1	0

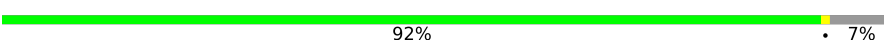


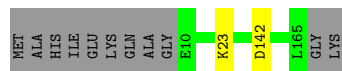
- Molecule 4: Small ribosomal subunit protein uS4

Chain i:  97%



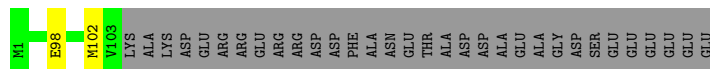
- Molecule 5: Small ribosomal subunit protein uS5

Chain j:  92%




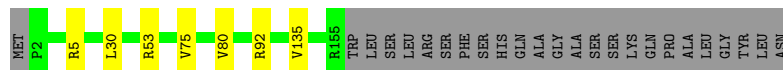
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform

Chain k:  75%



- Molecule 7: Small ribosomal subunit protein uS7

Chain l:  82%



- Molecule 8: Small ribosomal subunit protein uS8

Chain m:  98%




- Molecule 9: Small ribosomal subunit protein uS9

Chain n:  95%




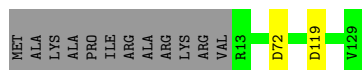
- Molecule 10: Small ribosomal subunit protein uS10

Chain o:  91%



- Molecule 11: Small ribosomal subunit protein uS11

Chain p:  89% 9%



- Molecule 12: Small ribosomal subunit protein uS12

Chain q:  98% ..



- Molecule 13: Small ribosomal subunit protein uS13

Chain r:  95% ..



- Molecule 14: Small ribosomal subunit protein uS14

Chain s:  99% .



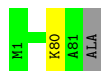
- Molecule 15: Small ribosomal subunit protein uS15

Chain t:  96% ..



- Molecule 16: Small ribosomal subunit protein bS16

Chain u:  98% ..




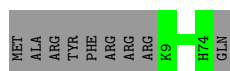
- Molecule 17: Small ribosomal subunit protein uS17

Chain v:  92% 6%




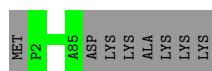
- Molecule 18: Small ribosomal subunit protein bS18

Chain w:  88% 12%



- Molecule 19: Small ribosomal subunit protein uS19

Chain x:  91% 9%



- Molecule 20: Small ribosomal subunit protein bS20

Chain y:  95% ..




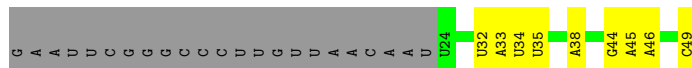
- Molecule 21: Small ribosomal subunit protein bS21

Chain z:  92% 7% .



- Molecule 22: mRNA

Chain 4:  35% 18% 47%




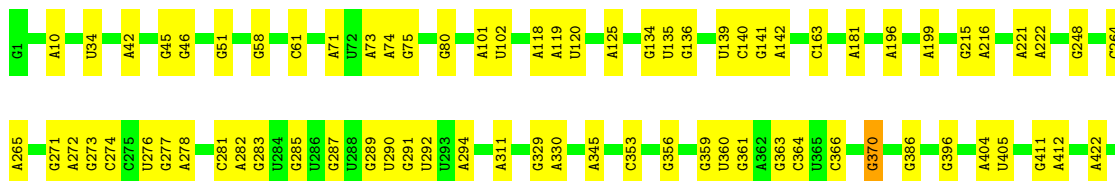
- Molecule 23: tRNA(fMet)

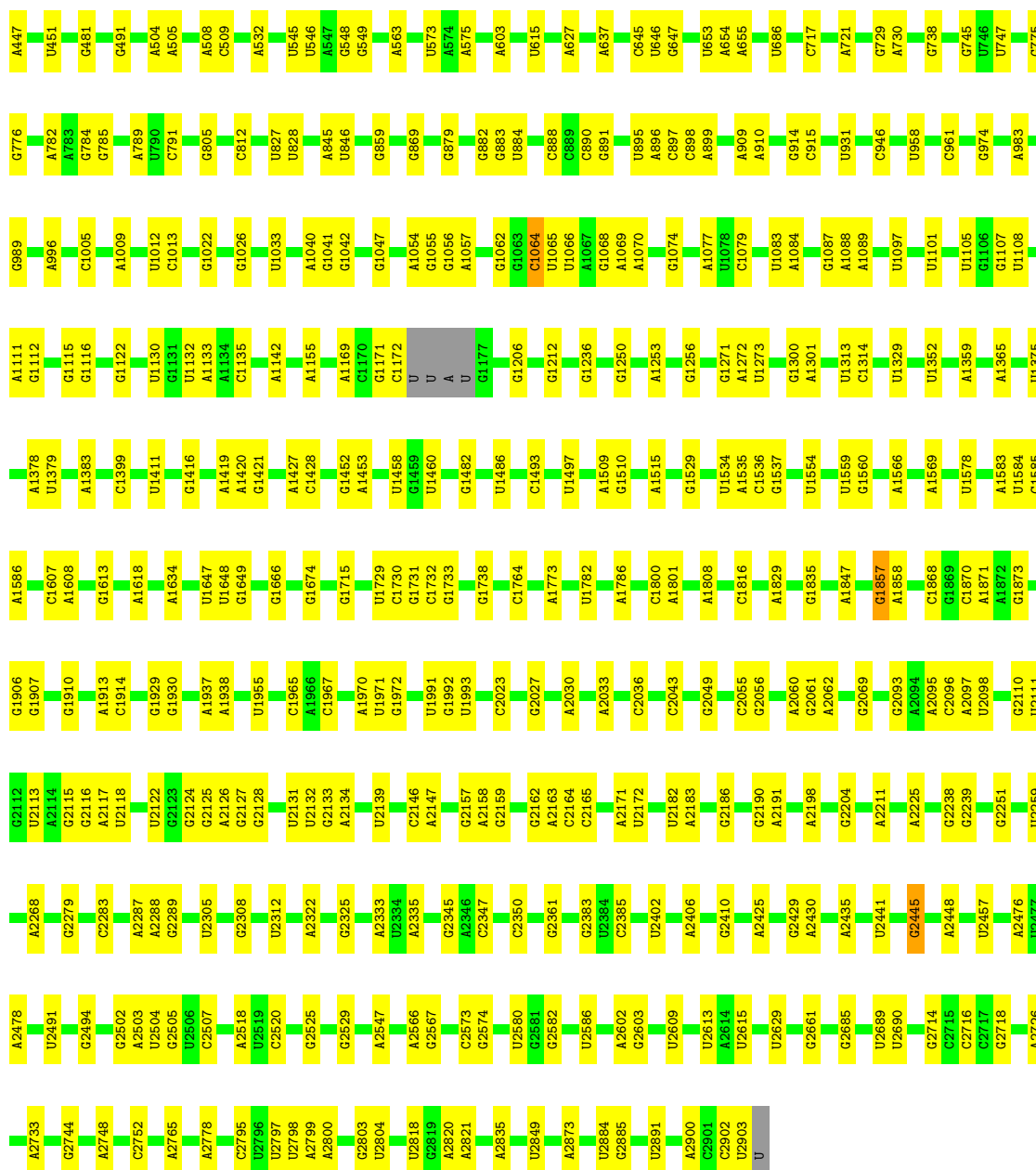
Chain 5:  63% 37%



- Molecule 24: 23S rRNA

Chain 1:  84% 15%





• Molecule 25: 5S rRNA

Chain 3: 88% 11%



• Molecule 26: Large ribosomal subunit protein uL2

Chain B: 99%



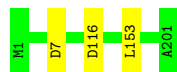
- Molecule 27: Large ribosomal subunit protein uL3

Chain C:  98% .



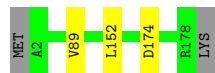
- Molecule 28: Large ribosomal subunit protein uL4

Chain D:  99% .



- Molecule 29: Large ribosomal subunit protein uL5

Chain E:  97% ..



- Molecule 30: Large ribosomal subunit protein uL6

Chain F:  97% ..



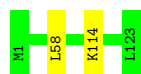
- Molecule 31: Large ribosomal subunit protein uL13

Chain J:  98% .



- Molecule 32: 50S ribosomal protein L14

Chain K:  98% .



- Molecule 33: 50S ribosomal protein L15

Chain L:  98% .



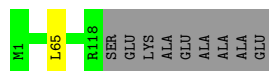
- Molecule 34: Large ribosomal subunit protein uL16

Chain M:  97% .



- Molecule 35: 50S ribosomal protein L17

Chain N:  92% . 7%



- Molecule 36: 50S ribosomal protein L18

Chain O:  98% ..



- Molecule 37: 50S ribosomal protein L19

Chain P:  99% .



- Molecule 38: 50S ribosomal protein L20

Chain Q:  99% .



- Molecule 39: 50S ribosomal protein L21

Chain R:  97% .



- Molecule 40: 50S ribosomal protein L22

Chain S:  98% .



- Molecule 41: 50S ribosomal protein L23

Chain T:  91% • 7%



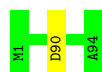
- Molecule 42: 50S ribosomal protein L24

Chain U:  97% ••



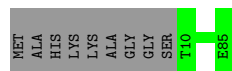
- Molecule 43: 50S ribosomal protein L25

Chain V:  99% •



- Molecule 44: 50S ribosomal protein L27

Chain W:  89% 11%



- Molecule 45: 50S ribosomal protein L28

Chain X:  99% •



- Molecule 46: 50S ribosomal protein L29

Chain Y:  98% •



- Molecule 47: 50S ribosomal protein L30

Chain Z:  98% •



- Molecule 48: 50S ribosomal protein L32

Chain b:  98% .



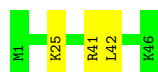
- Molecule 49: 50S ribosomal protein L33

Chain c:  91% . 7%



- Molecule 50: 50S ribosomal protein L34

Chain d:  93% 7%



- Molecule 51: 50S ribosomal protein L35

Chain e:  95% . .




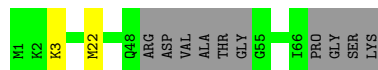
- Molecule 52: 50S ribosomal protein L36

Chain f:  97% .



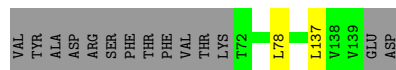
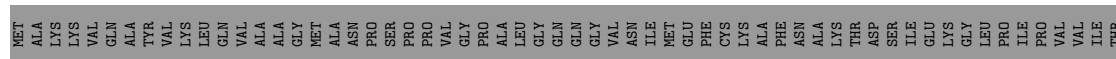
- Molecule 53: Large ribosomal subunit protein bL31A

Chain a:  83% . 14%

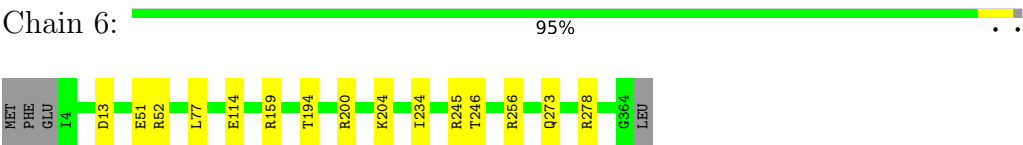


- Molecule 54: Large ribosomal subunit protein uL11

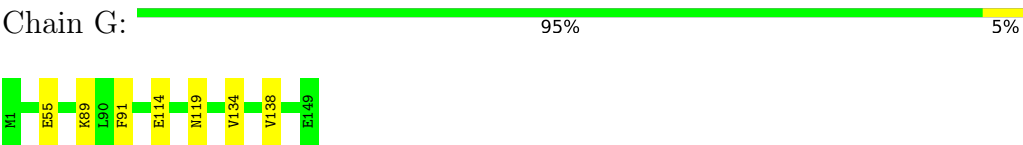
Chain I:  46% . 52%



● Molecule 55: Peptide chain release factor RF2



● Molecule 56: Large ribosomal subunit protein bL9



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (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: SPM, 5MU, 2MA, OMU, H2U, D2T, OMG, 6MZ, 2MG, 1MG, MA6, SPD, IAS, MG, K, 4D4, MS6, 3TD, PSU, G7M, ZN, 4OC, MEQ, UR3, PUT, OMC, 5MC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2	0.37	0/36631	0.81	2/57136 (0.0%)
2	g	0.27	0/1784	0.48	0/2403
3	h	0.26	0/1675	0.51	0/2256
4	i	0.26	0/1665	0.51	0/2227
5	j	0.28	0/1165	0.52	0/1568
6	k	0.27	0/858	0.51	0/1160
7	l	0.26	0/1230	0.53	0/1649
8	m	0.28	0/989	0.50	0/1326
9	n	0.26	0/1034	0.56	0/1375
10	o	0.27	0/796	0.56	0/1077
11	p	0.28	0/884	0.54	0/1191
12	q	0.28	0/960	0.59	0/1286
13	r	0.25	0/900	0.56	0/1204
14	s	0.27	0/817	0.53	0/1088
15	t	0.27	0/722	0.53	0/964
16	u	0.27	0/653	0.56	0/877
17	v	0.25	0/650	0.51	0/871
18	w	0.28	0/553	0.52	0/742
19	x	0.26	0/685	0.50	0/922
20	y	0.27	0/676	0.46	0/895
21	z	0.27	0/597	0.57	0/792
22	4	0.36	0/628	0.89	0/977
23	5	0.36	0/1859	0.81	0/2894
24	1	0.42	0/69147	0.80	10/107869 (0.0%)
25	3	0.34	0/2850	0.77	0/4444
26	B	0.29	0/2121	0.56	0/2852
27	C	0.28	0/1576	0.53	0/2119
28	D	0.28	0/1571	0.51	0/2113
29	E	0.27	0/1434	0.51	0/1926
30	F	0.27	0/1333	0.52	0/1805
31	J	0.28	0/1152	0.49	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	K	0.29	0/955	0.57	0/1279
33	L	0.28	0/1062	0.56	0/1413
34	M	0.28	0/1073	0.54	0/1433
35	N	0.29	0/958	0.58	0/1281
36	O	0.27	0/902	0.53	0/1209
37	P	0.29	0/929	0.54	0/1242
38	Q	0.30	0/960	0.53	0/1278
39	R	0.29	0/829	0.55	0/1107
40	S	0.28	0/864	0.52	0/1156
41	T	0.26	0/744	0.51	0/994
42	U	0.26	0/787	0.49	0/1051
43	V	0.27	0/766	0.49	0/1025
44	W	0.29	0/589	0.56	0/779
45	X	0.28	0/635	0.55	0/848
46	Y	0.26	0/502	0.48	0/667
47	Z	0.27	0/453	0.56	0/605
48	b	0.27	0/450	0.55	0/599
49	c	0.27	0/424	0.51	0/565
50	d	0.28	0/380	0.65	0/498
51	e	0.27	0/513	0.56	0/676
52	f	0.30	0/303	0.56	0/397
53	a	0.29	0/488	0.50	0/649
54	I	0.24	0/486	0.48	0/650
55	6	0.27	0/2884	0.49	0/3885
56	G	0.25	0/1122	0.46	0/1515
All	All	0.37	0/159653	0.74	12/238360 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	2096	C	N1-C2-O2	-9.14	113.42	118.90
24	1	2096	C	C2-N3-C4	-7.89	115.96	119.90
1	2	1133	G	N3-C2-N2	-7.68	114.52	119.90
1	2	1535	C	N1-C2-O2	-6.08	115.25	118.90
24	1	1313	U	C2-N1-C1'	5.88	124.76	117.70
24	1	1666	G	N3-C2-N2	-5.82	115.83	119.90
24	1	1064	C	C6-N1-C2	-5.81	117.97	120.30
24	1	1857	G	O4'-C1'-N9	5.55	112.64	108.20
24	1	1064	C	C5-C6-N1	5.52	123.76	121.00
24	1	729	G	O4'-C1'-N9	5.20	112.36	108.20
24	1	1314	C	C2-N1-C1'	5.20	124.52	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	370	G	O4'-C1'-N9	-5.16	104.07	108.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	g	222/241 (92%)	213 (96%)	9 (4%)	0	100	100
3	h	208/233 (89%)	202 (97%)	6 (3%)	0	100	100
4	i	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	j	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	k	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
7	l	152/179 (85%)	148 (97%)	4 (3%)	0	100	100
8	m	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	n	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	o	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	13	36
11	p	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
12	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	r	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	s	98/101 (97%)	98 (100%)	0	0	100	100
15	t	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	u	79/82 (96%)	75 (95%)	3 (4%)	1 (1%)	10	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	v	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	w	64/75 (85%)	64 (100%)	0	0	100	100
19	x	82/92 (89%)	82 (100%)	0	0	100	100
20	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
26	B	269/273 (98%)	266 (99%)	3 (1%)	0	100	100
27	C	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
28	D	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
29	E	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
30	F	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
31	J	140/142 (99%)	140 (100%)	0	0	100	100
32	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	L	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
34	M	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
35	N	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
36	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
37	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	Q	115/118 (98%)	115 (100%)	0	0	100	100
39	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
40	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	T	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
42	U	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
43	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	Y	60/63 (95%)	60 (100%)	0	0	100	100
47	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
48	b	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
49	c	49/55 (89%)	49 (100%)	0	0	100	100
50	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
53	a	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
54	I	66/142 (46%)	64 (97%)	2 (3%)	0	100	100
55	6	358/365 (98%)	352 (98%)	6 (2%)	0	100	100
56	G	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
All	All	6015/6420 (94%)	5880 (98%)	133 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	o	57	VAL
16	u	80	LYS

### 5.3.2 Protein sidechains [i](#)

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	g	186/199 (94%)	183 (98%)	3 (2%)	58	83
3	h	172/190 (90%)	168 (98%)	4 (2%)	45	75
4	i	172/173 (99%)	167 (97%)	5 (3%)	37	68
5	j	119/126 (94%)	117 (98%)	2 (2%)	56	81
6	k	90/116 (78%)	88 (98%)	2 (2%)	47	76
7	l	127/147 (86%)	120 (94%)	7 (6%)	18	44
8	m	104/105 (99%)	103 (99%)	1 (1%)	73	89
9	n	105/107 (98%)	101 (96%)	4 (4%)	28	59
10	o	86/90 (96%)	83 (96%)	3 (4%)	31	62
11	p	89/98 (91%)	88 (99%)	1 (1%)	70	88
12	q	102/103 (99%)	101 (99%)	1 (1%)	73	89
13	r	93/96 (97%)	90 (97%)	3 (3%)	34	65
14	s	83/84 (99%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	t	76/77 (99%)	73 (96%)	3 (4%)	27	58
16	u	65/65 (100%)	65 (100%)	0	100	100
17	v	73/78 (94%)	71 (97%)	2 (3%)	40	71
18	w	57/65 (88%)	57 (100%)	0	100	100
19	x	72/79 (91%)	72 (100%)	0	100	100
20	y	65/66 (98%)	62 (95%)	3 (5%)	23	52
21	z	60/61 (98%)	55 (92%)	5 (8%)	9	26
26	B	216/218 (99%)	214 (99%)	2 (1%)	75	91
27	C	163/163 (100%)	158 (97%)	5 (3%)	35	66
28	D	165/165 (100%)	162 (98%)	3 (2%)	54	80
29	E	148/150 (99%)	145 (98%)	3 (2%)	50	78
30	F	136/138 (99%)	132 (97%)	4 (3%)	37	68
31	J	116/116 (100%)	113 (97%)	3 (3%)	41	72
32	K	104/104 (100%)	102 (98%)	2 (2%)	52	79
33	L	103/103 (100%)	100 (97%)	3 (3%)	37	68
34	M	107/107 (100%)	104 (97%)	3 (3%)	38	69
35	N	98/103 (95%)	97 (99%)	1 (1%)	73	89
36	O	86/87 (99%)	85 (99%)	1 (1%)	67	87
37	P	99/100 (99%)	99 (100%)	0	100	100
38	Q	89/90 (99%)	89 (100%)	0	100	100
39	R	84/84 (100%)	81 (96%)	3 (4%)	30	61
40	S	93/93 (100%)	91 (98%)	2 (2%)	47	76
41	T	80/84 (95%)	78 (98%)	2 (2%)	42	73
42	U	83/85 (98%)	82 (99%)	1 (1%)	67	87
43	V	78/78 (100%)	77 (99%)	1 (1%)	65	86
44	W	58/63 (92%)	58 (100%)	0	100	100
45	X	67/68 (98%)	67 (100%)	0	100	100
46	Y	54/55 (98%)	54 (100%)	0	100	100
47	Z	48/49 (98%)	48 (100%)	0	100	100
48	b	47/48 (98%)	47 (100%)	0	100	100
49	c	46/49 (94%)	45 (98%)	1 (2%)	47	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	d	38/38 (100%)	35 (92%)	3 (8%)	10	28
51	e	51/52 (98%)	49 (96%)	2 (4%)	27	58
52	f	34/34 (100%)	33 (97%)	1 (3%)	37	68
53	a	55/62 (89%)	53 (96%)	2 (4%)	30	61
54	I	50/110 (46%)	48 (96%)	2 (4%)	27	57
55	6	305/310 (98%)	290 (95%)	15 (5%)	21	49
56	G	114/114 (100%)	107 (94%)	7 (6%)	15	40
All	All	5011/5245 (96%)	4890 (98%)	121 (2%)	45	74

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	g	23	TRP
2	g	73	LYS
2	g	117	LEU
3	h	54	ARG
3	h	107	ARG
3	h	179	ARG
3	h	185	ASN
4	i	8	LYS
4	i	14	ARG
4	i	29	ASP
4	i	44	ARG
4	i	47	ARG
5	j	23	LYS
5	j	142	ASP
6	k	98	GLU
6	k	102	MET
7	l	5	ARG
7	l	30	LEU
7	l	53	ARG
7	l	75	VAL
7	l	80	VAL
7	l	92	ARG
7	l	135	VAL
8	m	112	THR
9	n	4	ASN
9	n	22	LYS
9	n	100	LYS
9	n	123	ARG

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Mol	Chain	Res	Type
10	o	7	ARG
10	o	45	ARG
10	o	85	ASP
11	p	72	ASP
12	q	15	LYS
13	r	42	ASP
13	r	82	ASP
13	r	90	ARG
15	t	3	LEU
15	t	17	ARG
15	t	64	ARG
17	v	42	THR
17	v	57	ASP
20	y	3	ASN
20	y	27	MET
20	y	53	GLU
21	z	3	VAL
21	z	33	ARG
21	z	47	ARG
21	z	58	LYS
21	z	63	GLU
26	B	36	LYS
26	B	121	ASP
27	C	32	ASN
27	C	33	ARG
27	C	130	GLN
27	C	131	ASP
27	C	149	ASN
28	D	7	ASP
28	D	116	ASP
28	D	153	LEU
29	E	89	VAL
29	E	152	LEU
29	E	174	ASP
30	F	43	VAL
30	F	76	VAL
30	F	114	ASP
30	F	176	LYS
31	J	37	ARG
31	J	95	ARG
31	J	96	ARG
32	K	58	LEU

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Mol	Chain	Res	Type
32	K	114	LYS
33	L	85	VAL
33	L	93	ASN
33	L	112	LEU
34	M	7	THR
34	M	8	LYS
34	M	14	LYS
35	N	65	LEU
36	O	13	ARG
39	R	29	THR
39	R	55	ASP
39	R	79	ARG
40	S	68	ASP
40	S	109	ASP
41	T	68	LYS
41	T	69	ARG
42	U	37	GLU
43	V	90	ASP
49	c	28	ARG
50	d	25	LYS
50	d	41	ARG
50	d	42	LEU
51	e	31	HIS
51	e	33	LEU
52	f	11	CYS
53	a	3	LYS
53	a	22	MET
54	I	78	LEU
54	I	137	LEU
55	6	13	ASP
55	6	51	GLU
55	6	52	ARG
55	6	77	LEU
55	6	114	GLU
55	6	159	ARG
55	6	194	THR
55	6	200	ARG
55	6	204	LYS
55	6	234	ILE
55	6	245	ARG
55	6	246	THR
55	6	256	ARG

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Mol	Chain	Res	Type
55	6	273	GLN
55	6	278	ARG
56	G	55	GLU
56	G	89	LYS
56	G	91	PHE
56	G	114	GLU
56	G	119	ASN
56	G	134	VAL
56	G	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	g	18	HIS
2	g	42	ASN
2	g	109	GLN
2	g	168	HIS
3	h	123	GLN
4	i	131	ASN
5	j	122	ASN
5	j	146	ASN
5	j	148	ASN
7	l	68	ASN
8	m	67	GLN
12	q	75	GLN
14	s	66	GLN
16	u	9	HIS
17	v	51	ASN
19	x	14	HIS
20	y	13	GLN
20	y	82	GLN
21	z	64	ASN
26	B	153	GLN
27	C	173	GLN
28	D	92	HIS
29	E	63	GLN
30	F	22	GLN
30	F	45	HIS
30	F	88	GLN
30	F	116	GLN
31	J	138	GLN
32	K	29	HIS

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Mol	Chain	Res	Type
39	R	66	HIS
41	T	59	ASN
43	V	49	ASN
44	W	12	ASN
44	W	46	HIS
46	Y	39	GLN
47	Z	20	HIS
53	a	30	HIS
53	a	61	ASN
55	6	290	GLN
56	G	66	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1531/1542 (99%)	227 (14%)	6 (0%)
22	4	25/49 (51%)	8 (32%)	1 (4%)
23	5	73/76 (96%)	28 (38%)	0
24	1	2893/2904 (99%)	438 (15%)	8 (0%)
25	3	118/120 (98%)	13 (11%)	0
All	All	4640/4691 (98%)	714 (15%)	15 (0%)

All (714) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	7	A
1	2	9	G
1	2	22	G
1	2	32	A
1	2	39	G
1	2	47	C
1	2	48	C
1	2	50	A
1	2	51	A
1	2	71	A
1	2	74	A
1	2	77	A
1	2	80	A
1	2	89	U
1	2	91	U

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Mol	Chain	Res	Type
1	2	94	G
1	2	95	C
1	2	116	A
1	2	121	U
1	2	122	G
1	2	131	A
1	2	141	G
1	2	144	G
1	2	163	C
1	2	165	G
1	2	173	U
1	2	182	A
1	2	183	C
1	2	197	A
1	2	201	G
1	2	202	G
1	2	203	G
1	2	204	G
1	2	208	U
1	2	211	G
1	2	212	G
1	2	216	U
1	2	226	G
1	2	240	G
1	2	245	U
1	2	247	G
1	2	251	G
1	2	257	G
1	2	266	G
1	2	267	C
1	2	280	C
1	2	289	G
1	2	306	A
1	2	316	C
1	2	321	A
1	2	328	C
1	2	329	A
1	2	330	C
1	2	351	G
1	2	352	C
1	2	354	G
1	2	367	U

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Mol	Chain	Res	Type
1	2	372	C
1	2	373	A
1	2	384	G
1	2	406	G
1	2	412	A
1	2	413	G
1	2	414	A
1	2	415	A
1	2	417	G
1	2	421	U
1	2	422	C
1	2	423	G
1	2	424	G
1	2	429	U
1	2	436	C
1	2	446	G
1	2	453	G
1	2	456	A
1	2	457	G
1	2	458	U
1	2	459	A
1	2	463	U
1	2	464	U
1	2	467	U
1	2	468	A
1	2	469	C
1	2	478	A
1	2	479	U
1	2	480	U
1	2	481	G
1	2	486	U
1	2	495	A
1	2	509	A
1	2	511	C
1	2	518	C
1	2	521	G
1	2	524	G
1	2	527	G7M
1	2	531	U
1	2	547	A
1	2	559	A
1	2	562	U

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Mol	Chain	Res	Type
1	2	564	C
1	2	572	A
1	2	573	A
1	2	576	C
1	2	577	G
1	2	579	A
1	2	596	A
1	2	607	A
1	2	631	C
1	2	633	G
1	2	648	A
1	2	650	G
1	2	653	U
1	2	665	A
1	2	723	U
1	2	724	G
1	2	746	A
1	2	747	A
1	2	748	G
1	2	755	G
1	2	774	G
1	2	777	A
1	2	793	U
1	2	794	A
1	2	802	A
1	2	815	A
1	2	817	C
1	2	819	A
1	2	840	C
1	2	841	C
1	2	842	U
1	2	843	U
1	2	844	G
1	2	845	A
1	2	846	G
1	2	847	G
1	2	890	G
1	2	902	G
1	2	914	A
1	2	926	G
1	2	934	C
1	2	935	A

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Mol	Chain	Res	Type
1	2	953	G
1	2	960	U
1	2	963	G
1	2	966	2MG
1	2	969	A
1	2	975	A
1	2	976	G
1	2	977	A
1	2	983	A
1	2	984	C
1	2	992	U
1	2	994	A
1	2	1002	G
1	2	1003	G
1	2	1004	A
1	2	1006	G
1	2	1009	U
1	2	1010	U
1	2	1011	C
1	2	1024	G
1	2	1027	C
1	2	1029	U
1	2	1030	U
1	2	1031	C
1	2	1032	G
1	2	1033	G
1	2	1034	G
1	2	1035	A
1	2	1036	A
1	2	1039	G
1	2	1042	A
1	2	1044	A
1	2	1046	A
1	2	1065	U
1	2	1085	U
1	2	1086	U
1	2	1094	G
1	2	1095	U
1	2	1101	A
1	2	1137	C
1	2	1139	G
1	2	1157	A

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Mol	Chain	Res	Type
1	2	1159	U
1	2	1196	A
1	2	1197	A
1	2	1213	A
1	2	1227	A
1	2	1238	A
1	2	1258	G
1	2	1260	G
1	2	1275	A
1	2	1280	A
1	2	1286	U
1	2	1287	A
1	2	1298	U
1	2	1300	G
1	2	1302	C
1	2	1317	C
1	2	1320	C
1	2	1346	A
1	2	1353	G
1	2	1363	A
1	2	1364	U
1	2	1370	G
1	2	1378	C
1	2	1379	G
1	2	1381	U
1	2	1419	G
1	2	1441	A
1	2	1446	A
1	2	1451	U
1	2	1452	C
1	2	1453	G
1	2	1487	G
1	2	1491	G
1	2	1492	A
1	2	1497	G
1	2	1499	A
1	2	1503	A
1	2	1505	G
1	2	1506	U
1	2	1507	A
1	2	1517	G
1	2	1529	G

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Mol	Chain	Res	Type
1	2	1530	G
22	4	33	A
22	4	34	U
22	4	35	U
22	4	38	A
22	4	44	G
22	4	45	A
22	4	46	A
22	4	49	C
23	5	5	G
23	5	6	G
23	5	7	G
23	5	9	G
23	5	13	C
23	5	14	A
23	5	16	C
23	5	17	C
23	5	17(A)	U
23	5	18	G
23	5	19	G
23	5	20	U
23	5	21	A
23	5	25	C
23	5	31	G
23	5	42	G
23	5	43	A
23	5	47	U
23	5	48	C
23	5	51	C
23	5	52	G
23	5	53	G
23	5	54	U
23	5	58	A
23	5	65	C
23	5	69	C
23	5	70	G
23	5	71	C
24	1	10	A
24	1	34	U
24	1	42	A
24	1	45	G
24	1	46	G

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Mol	Chain	Res	Type
24	1	51	G
24	1	58	G
24	1	61	C
24	1	71	A
24	1	73	A
24	1	74	A
24	1	75	G
24	1	80	G
24	1	101	A
24	1	102	U
24	1	118	A
24	1	119	A
24	1	120	U
24	1	125	A
24	1	134	G
24	1	135	U
24	1	136	G
24	1	139	U
24	1	140	C
24	1	141	G
24	1	142	A
24	1	163	C
24	1	181	A
24	1	196	A
24	1	199	A
24	1	215	G
24	1	216	A
24	1	221	A
24	1	222	A
24	1	248	G
24	1	264	C
24	1	265	A
24	1	271	G
24	1	272	A
24	1	273	G
24	1	274	C
24	1	276	U
24	1	277	G
24	1	278	A
24	1	281	C
24	1	282	A
24	1	283	G

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Mol	Chain	Res	Type
24	1	285	G
24	1	287	G
24	1	289	G
24	1	290	U
24	1	291	G
24	1	292	U
24	1	294	A
24	1	311	A
24	1	329	G
24	1	330	A
24	1	345	A
24	1	353	C
24	1	356	G
24	1	359	G
24	1	360	U
24	1	361	G
24	1	363	G
24	1	364	C
24	1	366	C
24	1	370	G
24	1	386	G
24	1	396	G
24	1	405	U
24	1	411	G
24	1	412	A
24	1	422	A
24	1	447	A
24	1	451	U
24	1	481	G
24	1	491	G
24	1	504	A
24	1	505	A
24	1	508	A
24	1	509	C
24	1	532	A
24	1	545	U
24	1	546	U
24	1	548	G
24	1	549	G
24	1	563	A
24	1	573	U
24	1	575	A

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Mol	Chain	Res	Type
24	1	603	A
24	1	615	U
24	1	627	A
24	1	637	A
24	1	645	C
24	1	646	U
24	1	647	G
24	1	653	U
24	1	654	A
24	1	655	A
24	1	686	U
24	1	717	C
24	1	721	A
24	1	730	A
24	1	738	G
24	1	747	5MU
24	1	775	G
24	1	776	G
24	1	782	A
24	1	784	G
24	1	785	G
24	1	789	A
24	1	791	C
24	1	805	G
24	1	812	C
24	1	827	U
24	1	828	U
24	1	845	A
24	1	846	U
24	1	859	G
24	1	869	G
24	1	879	G
24	1	882	G
24	1	883	G
24	1	884	U
24	1	888	C
24	1	890	C
24	1	891	G
24	1	895	U
24	1	896	A
24	1	897	C
24	1	898	C

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Mol	Chain	Res	Type
24	1	899	A
24	1	909	A
24	1	910	A
24	1	914	G
24	1	915	C
24	1	931	U
24	1	946	C
24	1	958	U
24	1	961	C
24	1	974	G
24	1	983	A
24	1	989	G
24	1	996	A
24	1	1005	C
24	1	1009	A
24	1	1012	U
24	1	1013	C
24	1	1022	G
24	1	1026	G
24	1	1033	U
24	1	1040	A
24	1	1041	G
24	1	1042	G
24	1	1047	G
24	1	1054	A
24	1	1055	G
24	1	1056	G
24	1	1057	A
24	1	1062	G
24	1	1064	C
24	1	1065	U
24	1	1066	U
24	1	1068	G
24	1	1069	A
24	1	1070	A
24	1	1074	G
24	1	1077	A
24	1	1079	C
24	1	1083	U
24	1	1084	A
24	1	1087	G
24	1	1088	A

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Mol	Chain	Res	Type
24	1	1089	A
24	1	1097	U
24	1	1101	U
24	1	1105	U
24	1	1107	G
24	1	1108	U
24	1	1111	A
24	1	1112	G
24	1	1115	G
24	1	1116	G
24	1	1122	G
24	1	1130	U
24	1	1132	U
24	1	1133	A
24	1	1135	C
24	1	1142	A
24	1	1155	A
24	1	1169	A
24	1	1171	G
24	1	1172	C
24	1	1206	G
24	1	1212	G
24	1	1236	G
24	1	1250	G
24	1	1253	A
24	1	1256	G
24	1	1271	G
24	1	1272	A
24	1	1273	U
24	1	1300	G
24	1	1301	A
24	1	1329	U
24	1	1352	U
24	1	1359	A
24	1	1365	A
24	1	1375	U
24	1	1378	A
24	1	1379	U
24	1	1383	A
24	1	1399	C
24	1	1411	U
24	1	1416	G

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Mol	Chain	Res	Type
24	1	1419	A
24	1	1420	A
24	1	1421	G
24	1	1427	A
24	1	1428	C
24	1	1452	G
24	1	1453	A
24	1	1458	U
24	1	1460	U
24	1	1482	G
24	1	1486	U
24	1	1493	C
24	1	1497	U
24	1	1509	A
24	1	1510	G
24	1	1515	A
24	1	1529	G
24	1	1534	U
24	1	1535	A
24	1	1536	C
24	1	1537	G
24	1	1554	U
24	1	1559	U
24	1	1560	G
24	1	1566	A
24	1	1569	A
24	1	1578	U
24	1	1583	A
24	1	1584	U
24	1	1585	C
24	1	1586	A
24	1	1607	C
24	1	1608	A
24	1	1613	G
24	1	1634	A
24	1	1647	U
24	1	1648	U
24	1	1649	G
24	1	1674	G
24	1	1715	G
24	1	1729	U
24	1	1730	C

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Mol	Chain	Res	Type
24	1	1731	G
24	1	1732	C
24	1	1733	G
24	1	1738	G
24	1	1764	C
24	1	1773	A
24	1	1782	U
24	1	1786	A
24	1	1800	C
24	1	1801	A
24	1	1808	A
24	1	1816	C
24	1	1829	A
24	1	1847	A
24	1	1857	G
24	1	1858	A
24	1	1868	C
24	1	1870	C
24	1	1871	A
24	1	1873	G
24	1	1906	G
24	1	1907	G
24	1	1910	G
24	1	1913	A
24	1	1914	C
24	1	1929	G
24	1	1930	G
24	1	1937	A
24	1	1938	A
24	1	1955	U
24	1	1965	C
24	1	1967	C
24	1	1970	A
24	1	1971	U
24	1	1972	G
24	1	1991	U
24	1	1992	G
24	1	1993	U
24	1	2023	C
24	1	2027	G
24	1	2033	A
24	1	2036	C

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Mol	Chain	Res	Type
24	1	2043	C
24	1	2049	G
24	1	2055	C
24	1	2056	G
24	1	2060	A
24	1	2061	G
24	1	2062	A
24	1	2069	G7M
24	1	2093	G
24	1	2095	A
24	1	2097	A
24	1	2098	U
24	1	2110	G
24	1	2111	U
24	1	2113	U
24	1	2115	G
24	1	2116	G
24	1	2117	A
24	1	2118	U
24	1	2122	U
24	1	2124	G
24	1	2125	G
24	1	2126	A
24	1	2127	G
24	1	2128	G
24	1	2131	U
24	1	2132	U
24	1	2133	G
24	1	2134	A
24	1	2139	U
24	1	2147	A
24	1	2157	G
24	1	2158	A
24	1	2159	G
24	1	2162	G
24	1	2163	A
24	1	2164	C
24	1	2165	C
24	1	2171	A
24	1	2172	U
24	1	2182	U
24	1	2183	A

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Mol	Chain	Res	Type
24	1	2186	G
24	1	2190	G
24	1	2191	A
24	1	2198	A
24	1	2204	G
24	1	2211	A
24	1	2225	A
24	1	2238	G
24	1	2239	G
24	1	2259	U
24	1	2268	A
24	1	2279	G
24	1	2283	C
24	1	2287	A
24	1	2288	A
24	1	2289	G
24	1	2305	U
24	1	2308	G
24	1	2312	U
24	1	2322	A
24	1	2325	G
24	1	2333	A
24	1	2335	A
24	1	2345	G
24	1	2347	C
24	1	2350	C
24	1	2361	G
24	1	2383	G
24	1	2385	C
24	1	2402	U
24	1	2406	A
24	1	2410	G
24	1	2425	A
24	1	2429	G
24	1	2430	A
24	1	2435	A
24	1	2441	U
24	1	2445	2MG
24	1	2448	A
24	1	2476	A
24	1	2478	A
24	1	2491	U

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Mol	Chain	Res	Type
24	1	2494	G
24	1	2502	G
24	1	2504	PSU
24	1	2505	G
24	1	2507	C
24	1	2518	A
24	1	2520	C
24	1	2525	G
24	1	2529	G
24	1	2547	A
24	1	2566	A
24	1	2567	G
24	1	2573	C
24	1	2574	G
24	1	2582	G
24	1	2586	U
24	1	2602	A
24	1	2603	G
24	1	2609	U
24	1	2613	U
24	1	2615	U
24	1	2629	U
24	1	2661	G
24	1	2685	G
24	1	2689	U
24	1	2690	U
24	1	2714	G
24	1	2716	C
24	1	2718	G
24	1	2726	A
24	1	2733	A
24	1	2744	G
24	1	2748	A
24	1	2752	C
24	1	2765	A
24	1	2778	A
24	1	2795	C
24	1	2797	U
24	1	2798	U
24	1	2799	A
24	1	2800	A
24	1	2803	G

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Mol	Chain	Res	Type
24	1	2804	U
24	1	2818	U
24	1	2820	A
24	1	2821	A
24	1	2835	A
24	1	2849	U
24	1	2873	A
24	1	2884	U
24	1	2885	G
24	1	2891	U
24	1	2900	A
24	1	2902	C
24	1	2903	U
25	3	9	G
25	3	13	G
25	3	24	G
25	3	35	C
25	3	36	C
25	3	56	G
25	3	57	A
25	3	58	A
25	3	67	G
25	3	89	U
25	3	90	C
25	3	99	A
25	3	109	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	70	U
1	2	182	A
1	2	209	U
1	2	467	U
1	2	1026	G
1	2	1035	A
22	4	32	U
24	1	277	G
24	1	404	A
24	1	451	U
24	1	504	A
24	1	784	G

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Mol	Chain	Res	Type
24	1	2146	C
24	1	2162	G
24	1	2884	U

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

40 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	PSU	2	516	1,57	18,21,22	0.53	0	22,30,33	0.61	1 (4%)
1	5MC	2	1407	1	18,22,23	0.33	0	26,32,35	0.46	0
24	5MU	1	1939	59,24	19,22,23	0.32	0	28,32,35	0.42	0
1	UR3	2	1498	1	19,22,23	0.31	0	26,32,35	0.34	0
24	2MG	1	1835	24	18,26,27	0.99	3 (16%)	16,38,41	0.66	0
24	6MZ	1	1618	24	18,25,26	0.75	0	16,36,39	0.79	1 (6%)
1	5MC	2	967	1	18,22,23	0.31	0	26,32,35	0.43	0
24	PSU	1	2580	24	18,21,22	0.60	1 (5%)	22,30,33	0.67	1 (4%)
12	D2T	q	89	12	7,9,10	0.88	0	6,11,13	1.77	2 (33%)
24	1MG	1	745	24	18,26,27	0.95	2 (11%)	19,39,42	0.46	0
24	5MC	1	1962	59,24	18,22,23	0.30	0	26,32,35	0.43	0
24	OMU	1	2552	57,24	19,22,23	0.30	0	26,31,34	0.43	0
1	2MG	2	1207	1,59	18,26,27	0.96	1 (5%)	16,38,41	0.65	0
1	2MG	2	1516	1	18,26,27	0.98	2 (11%)	16,38,41	0.72	0
24	PSU	1	2504	59,24	18,21,22	0.54	0	22,30,33	0.62	0
24	PSU	1	746	57,24	18,21,22	0.62	0	22,30,33	0.36	0
24	2MA	1	2503	59,57,24	19,25,26	1.02	2 (10%)	21,37,40	3.03	5 (23%)
24	PSU	1	1911	24	18,21,22	0.51	0	22,30,33	0.57	0
55	MEQ	6	252	55	8,9,10	0.91	0	5,10,12	0.50	0
24	OMC	1	2498	57,24	19,22,23	0.34	0	26,31,34	0.45	0
1	4OC	2	1402	1,57	20,23,24	0.31	0	26,32,35	0.50	0
34	4D4	M	81	34	9,11,12	0.72	0	8,13,15	1.98	3 (37%)
24	PSU	1	2604	24	18,21,22	0.50	0	22,30,33	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PSU	1	2605	24	18,21,22	0.51	0	22,30,33	0.65	0
24	PSU	1	2457	24	18,21,22	0.56	0	22,30,33	0.59	1 (4%)
24	PSU	1	955	24	18,21,22	0.55	0	22,30,33	0.57	0
11	IAS	p	119	11	6,7,8	0.96	0	6,8,10	1.24	1 (16%)
27	MEQ	C	150	27	8,9,10	0.84	0	5,10,12	0.17	0
24	3TD	1	1915	57,24	19,22,23	0.53	0	21,32,35	0.64	0
24	2MG	1	2445	24	18,26,27	1.01	3 (16%)	16,38,41	0.62	0
1	MA6	2	1519	1	18,26,27	0.76	0	19,38,41	0.75	0
24	H2U	1	2449	24	18,21,22	0.31	0	21,30,33	0.45	0
24	6MZ	1	2030	24	18,25,26	0.77	0	16,36,39	0.78	1 (6%)
1	G7M	2	527	1,59	20,26,27	0.60	0	17,39,42	0.48	0
24	G7M	1	2069	59,24	20,26,27	0.58	0	17,39,42	0.45	0
24	5MU	1	747	24	19,22,23	0.32	0	28,32,35	0.32	0
24	OMG	1	2251	23,59,24	18,26,27	0.97	3 (16%)	19,38,41	0.58	0
1	2MG	2	966	1	18,26,27	0.98	2 (11%)	16,38,41	0.70	0
1	MA6	2	1518	1	18,26,27	0.76	0	19,38,41	0.74	0
24	PSU	1	1917	24	18,21,22	0.53	0	22,30,33	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2	516	1,57	-	0/7/25/26	0/2/2/2
1	5MC	2	1407	1	-	0/7/25/26	0/2/2/2
24	5MU	1	1939	59,24	-	0/7/25/26	0/2/2/2
1	UR3	2	1498	1	-	0/7/25/26	0/2/2/2
24	2MG	1	1835	24	-	0/5/27/28	0/3/3/3
24	6MZ	1	1618	24	-	0/5/27/28	0/3/3/3
1	5MC	2	967	1	-	0/7/25/26	0/2/2/2
24	PSU	1	2580	24	-	0/7/25/26	0/2/2/2
12	D2T	q	89	12	-	4/7/12/14	-
24	1MG	1	745	24	-	0/3/25/26	0/3/3/3
24	5MC	1	1962	59,24	-	0/7/25/26	0/2/2/2
24	OMU	1	2552	57,24	-	0/9/27/28	0/2/2/2
1	2MG	2	1207	1,59	-	0/5/27/28	0/3/3/3
1	2MG	2	1516	1	-	0/5/27/28	0/3/3/3
24	PSU	1	2504	59,24	-	0/7/25/26	0/2/2/2
24	PSU	1	746	57,24	-	1/7/25/26	0/2/2/2
24	2MA	1	2503	59,57,24	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	1	1911	24	-	0/7/25/26	0/2/2/2
55	MEQ	6	252	55	-	3/8/9/11	-
24	OMC	1	2498	57,24	-	0/9/27/28	0/2/2/2
1	4OC	2	1402	1,57	-	1/9/29/30	0/2/2/2
34	4D4	M	81	34	-	1/11/12/14	-
24	PSU	1	2604	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2605	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2457	24	-	0/7/25/26	0/2/2/2
24	PSU	1	955	24	-	0/7/25/26	0/2/2/2
11	IAS	p	119	11	-	1/7/7/8	-
27	MEQ	C	150	27	-	3/8/9/11	-
24	3TD	1	1915	57,24	-	0/7/25/26	0/2/2/2
24	2MG	1	2445	24	-	2/5/27/28	0/3/3/3
1	MA6	2	1519	1	-	1/7/29/30	0/3/3/3
24	H2U	1	2449	24	-	0/7/38/39	0/2/2/2
24	6MZ	1	2030	24	-	2/5/27/28	0/3/3/3
1	G7M	2	527	1,59	-	3/3/25/26	0/3/3/3
24	G7M	1	2069	59,24	-	2/3/25/26	0/3/3/3
24	5MU	1	747	24	-	0/7/25/26	0/2/2/2
24	OMG	1	2251	23,59,24	-	1/5/27/28	0/3/3/3
1	2MG	2	966	1	-	2/5/27/28	0/3/3/3
1	MA6	2	1518	1	-	0/7/29/30	0/3/3/3
24	PSU	1	1917	24	-	0/7/25/26	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	1835	2MG	C5-C6	-2.56	1.42	1.47
1	2	966	2MG	C5-C6	-2.56	1.42	1.47
24	1	745	1MG	C5-C4	-2.55	1.36	1.43
24	1	2445	2MG	C5-C6	-2.54	1.42	1.47
1	2	1207	2MG	C5-C6	-2.41	1.42	1.47
1	2	1516	2MG	C5-C6	-2.35	1.42	1.47
24	1	2251	OMG	C5-C6	-2.32	1.42	1.47
24	1	2503	2MA	C6-N6	-2.26	1.25	1.34
24	1	745	1MG	C8-N7	-2.17	1.31	1.35
24	1	1835	2MG	C8-N7	-2.09	1.31	1.35
24	1	2503	2MA	C6-N1	2.08	1.37	1.33
1	2	966	2MG	C8-N7	-2.08	1.31	1.35
24	1	2580	PSU	O4'-C1'	-2.08	1.41	1.43
24	1	2445	2MG	C8-N7	-2.07	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	2251	OMG	C5-C4	-2.07	1.37	1.43
24	1	2251	OMG	C8-N7	-2.07	1.31	1.35
1	2	1516	2MG	C5-C4	-2.06	1.37	1.43
24	1	2445	2MG	C5-C4	-2.05	1.37	1.43
24	1	1835	2MG	C5-C4	-2.02	1.37	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	2503	2MA	C5-C6-N1	-12.16	113.03	121.01
24	1	2503	2MA	C2-N3-C4	-3.88	112.37	115.52
34	M	81	4D4	NE-CZ-NH2	3.82	127.42	120.70
24	1	2503	2MA	C2-N1-C6	3.79	124.00	118.08
34	M	81	4D4	O-C-CA	-3.03	116.83	124.78
12	q	89	D2T	O-C-CA	-2.84	117.34	124.78
34	M	81	4D4	NH1-CZ-NE	-2.66	113.06	119.19
12	q	89	D2T	OD1-CG-CB	-2.51	117.19	122.44
11	p	119	IAS	OD1-CG-CB	-2.44	118.33	125.43
24	1	2503	2MA	N6-C6-N1	2.36	123.49	117.07
24	1	2580	PSU	O4'-C1'-C2'	2.35	108.46	105.14
24	1	1618	6MZ	C2-N1-C6	2.13	118.42	116.59
24	1	2030	6MZ	C2-N1-C6	2.11	118.40	116.59
1	2	516	PSU	O4'-C1'-C2'	2.11	108.12	105.14
24	1	2503	2MA	C5-C6-N6	2.06	123.49	120.35
24	1	2457	PSU	O4'-C1'-C2'	2.01	107.98	105.14

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	966	2MG	C3'-C4'-C5'-O5'
12	q	89	D2T	CA-CB-CG-OD1
12	q	89	D2T	CA-CB-CG-OD2
27	C	150	MEQ	N-CA-CB-CG
27	C	150	MEQ	C-CA-CB-CG
27	C	150	MEQ	O-C-CA-CB
24	1	2030	6MZ	O4'-C4'-C5'-O5'
24	1	2251	OMG	C1'-C2'-O2'-CM2
24	1	2445	2MG	C3'-C4'-C5'-O5'
1	2	527	G7M	C3'-C4'-C5'-O5'
1	2	966	2MG	O4'-C4'-C5'-O5'
24	1	2030	6MZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	527	G7M	O4'-C4'-C5'-O5'
24	1	2445	2MG	O4'-C4'-C5'-O5'
12	q	89	D2T	CG-CB-SB-CB1
1	2	527	G7M	C4'-C5'-O5'-P
55	6	252	MEQ	CA-CB-CG-CD
11	p	119	IAS	CA-CB-CG-OD1
12	q	89	D2T	SB-CB-CG-OD2
1	2	1519	MA6	O4'-C4'-C5'-O5'
1	2	1402	4OC	O4'-C4'-C5'-O5'
24	1	2069	G7M	O4'-C4'-C5'-O5'
24	1	746	PSU	O4'-C1'-C5-C6
24	1	2503	2MA	C4'-C5'-O5'-P
24	1	2503	2MA	O4'-C4'-C5'-O5'
55	6	252	MEQ	OE1-CD-CG-CB
55	6	252	MEQ	NE2-CD-CG-CB
34	M	81	4D4	O-C-CA-CB
24	1	2069	G7M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 493 ligands modelled in this entry, 460 are monoatomic - leaving 33 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	SPD	1	3209	-	9,9,9	0.09	0	8,8,8	0.16	0
58	PUT	1	3351	-	5,5,5	0.09	0	4,4,4	0.18	0
60	SPD	1	3335	-	9,9,9	0.11	0	8,8,8	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	SPM	1	3349	-	13,13,13	0.35	0	12,12,12	0.87	0
58	PUT	1	3327	-	5,5,5	0.11	0	4,4,4	0.16	0
58	PUT	1	3344	-	5,5,5	0.12	0	4,4,4	0.15	0
58	PUT	2	1726	-	5,5,5	0.12	0	4,4,4	0.15	0
60	SPD	1	3208	-	9,9,9	0.12	0	8,8,8	0.11	0
60	SPD	1	3211	-	9,9,9	0.09	0	8,8,8	0.16	0
60	SPD	1	3215	-	9,9,9	0.11	0	8,8,8	0.09	0
58	PUT	1	3332	-	5,5,5	0.12	0	4,4,4	0.17	0
60	SPD	1	3207	-	9,9,9	0.09	0	8,8,8	0.20	0
60	SPD	1	3213	-	9,9,9	0.08	0	8,8,8	0.13	0
58	PUT	2	1686	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	1	3331	-	5,5,5	0.12	0	4,4,4	0.19	0
58	PUT	1	3334	-	5,5,5	0.11	0	4,4,4	0.16	0
58	PUT	1	3337	-	5,5,5	0.08	0	4,4,4	0.18	0
61	SPM	1	3216	-	13,13,13	0.35	0	12,12,12	0.86	0
58	PUT	2	1725	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	1	3212	-	5,5,5	0.10	0	4,4,4	0.15	0
60	SPD	1	3214	-	9,9,9	0.08	0	8,8,8	0.15	0
58	PUT	C	301	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	1	3326	-	5,5,5	0.08	0	4,4,4	0.20	0
58	PUT	1	3329	-	5,5,5	0.10	0	4,4,4	0.16	0
58	PUT	1	3330	-	5,5,5	0.11	0	4,4,4	0.17	0
58	PUT	1	3333	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	1	3339	-	5,5,5	0.09	0	4,4,4	0.15	0
58	PUT	1	3328	-	5,5,5	0.09	0	4,4,4	0.19	0
60	SPD	1	3206	-	9,9,9	0.10	0	8,8,8	0.12	0
60	SPD	1	3210	-	9,9,9	0.09	0	8,8,8	0.12	0
58	PUT	2	1728	-	5,5,5	0.11	0	4,4,4	0.19	0
58	PUT	2	1685	-	5,5,5	0.13	0	4,4,4	0.15	0
58	PUT	1	3338	-	5,5,5	0.11	0	4,4,4	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SPD	1	3209	-	-	2/7/7/7	-
58	PUT	1	3351	-	-	3/3/3/3	-
60	SPD	1	3335	-	-	3/7/7/7	-
61	SPM	1	3349	-	-	6/11/11/11	-
58	PUT	1	3327	-	-	3/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PUT	1	3344	-	-	0/3/3/3	-
58	PUT	2	1726	-	-	3/3/3/3	-
60	SPD	1	3208	-	-	4/7/7/7	-
60	SPD	1	3211	-	-	2/7/7/7	-
60	SPD	1	3215	-	-	5/7/7/7	-
58	PUT	1	3332	-	-	1/3/3/3	-
60	SPD	1	3207	-	-	3/7/7/7	-
60	SPD	1	3213	-	-	3/7/7/7	-
58	PUT	2	1686	-	-	1/3/3/3	-
58	PUT	1	3331	-	-	1/3/3/3	-
58	PUT	1	3334	-	-	2/3/3/3	-
58	PUT	1	3337	-	-	0/3/3/3	-
61	SPM	1	3216	-	-	7/11/11/11	-
58	PUT	2	1725	-	-	0/3/3/3	-
58	PUT	1	3212	-	-	1/3/3/3	-
60	SPD	1	3214	-	-	0/7/7/7	-
58	PUT	C	301	-	-	1/3/3/3	-
58	PUT	1	3326	-	-	1/3/3/3	-
58	PUT	1	3329	-	-	1/3/3/3	-
58	PUT	1	3330	-	-	0/3/3/3	-
58	PUT	1	3333	-	-	0/3/3/3	-
58	PUT	1	3339	-	-	1/3/3/3	-
58	PUT	1	3328	-	-	2/3/3/3	-
60	SPD	1	3206	-	-	1/7/7/7	-
60	SPD	1	3210	-	-	5/7/7/7	-
58	PUT	2	1728	-	-	1/3/3/3	-
58	PUT	2	1685	-	-	2/3/3/3	-
58	PUT	1	3338	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	C	301	PUT	C1-C2-C3-C4
61	1	3349	SPM	N5-C6-C7-C8
60	1	3211	SPD	N6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
60	1	3215	SPD	C3-C4-C5-N6
61	1	3216	SPM	C7-C8-C9-N10
60	1	3210	SPD	N6-C7-C8-C9
60	1	3213	SPD	C3-C4-C5-N6
61	1	3216	SPM	C3-C4-N5-C6
58	1	3212	PUT	C1-C2-C3-C4
60	1	3210	SPD	C3-C4-C5-N6
61	1	3349	SPM	C2-C3-C4-N5
58	1	3339	PUT	C1-C2-C3-C4
58	2	1728	PUT	C1-C2-C3-C4
58	1	3338	PUT	C1-C2-C3-C4
61	1	3349	SPM	C7-C8-C9-N10
58	1	3332	PUT	C1-C2-C3-C4
61	1	3349	SPM	N10-C11-C12-C13
60	1	3335	SPD	C3-C4-C5-N6
60	1	3206	SPD	C8-C7-N6-C5
60	1	3210	SPD	C4-C5-N6-C7
60	1	3215	SPD	C4-C5-N6-C7
60	1	3207	SPD	C2-C3-C4-C5
58	1	3328	PUT	N1-C1-C2-C3
58	1	3351	PUT	C2-C3-C4-N2
58	1	3351	PUT	N1-C1-C2-C3
60	1	3210	SPD	C2-C3-C4-C5
60	1	3208	SPD	N6-C7-C8-C9
60	1	3207	SPD	C3-C4-C5-N6
58	1	3329	PUT	C1-C2-C3-C4
60	1	3213	SPD	C2-C3-C4-C5
58	1	3328	PUT	C2-C3-C4-N2
58	2	1685	PUT	N1-C1-C2-C3
58	2	1686	PUT	N1-C1-C2-C3
60	1	3215	SPD	N1-C2-C3-C4
60	1	3215	SPD	C7-C8-C9-N10
58	1	3327	PUT	C1-C2-C3-C4
61	1	3216	SPM	C6-C7-C8-C9
58	2	1685	PUT	C1-C2-C3-C4
58	1	3351	PUT	C1-C2-C3-C4
60	1	3335	SPD	N6-C7-C8-C9
61	1	3216	SPM	C12-C11-N10-C9
61	1	3349	SPM	C7-C6-N5-C4
60	1	3209	SPD	C3-C4-C5-N6
58	1	3334	PUT	N1-C1-C2-C3
60	1	3207	SPD	N6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
58	2	1726	PUT	C1-C2-C3-C4
60	1	3208	SPD	C8-C7-N6-C5
60	1	3208	SPD	C3-C4-C5-N6
60	1	3215	SPD	C8-C7-N6-C5
61	1	3216	SPM	C8-C9-N10-C11
60	1	3209	SPD	C8-C7-N6-C5
60	1	3335	SPD	C8-C7-N6-C5
58	2	1726	PUT	N1-C1-C2-C3
58	1	3327	PUT	C2-C3-C4-N2
58	1	3327	PUT	N1-C1-C2-C3
60	1	3210	SPD	C8-C7-N6-C5
61	1	3216	SPM	C7-C6-N5-C4
60	1	3211	SPD	C7-C8-C9-N10
61	1	3216	SPM	C11-C12-C13-N14
61	1	3349	SPM	C11-C12-C13-N14
60	1	3208	SPD	C4-C5-N6-C7
58	2	1726	PUT	C2-C3-C4-N2
58	1	3326	PUT	C1-C2-C3-C4
60	1	3213	SPD	C8-C7-N6-C5
58	1	3331	PUT	C1-C2-C3-C4
58	1	3334	PUT	C1-C2-C3-C4

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](#)

There are no chain breaks in this entry.