



Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:34 pm GMT

PDB ID : 8P7Y
EMDB ID : EMD-17135
Title : Mycoplasma pneumoniae 70S ribosome with second S4 protein on large subunit
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-05-31
Resolution : 3.70 Å (reported)
Based on initial models : 7OOD, 7OOC

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

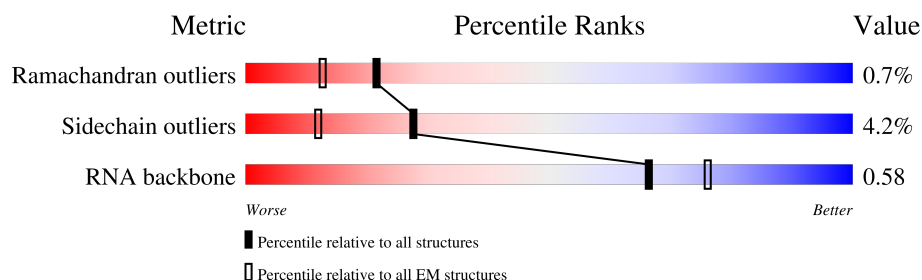
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.





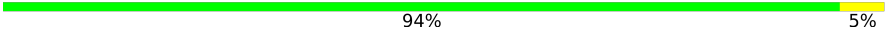



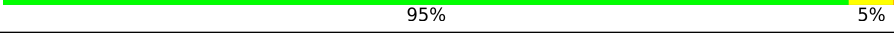

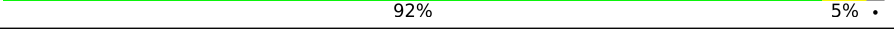

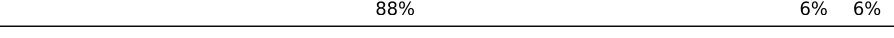
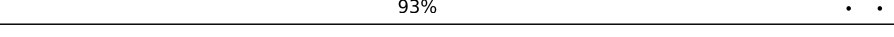

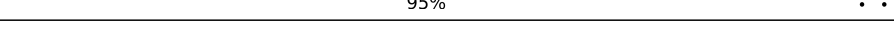
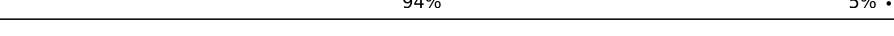

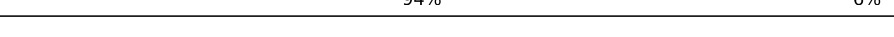

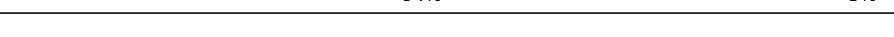






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	48	
2	1	59	
3	2	37	
4	3	2907	
5	4	108	
6	5	1520	
7	6	76	
8	7	75	
9	8	76	


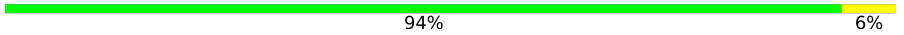
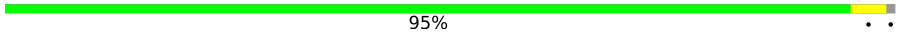

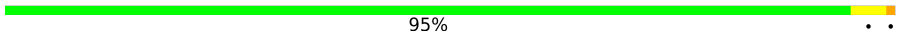


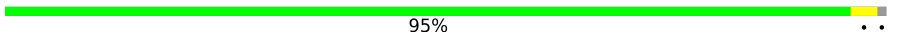
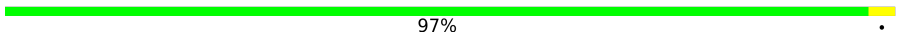
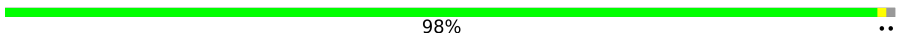



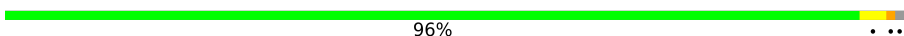




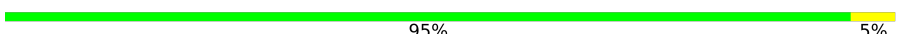


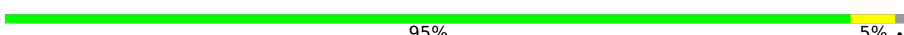



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Mol	Chain	Length	Quality of chain
10	A	294	
11	B	273	
12	C	205	
12	U	205	
13	D	219	
14	E	215	
15	F	155	
16	G	142	
17	H	132	
18	I	108	
19	J	121	
20	K	139	
21	L	124	
22	M	61	
23	N	86	
24	O	94	
25	P	85	
26	Q	104	
27	R	87	
28	S	87	
29	T	60	
30	X	444	
31	Y	21	
32	Z	36	
33	a	287	

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Mol	Chain	Length	Quality of chain
34	b	287	 76%5%20%
35	c	212	 94%6%
36	d	180	 95%..
37	e	184	 91%..
38	f	149	 95%..
39	g	161	 75%.22%
40	h	137	 93%.7%
41	i	146	 95%..
42	j	122	 97%.
43	k	151	 98%..
44	l	139	 94%..
45	m	124	 90%6%.
46	n	116	 94%6%
47	o	119	 96%..
48	p	127	 91%.7%
49	q	100	 91%8%.
50	r	159	 86%.11%
51	s	237	 39%.60%
52	t	111	 95%5%
53	u	104	 82%.15%
54	v	65	 92%6%.
55	w	111	 95%5%.
56	x	97	 91%8%.
57	y	57	 88%11%.
58	z	53	 92%.6%

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 153255 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 protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	48	Total	C	N	O	S	0	0
			392	242	85	63	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	2893	Total	C	N	O	P	0	0
			61995	27704	11293	20105	2893		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	108	Total	C	N	O	P	0	0
			2305	1030	415	752	108		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	1507	Total	C	N	O	P	0	0
			32258	14420	5847	10484	1507		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	76	Total	C	N	O	P	0	0
			1620	723	287	534	76		

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	75	Total	C	N	O	P	0	0
			1599	712	279	533	75		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	76	Total	C	N	O	P	0	0
			1615	722	284	533	76		

- Molecule 10 is a protein called 30S ribosomal protein S2.

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

- Molecule 11 is a protein called 30S ribosomal protein S3.

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

- Molecule 12 is a protein called 30S ribosomal protein S4.

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

- Molecule 13 is a protein called 30S ribosomal protein S5.

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

- Molecule 14 is a protein called 30S ribosomal protein S6.

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

- Molecule 15 is a protein called 30S ribosomal protein S7.

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

- Molecule 16 is a protein called 30S ribosomal protein S8.

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

- Molecule 17 is a protein called 30S ribosomal protein S9.

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

- Molecule 18 is a protein called 30S ribosomal protein S10.

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

- Molecule 19 is a protein called 30S ribosomal protein S11.

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

- Molecule 20 is a protein called 30S ribosomal protein S12.

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

- Molecule 21 is a protein called 30S ribosomal protein S13.

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

- Molecule 22 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 23 is a protein called 30S ribosomal protein S15.

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

- Molecule 24 is a protein called 30S ribosomal protein S16.

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

- Molecule 25 is a protein called 30S ribosomal protein S17.

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

- Molecule 26 is a protein called 30S ribosomal protein S18.

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

- Molecule 27 is a protein called 30S ribosomal protein S19.

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

- Molecule 28 is a protein called 30S ribosomal protein S20.

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

- Molecule 29 is a protein called 30S ribosomal protein S21.

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

- Molecule 30 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	30	Total	C	N	O	S	0	0
			242	155	43	43	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	21	Total	C	N	O	P	0	0
			446	200	80	145	21		

- Molecule 32 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Z	36	Total	C	N	O	0	0
			187	112	37	38		

- Molecule 33 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	230	Total	C	N	O	S	0	0
			1769	1124	319	319	7		

- Molecule 35 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	149	Total	C	N	O	S	0	0
			1210	780	212	215	3		

- Molecule 39 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 40 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 41 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 42 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 43 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 44 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 45 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 46 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 47 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 48 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 49 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

- Molecule 51 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 52 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 53 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	88	Total	C	N	O	S	0	0
			670	416	132	121	1		

- Molecule 54 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 55 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	110	Total	C	N	O		0	0
			906	576	168	162			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	96	Total	C	N	O	S	0	0
			761	481	133	143	4		

- Molecule 57 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

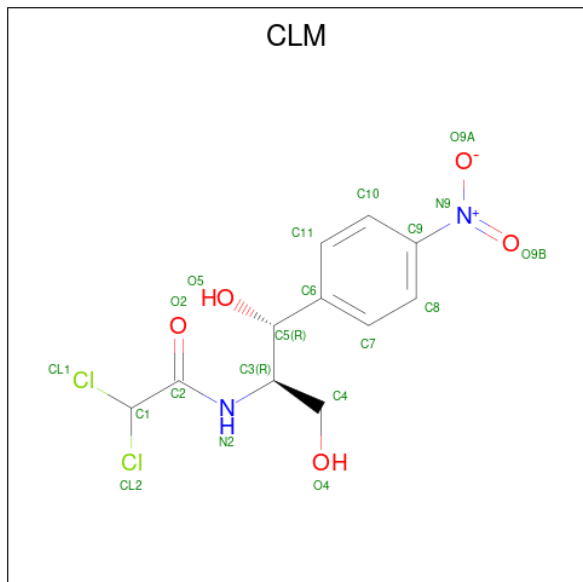
- Molecule 58 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	2	1	Total	Zn	0
			1	1	
59	M	1	Total	Zn	0
			1	1	
59	Q	1	Total	Zn	0
			1	1	
59	x	1	Total	Zn	0
			1	1	
59	y	1	Total	Zn	0
			1	1	
59	z	1	Total	Zn	0
			1	1	

- Molecule 60 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total	K	0
			1	1	

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

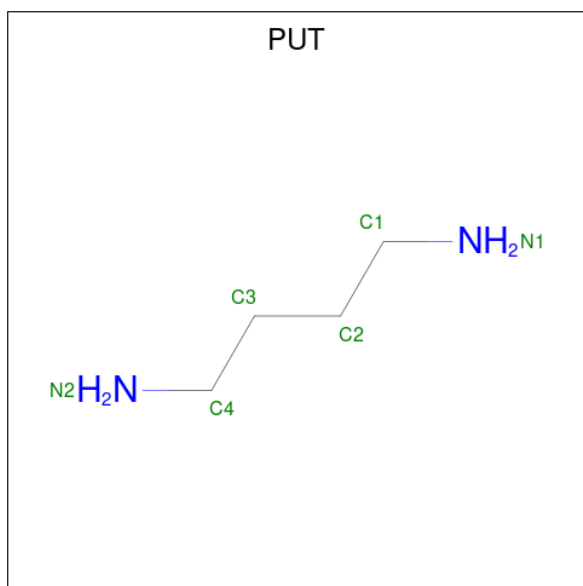
Mol	Chain	Residues	Atoms		AltConf
62	3	221	Total	Mg	0
			221	221	
62	4	1	Total	Mg	0
			1	1	
62	5	90	Total	Mg	0
			90	90	
62	6	1	Total	Mg	0
			1	1	
62	7	2	Total	Mg	0
			2	2	
62	8	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
62	K	1	Total 1	Mg 1	0
62	P	1	Total 1	Mg 1	0
62	Y	2	Total 2	Mg 2	0
62	b	2	Total 2	Mg 2	0
62	i	1	Total 1	Mg 1	0
62	y	2	Total 2	Mg 2	0

- Molecule 63 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



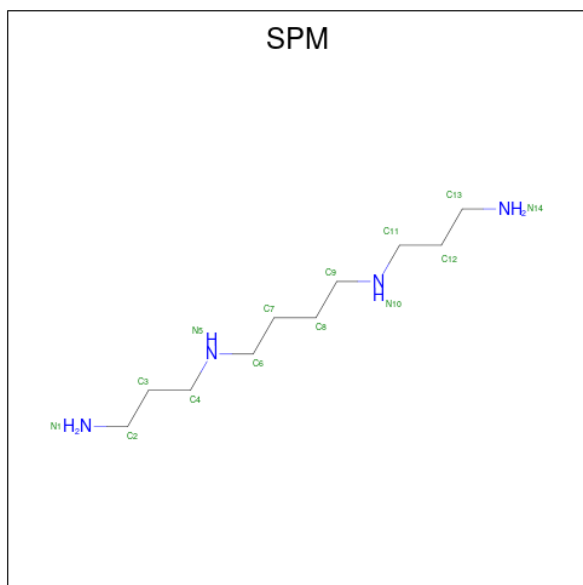
Mol	Chain	Residues	Atoms			AltConf
63	3	1	Total 6	C 4	N 2	0
63	3	1	Total 6	C 4	N 2	0
63	3	1	Total 6	C 4	N 2	0
63	3	1	Total 6	C 4	N 2	0
63	3	1	Total 6	C 4	N 2	0

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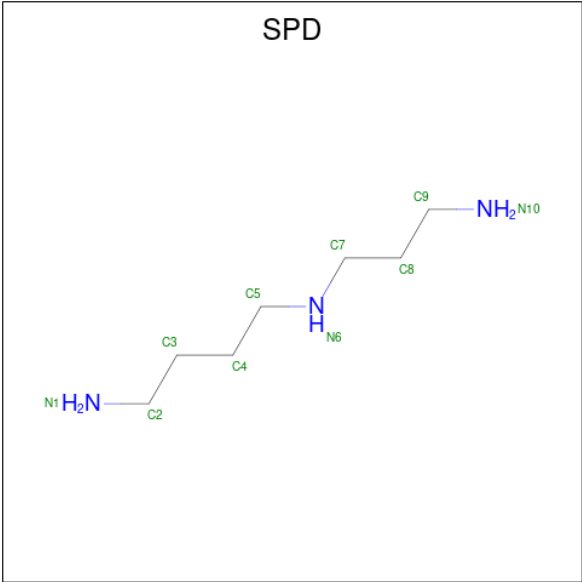
Mol	Chain	Residues	Atoms			AltConf
63	3	1	Total	C	N	0
			6	4	2	
63	3	1	Total	C	N	0
			6	4	2	
63	5	1	Total	C	N	0
			6	4	2	

- Molecule 64 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
64	3	1	Total	C	N	0
			14	10	4	
64	3	1	Total	C	N	0
			14	10	4	
64	3	1	Total	C	N	0
			14	10	4	
64	b	1	Total	C	N	0
			14	10	4	

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



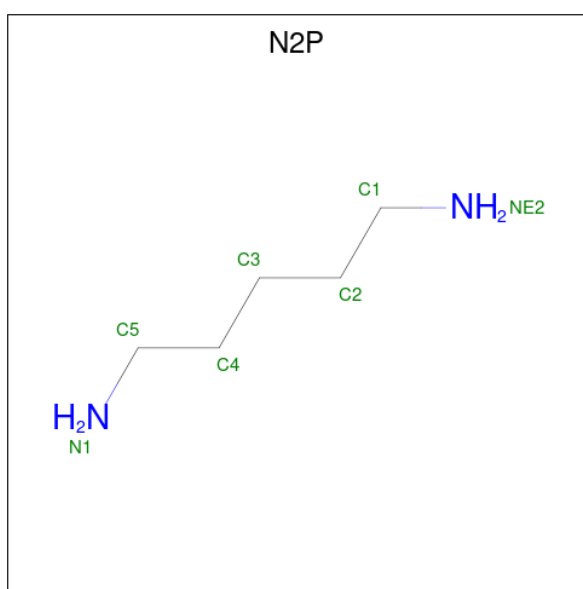
Mol	Chain	Residues	Atoms			AltConf
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	

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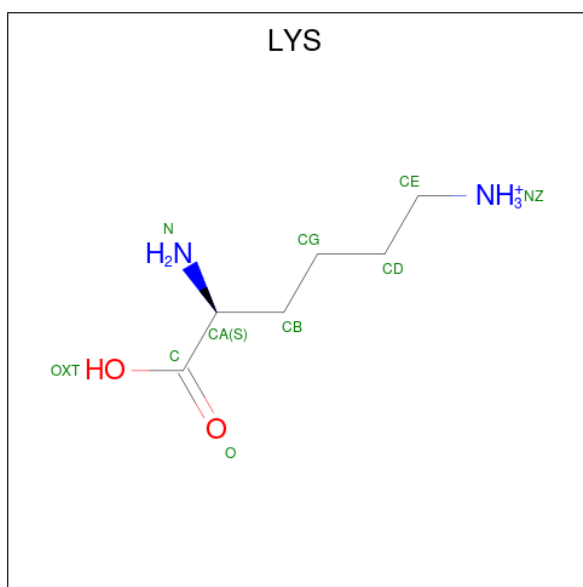
Mol	Chain	Residues	Atoms			AltConf
65	3	1	Total	C	N	0
			10	7	3	
65	3	1	Total	C	N	0
			10	7	3	
65	5	1	Total	C	N	0
			10	7	3	
65	5	1	Total	C	N	0
			10	7	3	

- Molecule 66 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			AltConf
66	3	1	Total	C	N	0
			7	5	2	
66	3	1	Total	C	N	0
			7	5	2	
66	3	1	Total	C	N	0
			7	5	2	
66	5	1	Total	C	N	0
			7	5	2	

- Molecule 67 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



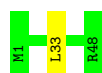
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	8	1	9	6	2	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L34

Chain 0:  98% .



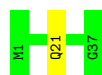
- Molecule 2: 50S ribosomal protein L35

Chain 1:  95% 5%




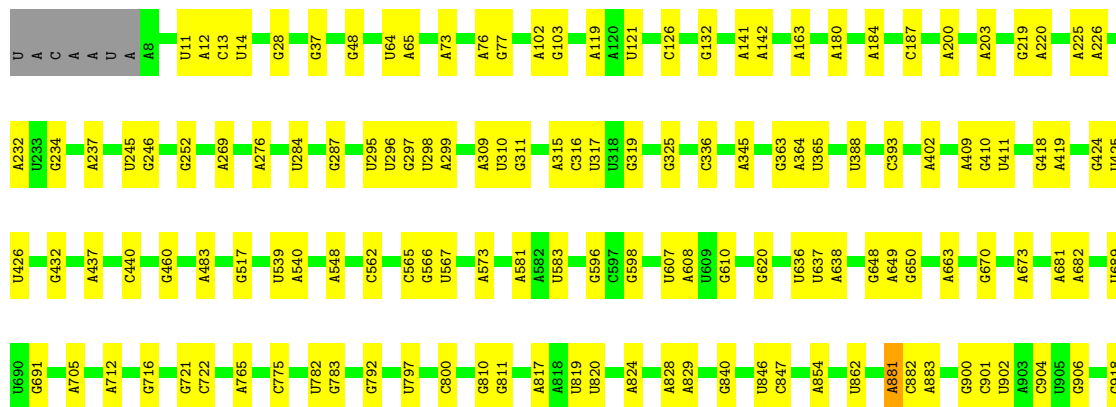
- Molecule 3: 50S ribosomal protein L36

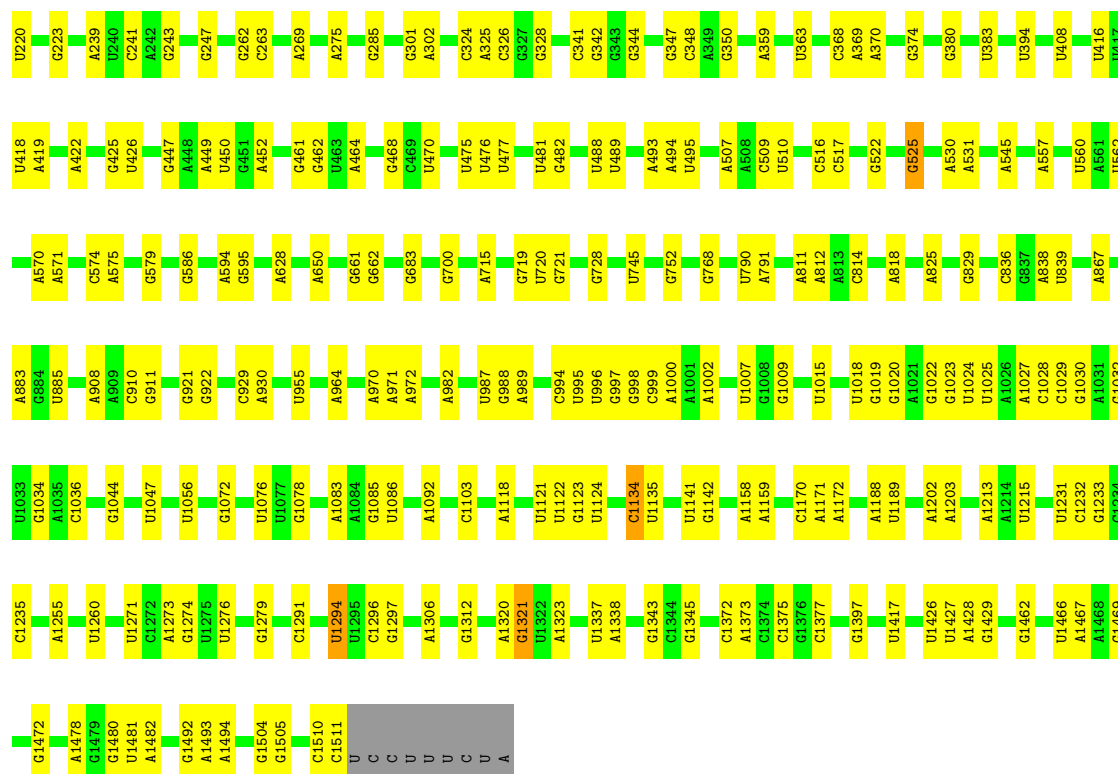
Chain 2:  97% .



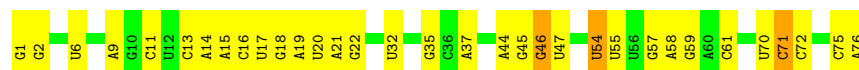
- Molecule 4: 23S ribosomal RNA

Chain 3:  81% 18%

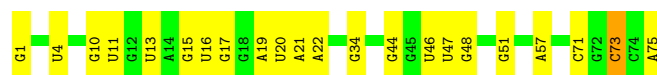




• Molecule 7: tRNA-Ala (E-site)



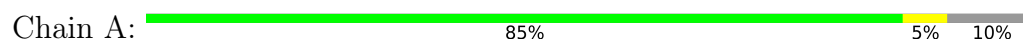
• Molecule 8: tRNA-Asp (P-site)



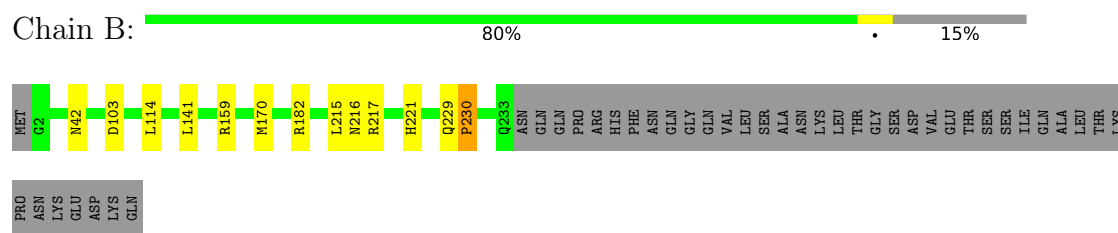
• Molecule 9: tRNA-Lys (A-site)



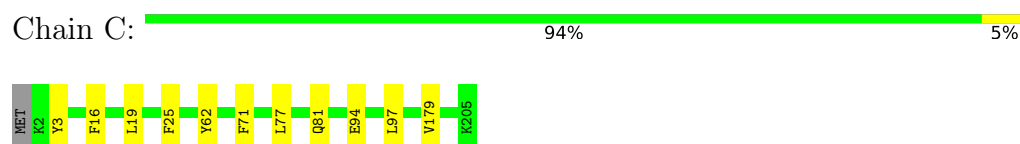
• Molecule 10: 30S ribosomal protein S2



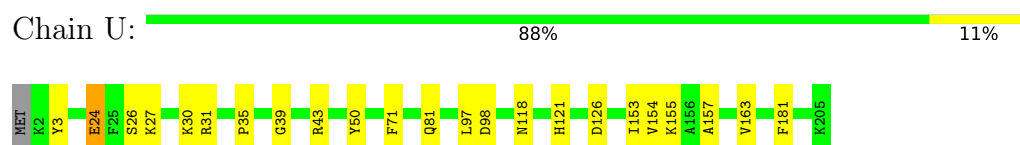
- Molecule 11: 30S ribosomal protein S3



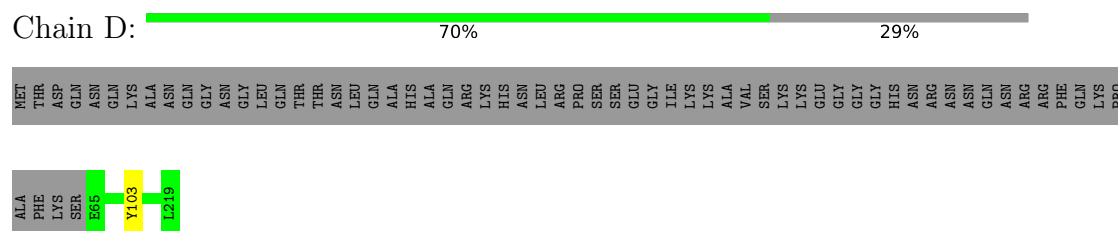
- Molecule 12: 30S ribosomal protein S4



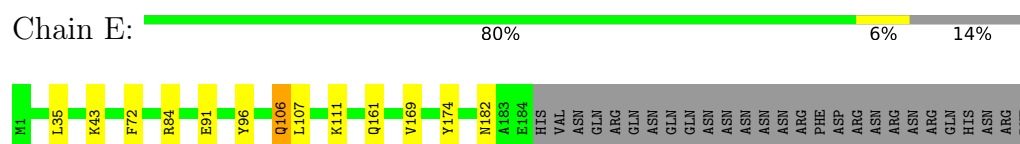
- Molecule 12: 30S ribosomal protein S4



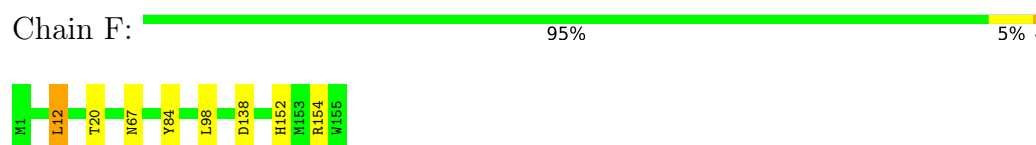
- Molecule 13: 30S ribosomal protein S5



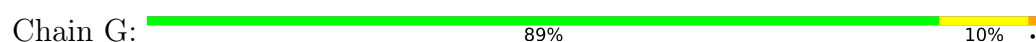
- Molecule 14: 30S ribosomal protein S6



- Molecule 15: 30S ribosomal protein S7



- Molecule 16: 30S ribosomal protein S8





- Molecule 17: 30S ribosomal protein S9

Chain H: 92% 5% .



- Molecule 18: 30S ribosomal protein S10

Chain I: 91% 5% . .



- Molecule 19: 30S ribosomal protein S11

Chain J: 88% 6% 6%



- Molecule 20: 30S ribosomal protein S12

Chain K: 93% . .



- Molecule 21: 30S ribosomal protein S13

Chain L: 90% 7% . .



- Molecule 22: 30S ribosomal protein S14 type Z

Chain M: 95% . .



- Molecule 23: 30S ribosomal protein S15

Chain N: 94% 5% .



- Molecule 24: 30S ribosomal protein S16

Chain O: 86% 6% 7%



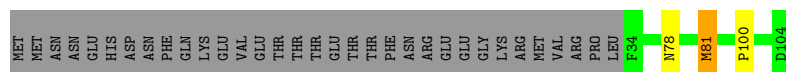
- Molecule 25: 30S ribosomal protein S17

Chain P: 94% 6%



- Molecule 26: 30S ribosomal protein S18

Chain Q: 65% 2% 32%



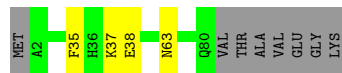
- Molecule 27: 30S ribosomal protein S19

Chain R: 94% 5%



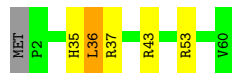
- Molecule 28: 30S ribosomal protein S20

Chain S: 86% 5% 9%



- Molecule 29: 30S ribosomal protein S21

Chain T: 90% 7% 2%



- Molecule 30: Trigger factor

Chain X: 6% 93% 1%

Chain c:  94% 6%



- Molecule 36: 50S ribosomal protein L5

Chain d:  95% ..



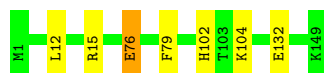
- Molecule 37: 50S ribosomal protein L6

Chain e:  91% . .



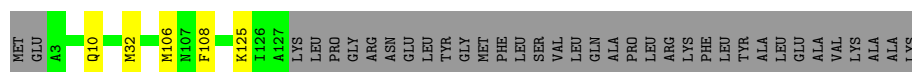
- Molecule 38: 50S ribosomal protein L9

Chain f:  95% . .



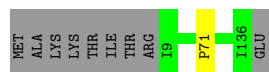
- Molecule 39: 50S ribosomal protein L10

Chain g:  75% . 22%



- Molecule 40: 50S ribosomal protein L11

Chain h:  93% . 7%



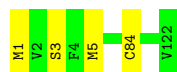
- Molecule 41: 50S ribosomal protein L13

Chain i:  95% . .



- Molecule 42: 50S ribosomal protein L14

Chain j:  97% .



- Molecule 43: 50S ribosomal protein L15

Chain k:  98% ..



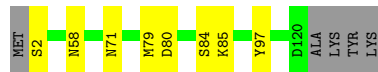
- Molecule 44: 50S ribosomal protein L16

Chain l:  94% . .



- Molecule 45: 50S ribosomal protein L17

Chain m:  90% 6% .



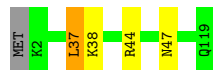
- Molecule 46: 50S ribosomal protein L18

Chain n:  94% 6%



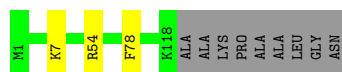
- Molecule 47: 50S ribosomal protein L19

Chain o:  96% . . .



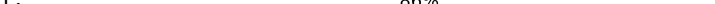
- Molecule 48: 50S ribosomal protein L20

Chain p:  91% . 7%



- Molecule 49: 50S ribosomal protein L21

Category	Count
M1	100
S9	100
K10	100
Y49	100
L50	100
E51	100
K52	100
N69	100
Y83	100
H99	100
ASP	100

- Chain r:  86% . 11%

M1			S81			L107	S108	D109			N112			L117			E130		A142	VAL	THR	SER	SER	VAL	VAL	VAL	LYS	ALA	PRO	SER	SER	LYS	THR	GLN	GLY	GLY	VAL	GLN	LYS
----	--	--	-----	--	--	------	------	------	--	--	------	--	--	------	--	--	------	--	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain s:  39% . 60%

[illegible]

- Chain t:  95% 5%

- Chain u: 82% • 15%

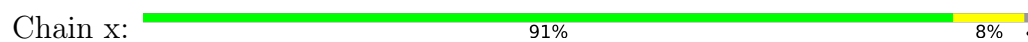
MET	ASN	ASN	LYS	TYR	PHE	LEU	THR	LYS	ILE	ASP	LEU	GLN	PHE	PHE	ALA	S17	S23	R94	V95	S96	A104
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Chain v: 92% 6%

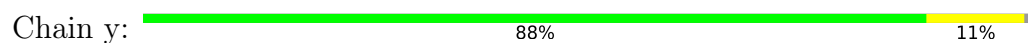
- Chain w:  95% 5% 0%



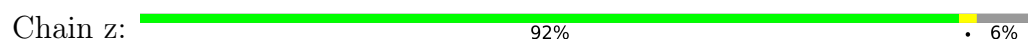
- Molecule 56: 50S ribosomal protein L31



- Molecule 57: 50S ribosomal protein L32



- Molecule 58: 50S ribosomal protein L33 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	10154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, B8T, 1MG, SPM, 5MC, PUT, SPD, MA6, ZN, 2MA, N2P, 7MG, CLM, MG, OMG

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	0	0.29	0/395	0.69	0/518
2	1	0.27	0/484	0.60	0/637
3	2	0.26	0/306	0.65	0/401
4	3	0.17	0/69363	0.71	19/108161 (0.0%)
5	4	0.16	0/2578	0.72	0/4016
6	5	0.16	0/35992	0.71	8/56111 (0.0%)
7	6	0.40	1/1810 (0.1%)	0.91	5/2817 (0.2%)
8	7	0.30	1/1785 (0.1%)	0.81	1/2779 (0.0%)
9	8	0.49	3/1804 (0.2%)	1.04	8/2807 (0.3%)
10	A	0.34	0/2172	0.75	5/2934 (0.2%)
11	B	0.31	0/1863	0.76	4/2516 (0.2%)
12	C	0.32	0/1700	0.70	1/2278 (0.0%)
12	U	0.40	1/1700 (0.1%)	0.85	1/2278 (0.0%)
13	D	0.31	0/1206	0.68	0/1616
14	E	0.35	0/1536	0.77	4/2072 (0.2%)
15	F	0.31	0/1274	0.76	2/1710 (0.1%)
16	G	0.36	0/1126	0.94	12/1517 (0.8%)
17	H	0.37	0/1056	0.76	2/1409 (0.1%)
18	I	0.30	0/843	0.76	3/1132 (0.3%)
19	J	0.35	0/844	0.70	0/1136
20	K	0.30	0/1089	0.70	0/1461
21	L	0.31	0/1002	0.87	4/1340 (0.3%)
22	M	0.36	0/483	0.75	1/643 (0.2%)
23	N	0.25	0/695	0.71	2/926 (0.2%)
24	O	0.34	0/718	0.81	2/962 (0.2%)
25	P	0.28	0/702	0.69	0/934
26	Q	0.42	0/601	0.95	2/801 (0.2%)
27	R	0.35	0/716	0.68	0/958
28	S	0.32	0/645	0.71	0/857
29	T	0.46	0/524	0.85	1/685 (0.1%)
30	X	0.28	0/245	0.64	0/325
31	Y	0.28	0/498	0.88	0/773

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.75	0/26	1.33	0/33
33	a	0.29	0/2267	0.65	1/3044 (0.0%)
34	b	0.29	0/1803	0.59	1/2424 (0.0%)
35	c	0.29	0/1681	0.58	1/2257 (0.0%)
36	d	0.30	0/1437	0.67	0/1931
37	e	0.30	0/1420	0.64	2/1912 (0.1%)
38	f	0.32	0/1233	0.64	0/1653
39	g	0.27	0/960	0.64	0/1284
40	h	0.28	0/968	0.66	3/1298 (0.2%)
41	i	0.31	0/1186	0.70	2/1592 (0.1%)
42	j	0.33	0/953	0.73	1/1275 (0.1%)
43	k	0.31	0/1187	0.64	0/1581
44	l	0.39	0/1104	0.73	1/1481 (0.1%)
45	m	0.28	0/973	0.65	1/1309 (0.1%)
46	n	0.30	0/927	0.74	0/1239
47	o	0.29	0/976	0.68	1/1296 (0.1%)
48	p	0.27	0/996	0.63	0/1325
49	q	0.29	0/828	0.64	0/1111
50	r	0.32	0/1100	0.69	2/1471 (0.1%)
51	s	0.29	0/752	0.61	0/1015
52	t	0.29	0/878	0.70	3/1165 (0.3%)
53	u	0.29	0/678	0.64	0/902
54	v	0.39	0/526	0.82	2/703 (0.3%)
55	w	0.26	0/916	0.60	1/1222 (0.1%)
56	x	0.28	0/776	0.67	1/1033 (0.1%)
57	y	0.26	0/457	0.70	0/601
58	z	0.32	0/412	0.63	0/547
All	All	0.23	6/165175 (0.0%)	0.72	110/246214 (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
12	U	0	2
22	M	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	76	A	C6-N6	15.02	1.46	1.33
8	7	1	G	OP3-P	-7.62	1.52	1.61
7	6	1	G	OP3-P	-7.59	1.52	1.61
9	8	76	A	N7-C5	-6.67	1.35	1.39
9	8	76	A	N9-C8	-6.22	1.32	1.37
12	U	31	ARG	CA-C	5.98	1.68	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	76	A	C2-N3-C4	22.02	121.61	110.60
9	8	76	A	N1-C2-N3	-15.22	121.69	129.30
9	8	76	A	N3-C4-C5	-12.67	117.93	126.80
10	A	173	PRO	CA-N-CD	-11.43	95.50	111.50
4	3	2166	U	O5'-P-OP1	-10.79	95.99	105.70
26	Q	100	PRO	CA-N-CD	-10.27	97.13	111.50
9	8	76	A	N3-C4-N9	10.12	135.50	127.40
18	I	9	TYR	C-N-CD	-9.73	99.19	120.60
9	8	76	A	N7-C8-N9	-9.51	109.05	113.80
7	6	32	U	P-O3'-C3'	-9.44	108.38	119.70
9	8	76	A	C5-N7-C8	9.08	108.44	103.90
21	L	89	LEU	CA-CB-CG	8.91	135.80	115.30
21	L	75	LEU	CA-CB-CG	8.22	134.21	115.30
16	G	14	PRO	CA-N-CD	-8.11	100.14	111.50
4	3	388	U	O5'-P-OP1	-7.89	98.60	105.70
11	B	182	ARG	CG-CD-NE	7.80	128.18	111.80
40	h	71	PRO	N-CD-CG	-7.78	91.54	103.20
9	8	76	A	C8-N9-C4	7.73	108.89	105.80
4	3	900	G	O5'-P-OP2	-7.64	98.82	105.70
21	L	96	PRO	CA-N-CD	-7.59	100.87	111.50
7	6	54	U	P-O3'-C3'	-7.59	110.59	119.70
8	7	73	C	P-O3'-C3'	-7.52	110.68	119.70
12	U	31	ARG	O-C-N	-7.44	110.80	122.70
9	8	76	A	C4-C5-N7	-7.31	107.05	110.70
4	3	2184	A	C5'-C4'-O4'	7.30	117.86	109.10
4	3	1486	U	C2-N1-C1'	7.17	126.31	117.70
11	B	141	LEU	CA-CB-CG	7.14	131.73	115.30
50	r	109	ASP	CB-CG-OD1	7.11	124.70	118.30
6	5	1323	A	O5'-P-OP1	7.11	119.23	110.70
56	x	100	LEU	CA-CB-CG	7.10	131.62	115.30
17	H	45	LEU	CA-CB-CG	7.03	131.46	115.30
41	i	63	ASP	CB-CG-OD1	6.94	124.55	118.30
16	G	13	ASP	CB-CG-OD1	6.82	124.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	57	LYS	CD-CE-NZ	6.82	127.39	111.70
40	h	71	PRO	CA-N-CD	-6.81	101.97	111.50
6	5	1294	U	C6-N1-C2	-6.67	117.00	121.00
4	3	1486	U	N1-C2-O2	6.61	127.43	122.80
29	T	36	LEU	CA-CB-CG	6.60	130.47	115.30
11	B	230	PRO	CA-N-CD	-6.59	102.27	111.50
6	5	1294	U	N3-C2-O2	-6.57	117.60	122.20
18	I	46	LEU	C-N-CD	-6.53	106.24	120.60
4	3	393	C	C6-N1-C2	-6.52	117.69	120.30
18	I	10	PRO	CA-N-CD	-6.52	102.37	111.50
6	5	1323	A	OP2-P-O3'	6.47	119.44	105.20
16	G	60	LEU	CB-CG-CD2	-6.37	100.17	111.00
54	v	33	LEU	CB-CG-CD2	-6.26	100.36	111.00
4	3	2182	C	C6-N1-C2	-6.24	117.80	120.30
11	B	215	LEU	CA-CB-CG	6.15	129.45	115.30
52	t	95	PRO	CA-N-CD	-6.14	102.90	111.50
16	G	7	PRO	N-CD-CG	-6.12	94.02	103.20
4	3	1486	U	N3-C2-O2	-6.10	117.93	122.20
45	m	80	ASP	CB-CG-OD1	6.07	123.76	118.30
4	3	2182	C	N1-C2-O2	6.04	122.52	118.90
10	A	210	LEU	CA-CB-CG	6.03	129.18	115.30
15	F	98	LEU	CA-CB-CG	5.93	128.95	115.30
24	O	43	LEU	CA-CB-CG	5.92	128.91	115.30
16	G	48	LEU	CB-CG-CD1	-5.88	101.00	111.00
17	H	21	LEU	CA-CB-CG	5.83	128.71	115.30
16	G	5	THR	C-N-CA	5.80	136.19	121.70
40	h	71	PRO	CA-CB-CG	-5.72	93.14	104.00
10	A	179	ASP	CB-CG-OD1	5.70	123.43	118.30
12	C	19	LEU	CA-CB-CG	5.69	128.38	115.30
16	G	14	PRO	N-CD-CG	-5.68	94.68	103.20
16	G	74	LEU	CA-CB-CG	5.67	128.33	115.30
6	5	1321	G	OP1-P-O3'	5.64	117.61	105.20
14	E	107	LEU	CA-CB-CG	5.63	128.26	115.30
26	Q	81	MET	CA-CB-CG	5.62	122.86	113.30
14	E	35	LEU	CA-CB-CG	5.62	128.23	115.30
7	6	46	G	P-O3'-C3'	5.62	126.44	119.70
33	a	128	ILE	CG1-CB-CG2	-5.61	99.07	111.40
4	3	1341	U	C2-N1-C1'	5.60	124.42	117.70
6	5	1103	C	N3-C4-C5	-5.59	119.66	121.90
16	G	7	PRO	CA-N-CD	-5.55	103.72	111.50
7	6	71	C	C6-N1-C2	-5.53	118.09	120.30
4	3	1303	U	C2-N1-C1'	5.51	124.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	123	MET	CA-CB-CG	5.49	122.64	113.30
23	N	78	LEU	CA-CB-CG	5.47	127.88	115.30
35	c	193	LEU	CA-CB-CG	5.46	127.86	115.30
16	G	14	PRO	CA-CB-CG	-5.43	93.69	104.00
4	3	2182	C	N3-C2-O2	-5.42	118.11	121.90
42	j	5	MET	CA-CB-CG	5.41	122.49	113.30
6	5	1294	U	C5-C6-N1	5.38	125.39	122.70
37	e	30	PRO	CA-N-CD	-5.38	103.97	111.50
15	F	12	LEU	C-N-CD	-5.36	108.80	120.60
34	b	13	MET	CB-CG-SD	-5.35	96.35	112.40
10	A	17	LEU	CA-CB-CG	5.34	127.58	115.30
4	3	2184	A	C4'-C3'-O3'	5.32	123.65	113.00
10	A	151	MET	CA-CB-CG	5.32	122.35	113.30
52	t	95	PRO	N-CD-CG	-5.31	95.24	103.20
4	3	1303	U	N1-C2-O2	5.29	126.50	122.80
4	3	2184	A	C5'-C4'-C3'	5.28	124.45	116.00
23	N	63	LEU	CA-CB-CG	5.26	127.41	115.30
50	r	130	GLU	CA-CB-CG	5.26	124.96	113.40
4	3	881	A	P-O3'-C3'	5.23	125.97	119.70
37	e	92	LEU	CA-CB-CG	5.22	127.30	115.30
54	v	44	LYS	CD-CE-NZ	-5.22	99.70	111.70
4	3	393	C	P-O3'-C3'	5.18	125.92	119.70
52	t	111	LEU	CA-CB-CG	5.16	127.17	115.30
47	o	37	LEU	CA-CB-CG	5.13	127.09	115.30
41	i	11	GLN	CA-CB-CG	5.12	124.67	113.40
55	w	7	LEU	CA-CB-CG	-5.10	103.57	115.30
21	L	19	LEU	CA-CB-CG	5.09	127.01	115.30
14	E	107	LEU	CB-CG-CD2	-5.09	102.35	111.00
7	6	71	C	N1-C2-O2	5.08	121.95	118.90
16	G	60	LEU	CA-CB-CG	5.08	126.98	115.30
24	O	41	PRO	CA-N-CD	-5.06	104.41	111.50
14	E	106	GLN	CA-CB-CG	5.05	124.51	113.40
4	3	1303	U	N3-C2-O2	-5.03	118.68	122.20
6	5	1134	C	C2-N1-C1'	5.02	124.32	118.80
44	l	82	ARG	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	M	23	ARG	Sidechain
12	U	121	HIS	Peptide

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Mol	Chain	Res	Type	Group
12	U	153	ILE	Peptide

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	
1	0	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	A	262/294 (89%)	236 (90%)	24 (9%)	2 (1%)	16	49
11	B	230/273 (84%)	203 (88%)	23 (10%)	4 (2%)	7	36
12	C	202/205 (98%)	167 (83%)	33 (16%)	2 (1%)	13	44
12	U	202/205 (98%)	147 (73%)	39 (19%)	16 (8%)	1	10
13	D	153/219 (70%)	143 (94%)	10 (6%)	0	100	100
14	E	182/215 (85%)	156 (86%)	25 (14%)	1 (0%)	25	57
15	F	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	10	40
16	G	139/142 (98%)	133 (96%)	6 (4%)	0	100	100
17	H	127/132 (96%)	113 (89%)	14 (11%)	0	100	100
18	I	102/108 (94%)	89 (87%)	12 (12%)	1 (1%)	13	44
19	J	112/121 (93%)	106 (95%)	5 (4%)	1 (1%)	14	47
20	K	133/139 (96%)	116 (87%)	14 (10%)	3 (2%)	5	31
21	L	121/124 (98%)	109 (90%)	10 (8%)	2 (2%)	7	36
22	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	N	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
24	O	85/94 (90%)	79 (93%)	6 (7%)	0	100	100
25	P	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	11	41
26	Q	69/104 (66%)	64 (93%)	5 (7%)	0	100	100
27	R	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
28	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	10	40
29	T	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	X	28/444 (6%)	25 (89%)	3 (11%)	0	100	100
32	Z	3/36 (8%)	3 (100%)	0	0	100	100
33	a	283/287 (99%)	269 (95%)	13 (5%)	1 (0%)	30	62
34	b	228/287 (79%)	219 (96%)	9 (4%)	0	100	100
35	c	209/212 (99%)	196 (94%)	13 (6%)	0	100	100
36	d	177/180 (98%)	171 (97%)	6 (3%)	0	100	100
37	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
38	f	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	9	39
39	g	123/161 (76%)	119 (97%)	4 (3%)	0	100	100
40	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
41	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
42	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
43	k	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
44	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
45	m	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
46	n	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
47	o	116/119 (98%)	108 (93%)	8 (7%)	0	100	100
48	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
49	q	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
50	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
51	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
52	t	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
53	u	86/104 (83%)	83 (96%)	3 (4%)	0	100	100
54	v	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	w	108/111 (97%)	104 (96%)	4 (4%)	0	100	100
56	x	94/97 (97%)	70 (74%)	22 (23%)	2 (2%)	5	33
57	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
58	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6248/7355 (85%)	5762 (92%)	445 (7%)	41 (1%)	21	51

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	B	229	GLN
11	B	230	PRO
20	K	56	LYS
25	P	54	LEU
12	U	39	GLY
12	U	126	ASP
12	U	163	VAL
38	f	76	GLU
12	C	81	GLN
12	C	179	VAL
12	U	3	TYR
12	U	24	GLU
12	U	30	LYS
12	U	81	GLN
12	U	154	VAL
12	U	155	LYS
11	B	217	ARG
12	U	27	LYS
10	A	54	ASP
10	A	219	ASN
11	B	216	ASN
15	F	20	THR
20	K	57	LYS
20	K	72	ASN
28	S	37	LYS
12	U	157	ALA
12	U	181	PHE
33	a	128	ILE
38	f	12	LEU
56	x	49	GLU
56	x	59	ALA
14	E	169	VAL

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Mol	Chain	Res	Type
15	F	12	LEU
19	J	114	CYS
21	L	123	SER
12	U	43	ARG
12	U	50	TYR
12	U	26	SER
18	I	100	VAL
21	L	116	VAL
12	U	35	PRO

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	
1	0	41/41 (100%)	40 (98%)	1 (2%)	44	63
2	1	51/51 (100%)	48 (94%)	3 (6%)	16	44
3	2	35/35 (100%)	34 (97%)	1 (3%)	37	59
10	A	238/262 (91%)	229 (96%)	9 (4%)	28	53
11	B	195/232 (84%)	189 (97%)	6 (3%)	35	57
12	C	182/183 (100%)	174 (96%)	8 (4%)	24	50
12	U	182/183 (100%)	177 (97%)	5 (3%)	40	61
13	D	125/178 (70%)	124 (99%)	1 (1%)	79	85
14	E	165/196 (84%)	155 (94%)	10 (6%)	15	43
15	F	132/132 (100%)	127 (96%)	5 (4%)	28	53
16	G	123/124 (99%)	115 (94%)	8 (6%)	14	41
17	H	112/115 (97%)	107 (96%)	5 (4%)	23	50
18	I	97/99 (98%)	94 (97%)	3 (3%)	35	57
19	J	91/97 (94%)	85 (93%)	6 (7%)	14	41
20	K	117/120 (98%)	114 (97%)	3 (3%)	41	61
21	L	104/105 (99%)	97 (93%)	7 (7%)	13	40
22	M	47/48 (98%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	N	77/78 (99%)	75 (97%)	2 (3%)	41	61
24	O	76/82 (93%)	72 (95%)	4 (5%)	19	46
25	P	75/75 (100%)	71 (95%)	4 (5%)	19	46
26	Q	62/94 (66%)	60 (97%)	2 (3%)	34	57
27	R	76/77 (99%)	72 (95%)	4 (5%)	19	46
28	S	71/77 (92%)	68 (96%)	3 (4%)	25	51
29	T	55/56 (98%)	50 (91%)	5 (9%)	7	30
30	X	27/406 (7%)	24 (89%)	3 (11%)	5	24
32	Z	2/2 (100%)	2 (100%)	0	100	100
33	a	241/243 (99%)	238 (99%)	3 (1%)	67	79
34	b	187/233 (80%)	175 (94%)	12 (6%)	14	42
35	c	183/184 (100%)	172 (94%)	11 (6%)	16	43
36	d	153/154 (99%)	145 (95%)	8 (5%)	19	46
37	e	153/159 (96%)	147 (96%)	6 (4%)	27	53
38	f	134/134 (100%)	128 (96%)	6 (4%)	23	50
39	g	100/129 (78%)	95 (95%)	5 (5%)	20	47
40	h	102/110 (93%)	102 (100%)	0	100	100
41	i	126/128 (98%)	123 (98%)	3 (2%)	44	63
42	j	103/103 (100%)	100 (97%)	3 (3%)	37	59
43	k	125/126 (99%)	123 (98%)	2 (2%)	58	74
44	l	113/115 (98%)	108 (96%)	5 (4%)	24	50
45	m	105/109 (96%)	98 (93%)	7 (7%)	13	40
46	n	99/99 (100%)	92 (93%)	7 (7%)	12	39
47	o	104/105 (99%)	100 (96%)	4 (4%)	28	53
48	p	104/108 (96%)	101 (97%)	3 (3%)	37	59
49	q	90/91 (99%)	82 (91%)	8 (9%)	8	31
50	r	118/132 (89%)	114 (97%)	4 (3%)	32	56
51	s	84/208 (40%)	82 (98%)	2 (2%)	44	63
52	t	96/96 (100%)	93 (97%)	3 (3%)	35	57
53	u	70/85 (82%)	67 (96%)	3 (4%)	25	50
54	v	59/60 (98%)	57 (97%)	2 (3%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	w	97/98 (99%)	93 (96%)	4 (4%)	26	52
56	x	85/86 (99%)	80 (94%)	5 (6%)	16	44
57	y	48/49 (98%)	42 (88%)	6 (12%)	3	19
58	z	47/50 (94%)	46 (98%)	1 (2%)	48	67
All	All	5484/6342 (86%)	5253 (96%)	231 (4%)	27	51

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	33	LEU
2	1	28	HIS
2	1	39	ARG
2	1	50	SER
3	2	21	GLN
10	A	16	GLU
10	A	66	GLN
10	A	84	PHE
10	A	107	PHE
10	A	126	SER
10	A	160	GLU
10	A	210	LEU
10	A	249	LYS
10	A	260	GLN
11	B	42	ASN
11	B	103	ASP
11	B	114	LEU
11	B	159	ARG
11	B	170	MET
11	B	221	HIS
12	C	3	TYR
12	C	16	PHE
12	C	25	PHE
12	C	62	TYR
12	C	71	PHE
12	C	77	LEU
12	C	94	GLU
12	C	97	LEU
13	D	103	TYR
14	E	43	LYS
14	E	72	PHE
14	E	84	ARG

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Mol	Chain	Res	Type
14	E	91	GLU
14	E	96	TYR
14	E	106	GLN
14	E	111	LYS
14	E	161	GLN
14	E	174	TYR
14	E	182	ASN
15	F	67	ASN
15	F	84	TYR
15	F	138	ASP
15	F	152	HIS
15	F	154	ARG
16	G	12	PHE
16	G	13	ASP
16	G	57	PHE
16	G	85	ASN
16	G	91	SER
16	G	101	PHE
16	G	106	LEU
16	G	109	ASN
17	H	5	SER
17	H	11	ARG
17	H	14	SER
17	H	50	MET
17	H	125	ARG
18	I	9	TYR
18	I	18	SER
18	I	21	SER
19	J	21	ASN
19	J	39	SER
19	J	68	LYS
19	J	72	MET
19	J	95	ASN
19	J	112	ASN
20	K	32	ASN
20	K	47	CYS
20	K	128	SER
21	L	3	ARG
21	L	11	ASN
21	L	31	GLN
21	L	68	ASP
21	L	71	ARG

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Mol	Chain	Res	Type
21	L	75	LEU
21	L	89	LEU
23	N	16	ASP
23	N	69	HIS
24	O	14	TYR
24	O	18	ARG
24	O	46	ASN
24	O	79	TRP
25	P	29	ARG
25	P	49	ASN
25	P	56	LYS
25	P	79	LYS
26	Q	78	ASN
26	Q	81	MET
27	R	17	LYS
27	R	26	GLU
27	R	61	TYR
27	R	79	ASN
28	S	35	PHE
28	S	38	GLU
28	S	63	ASN
29	T	35	HIS
29	T	36	LEU
29	T	37	ARG
29	T	43	ARG
29	T	53	ARG
12	U	24	GLU
12	U	71	PHE
12	U	97	LEU
12	U	98	ASP
12	U	118	ASN
30	X	29	LYS
30	X	45	LYS
30	X	56	TYR
33	a	9	ARG
33	a	262	HIS
33	a	270	MET
34	b	1	MET
34	b	24	LEU
34	b	35	GLN
34	b	52	LEU
34	b	53	SER

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Mol	Chain	Res	Type
34	b	79	LYS
34	b	100	ASN
34	b	114	SER
34	b	158	ARG
34	b	189	MET
34	b	194	SER
34	b	227	GLU
35	c	10	ASP
35	c	12	SER
35	c	19	LYS
35	c	27	LYS
35	c	151	LYS
35	c	162	ASN
35	c	173	SER
35	c	176	LYS
35	c	179	GLN
35	c	195	ASN
35	c	197	LEU
36	d	8	TYR
36	d	31	LEU
36	d	46	ASP
36	d	47	SER
36	d	88	LYS
36	d	96	MET
36	d	114	PHE
36	d	133	LYS
37	e	3	LYS
37	e	7	ARG
37	e	24	HIS
37	e	41	ASN
37	e	86	PHE
37	e	168	PHE
38	f	15	ARG
38	f	76	GLU
38	f	79	PHE
38	f	102	HIS
38	f	104	LYS
38	f	132	GLU
39	g	10	GLN
39	g	32	MET
39	g	106	MET
39	g	108	PHE

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Mol	Chain	Res	Type
39	g	125	LYS
41	i	46	ASP
41	i	89	LYS
41	i	95	MET
42	j	1	MET
42	j	3	SER
42	j	84	CYS
43	k	76	GLU
43	k	113	LYS
44	l	73	SER
44	l	103	MET
44	l	108	ASN
44	l	133	LYS
44	l	134	ARG
45	m	2	SER
45	m	58	ASN
45	m	71	ASN
45	m	79	MET
45	m	84	SER
45	m	85	LYS
45	m	97	TYR
46	n	1	MET
46	n	12	HIS
46	n	25	ASP
46	n	55	SER
46	n	57	SER
46	n	62	LEU
46	n	92	ASP
47	o	37	LEU
47	o	38	LYS
47	o	44	ARG
47	o	47	ASN
48	p	7	LYS
48	p	54	ARG
48	p	78	PHE
49	q	9	SER
49	q	10	LYS
49	q	49	TYR
49	q	51	GLU
49	q	52	LYS
49	q	69	ASN
49	q	83	TYR

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Mol	Chain	Res	Type
49	q	99	HIS
50	r	81	SER
50	r	107	LEU
50	r	112	ASN
50	r	117	LEU
51	s	51	LYS
51	s	84	THR
52	t	40	ASN
52	t	72	SER
52	t	84	GLN
53	u	23	SER
53	u	94	ARG
53	u	96	SER
54	v	5	ASP
54	v	26	ARG
55	w	37	GLU
55	w	55	LEU
55	w	71	LYS
55	w	101	SER
56	x	5	PHE
56	x	11	SER
56	x	22	SER
56	x	32	LYS
56	x	93	SER
57	y	6	ARG
57	y	10	LYS
57	y	43	CYS
57	y	52	ARG
57	y	54	LYS
57	y	55	LYS
58	z	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
10	A	219	ASN
11	B	6	ASN
11	B	231	ASN
12	C	121	HIS
14	E	101	ASN
15	F	19	ASN
15	F	67	ASN

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Mol	Chain	Res	Type
16	G	85	ASN
17	H	43	ASN
19	J	111	HIS
20	K	29	ASN
28	S	20	ASN
28	S	72	ASN
12	U	37	GLN
12	U	171	ASN
34	b	157	GLN
34	b	225	GLN
35	c	76	GLN
35	c	83	HIS
35	c	195	ASN
37	e	77	ASN
38	f	78	HIS
41	i	11	GLN
41	i	13	ASN
41	i	80	HIS
45	m	59	ASN
47	o	78	ASN
53	u	43	GLN
54	v	32	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	Y	20/21 (95%)	14 (70%)	4 (20%)
4	3	2891/2907 (99%)	520 (17%)	21 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	1503/1520 (98%)	253 (16%)	7 (0%)
7	6	75/76 (98%)	29 (38%)	6 (8%)
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	4745/4783 (99%)	888 (18%)	40 (0%)

All (888) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C

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Mol	Chain	Res	Type
4	3	14	U
4	3	28	G
4	3	37	G
4	3	48	G
4	3	64	U
4	3	65	A
4	3	73	A
4	3	76	A
4	3	77	G
4	3	102	A
4	3	103	G
4	3	119	A
4	3	121	U
4	3	126	C
4	3	132	G
4	3	141	A
4	3	142	A
4	3	163	A
4	3	180	A
4	3	184	A
4	3	187	C
4	3	200	A
4	3	203	A
4	3	219	G
4	3	220	A
4	3	225	A
4	3	226	A
4	3	232	A
4	3	234	G
4	3	237	A
4	3	245	U
4	3	246	G
4	3	252	G
4	3	269	A
4	3	276	A
4	3	284	U
4	3	287	G
4	3	295	U
4	3	296	U
4	3	297	G
4	3	298	U
4	3	299	A

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Mol	Chain	Res	Type
4	3	309	A
4	3	310	U
4	3	311	G
4	3	315	A
4	3	316	C
4	3	317	U
4	3	319	G
4	3	325	G
4	3	336	C
4	3	345	A
4	3	363	G
4	3	364	A
4	3	365	U
4	3	402	A
4	3	409	A
4	3	410	G
4	3	411	U
4	3	418	G
4	3	419	A
4	3	424	G
4	3	425	U
4	3	426	U
4	3	432	G
4	3	437	A
4	3	440	C
4	3	460	G
4	3	483	A
4	3	517	G
4	3	539	U
4	3	540	A
4	3	548	A
4	3	562	C
4	3	565	C
4	3	566	G
4	3	567	U
4	3	573	A
4	3	581	A
4	3	583	U
4	3	596	G
4	3	598	G
4	3	607	U
4	3	608	A

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Mol	Chain	Res	Type
4	3	610	G
4	3	620	G
4	3	636	U
4	3	637	U
4	3	638	A
4	3	648	G
4	3	649	A
4	3	650	G
4	3	663	A
4	3	670	G
4	3	673	A
4	3	681	A
4	3	682	A
4	3	689	U
4	3	691	G
4	3	705	A
4	3	712	A
4	3	716	G
4	3	721	G
4	3	722	C
4	3	765	A
4	3	775	C
4	3	782	U
4	3	792	G
4	3	797	U
4	3	800	C
4	3	810	G
4	3	811	G
4	3	817	A
4	3	819	U
4	3	820	U
4	3	824	A
4	3	828	A
4	3	829	A
4	3	840	G
4	3	846	U
4	3	847	C
4	3	854	A
4	3	862	U
4	3	881	A
4	3	882	C
4	3	883	A

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Mol	Chain	Res	Type
4	3	901	C
4	3	902	U
4	3	904	C
4	3	906	G
4	3	918	G
4	3	924	C
4	3	926	U
4	3	927	A
4	3	928	G
4	3	930	C
4	3	932	U
4	3	934	C
4	3	935	U
4	3	936	G
4	3	944	U
4	3	947	A
4	3	949	C
4	3	951	C
4	3	952	U
4	3	953	G
4	3	970	U
4	3	981	A
4	3	982	G
4	3	994	U
4	3	997	G
4	3	998	C
4	3	1008	A
4	3	1010	G
4	3	1016	A
4	3	1019	A
4	3	1026	A
4	3	1032	A
4	3	1039	G
4	3	1045	A
4	3	1049	U
4	3	1058	U
4	3	1060	G
4	3	1061	A
4	3	1068	U
4	3	1074	A
4	3	1080	A
4	3	1082	A

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Mol	Chain	Res	Type
4	3	1084	C
4	3	1095	U
4	3	1096	U
4	3	1097	G
4	3	1098	G
4	3	1099	C
4	3	1102	A
4	3	1104	A
4	3	1105	A
4	3	1106	G
4	3	1107	C
4	3	1110	C
4	3	1111	C
4	3	1113	U
4	3	1114	C
4	3	1115	G
4	3	1120	A
4	3	1122	G
4	3	1123	A
4	3	1125	U
4	3	1130	A
4	3	1132	C
4	3	1138	A
4	3	1145	G
4	3	1146	A
4	3	1147	G
4	3	1165	U
4	3	1167	U
4	3	1168	A
4	3	1170	C
4	3	1176	U
4	3	1177	A
4	3	1178	A
4	3	1204	A
4	3	1208	A
4	3	1209	U
4	3	1210	A
4	3	1212	C
4	3	1215	G
4	3	1234	U
4	3	1235	U
4	3	1236	G

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Mol	Chain	Res	Type
4	3	1242	G
4	3	1246	U
4	3	1250	A
4	3	1251	G
4	3	1253	G
4	3	1256	A
4	3	1257	G
4	3	1266	G
4	3	1268	U
4	3	1280	G
4	3	1281	A
4	3	1283	A
4	3	1285	U
4	3	1286	G
4	3	1292	A
4	3	1301	G
4	3	1304	U
4	3	1313	G
4	3	1325	C
4	3	1328	A
4	3	1329	U
4	3	1330	U
4	3	1369	U
4	3	1378	C
4	3	1380	U
4	3	1388	G
4	3	1393	A
4	3	1406	A
4	3	1407	U
4	3	1412	A
4	3	1423	A
4	3	1424	U
4	3	1431	A
4	3	1444	C
4	3	1445	U
4	3	1446	G
4	3	1448	U
4	3	1456	C
4	3	1463	G
4	3	1467	U
4	3	1480	A
4	3	1481	U

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Mol	Chain	Res	Type
4	3	1483	G
4	3	1486	U
4	3	1487	U
4	3	1502	A
4	3	1504	G
4	3	1508	G
4	3	1510	A
4	3	1513	A
4	3	1514	U
4	3	1515	A
4	3	1519	A
4	3	1522	U
4	3	1534	A
4	3	1535	A
4	3	1541	A
4	3	1546	U
4	3	1550	G
4	3	1569	A
4	3	1570	A
4	3	1571	G
4	3	1580	G
4	3	1582	G
4	3	1584	U
4	3	1585	A
4	3	1588	A
4	3	1603	A
4	3	1612	U
4	3	1617	U
4	3	1618	U
4	3	1619	A
4	3	1641	A
4	3	1642	G
4	3	1643	A
4	3	1644	A
4	3	1645	C
4	3	1650	A
4	3	1651	C
4	3	1661	A
4	3	1668	G
4	3	1680	A
4	3	1681	G
4	3	1682	C

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Mol	Chain	Res	Type
4	3	1694	A
4	3	1708	G
4	3	1727	U
4	3	1737	G
4	3	1748	U
4	3	1749	A
4	3	1764	U
4	3	1769	A
4	3	1770	A
4	3	1771	C
4	3	1780	A
4	3	1789	C
4	3	1791	A
4	3	1807	C
4	3	1808	C
4	3	1809	A
4	3	1816	A
4	3	1823	U
4	3	1836	A
4	3	1854	A
4	3	1855	A
4	3	1866	G
4	3	1869	G
4	3	1878	A
4	3	1886	C
4	3	1910	G
4	3	1913	G
4	3	1920	A
4	3	1936	G
4	3	1937	G
4	3	1938	U
4	3	1943	A
4	3	1944	A
4	3	1962	U
4	3	1974	U
4	3	1977	A
4	3	1978	U
4	3	1979	G
4	3	1998	U
4	3	1999	G
4	3	2000	U
4	3	2004	G

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Mol	Chain	Res	Type
4	3	2028	G
4	3	2030	A
4	3	2038	A
4	3	2040	A
4	3	2041	C
4	3	2042	A
4	3	2050	G
4	3	2057	C
4	3	2062	C
4	3	2063	G
4	3	2067	A
4	3	2068	G
4	3	2069	A
4	3	2076	G
4	3	2084	A
4	3	2099	U
4	3	2100	G
4	3	2106	G
4	3	2108	C
4	3	2110	U
4	3	2111	U
4	3	2112	A
4	3	2114	C
4	3	2115	A
4	3	2116	U
4	3	2117	G
4	3	2118	U
4	3	2119	A
4	3	2123	A
4	3	2124	A
4	3	2125	U
4	3	2126	A
4	3	2130	A
4	3	2131	G
4	3	2133	A
4	3	2134	G
4	3	2139	C
4	3	2140	G
4	3	2144	C
4	3	2150	C
4	3	2152	C
4	3	2153	U

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Mol	Chain	Res	Type
4	3	2154	A
4	3	2157	A
4	3	2164	G
4	3	2166	U
4	3	2169	G
4	3	2170	A
4	3	2173	G
4	3	2175	U
4	3	2180	U
4	3	2181	A
4	3	2182	C
4	3	2183	U
4	3	2184	A
4	3	2185	C
4	3	2193	U
4	3	2194	G
4	3	2195	U
4	3	2198	G
4	3	2199	C
4	3	2200	U
4	3	2201	G
4	3	2202	U
4	3	2207	A
4	3	2211	G
4	3	2212	U
4	3	2219	U
4	3	2220	A
4	3	2221	U
4	3	2227	U
4	3	2228	U
4	3	2233	A
4	3	2246	G
4	3	2247	G
4	3	2259	OMG
4	3	2274	A
4	3	2276	A
4	3	2287	G
4	3	2291	U
4	3	2295	A
4	3	2298	G
4	3	2305	C
4	3	2311	G

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Mol	Chain	Res	Type
4	3	2313	U
4	3	2316	G
4	3	2319	A
4	3	2327	U
4	3	2329	G
4	3	2333	G
4	3	2335	A
4	3	2336	A
4	3	2342	U
4	3	2343	A
4	3	2344	A
4	3	2353	G
4	3	2355	C
4	3	2358	U
4	3	2366	A
4	3	2391	G
4	3	2393	C
4	3	2397	G
4	3	2410	C
4	3	2411	C
4	3	2414	U
4	3	2422	G
4	3	2431	U
4	3	2433	A
4	3	2437	G
4	3	2438	A
4	3	2443	A
4	3	2449	U
4	3	2456	A
4	3	2477	A
4	3	2481	U
4	3	2482	U
4	3	2483	C
4	3	2484	A
4	3	2486	A
4	3	2488	C
4	3	2499	U
4	3	2510	G
4	3	2512	U
4	3	2513	G
4	3	2521	A
4	3	2526	A

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Mol	Chain	Res	Type
4	3	2537	G
4	3	2543	G
4	3	2574	A
4	3	2575	G
4	3	2580	A
4	3	2585	A
4	3	2593	U
4	3	2594	C
4	3	2605	G
4	3	2610	A
4	3	2617	U
4	3	2618	C
4	3	2621	U
4	3	2623	U
4	3	2637	A
4	3	2638	G
4	3	2654	U
4	3	2668	A
4	3	2669	G
4	3	2697	C
4	3	2698	U
4	3	2722	G
4	3	2734	C
4	3	2737	G
4	3	2741	A
4	3	2752	G
4	3	2756	A
4	3	2760	C
4	3	2764	U
4	3	2765	A
4	3	2773	A
4	3	2786	A
4	3	2798	A
4	3	2799	U
4	3	2804	C
4	3	2806	A
4	3	2807	G
4	3	2808	A
4	3	2810	A
4	3	2813	A
4	3	2822	C
4	3	2824	A

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Mol	Chain	Res	Type
4	3	2829	G
4	3	2839	A
4	3	2853	U
4	3	2862	U
4	3	2863	G
4	3	2871	G
4	3	2876	G
4	3	2884	C
4	3	2887	A
4	3	2888	U
4	3	2895	A
4	3	2896	G
4	3	2899	C
5	4	9	C
5	4	10	C
5	4	11	A
5	4	13	G
5	4	14	U
5	4	22	G
5	4	23	A
5	4	28	C
5	4	33	U
5	4	35	C
5	4	39	U
5	4	41	C
5	4	48	A
5	4	49	G
5	4	54	U
5	4	56	A
5	4	60	C
5	4	64	G
5	4	65	G
5	4	80	G
5	4	82	U
5	4	83	U
5	4	84	C
5	4	85	A
5	4	88	G
5	4	89	A
5	4	99	A
5	4	106	A
5	4	108	C

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Mol	Chain	Res	Type
6	5	6	C
6	5	10	G
6	5	33	A
6	5	40	G
6	5	48	C
6	5	49	C
6	5	52	A
6	5	57	U
6	5	61	A
6	5	106	C
6	5	114	C
6	5	115	A
6	5	117	U
6	5	120	A
6	5	149	G
6	5	154	G
6	5	163	G
6	5	167	A
6	5	171	A
6	5	173	U
6	5	176	G
6	5	180	C
6	5	182	C
6	5	185	G
6	5	186	A
6	5	189	C
6	5	190	A
6	5	197	A
6	5	198	A
6	5	199	A
6	5	220	U
6	5	223	G
6	5	239	A
6	5	241	C
6	5	243	G
6	5	247	G
6	5	262	G
6	5	263	C
6	5	269	A
6	5	275	A
6	5	285	G
6	5	301	G

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Mol	Chain	Res	Type
6	5	302	A
6	5	324	C
6	5	325	A
6	5	326	C
6	5	328	G
6	5	341	C
6	5	342	G
6	5	344	G
6	5	347	G
6	5	348	C
6	5	350	G
6	5	359	A
6	5	363	U
6	5	368	C
6	5	369	A
6	5	370	A
6	5	374	G
6	5	380	G
6	5	383	U
6	5	394	U
6	5	408	U
6	5	416	U
6	5	418	U
6	5	419	A
6	5	422	A
6	5	425	G
6	5	426	U
6	5	447	G
6	5	449	A
6	5	450	U
6	5	452	A
6	5	461	G
6	5	462	G
6	5	464	A
6	5	468	G
6	5	470	U
6	5	475	U
6	5	476	U
6	5	477	U
6	5	481	U
6	5	482	G
6	5	488	U

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Mol	Chain	Res	Type
6	5	489	U
6	5	493	A
6	5	494	A
6	5	495	U
6	5	507	A
6	5	509	C
6	5	510	U
6	5	516	C
6	5	517	C
6	5	522	G
6	5	525	7MG
6	5	530	A
6	5	531	A
6	5	545	A
6	5	557	A
6	5	560	U
6	5	562	U
6	5	570	A
6	5	571	A
6	5	574	C
6	5	575	A
6	5	579	G
6	5	586	G
6	5	594	A
6	5	595	G
6	5	628	A
6	5	650	A
6	5	661	G
6	5	662	G
6	5	683	G
6	5	700	G
6	5	715	A
6	5	719	G
6	5	720	U
6	5	721	G
6	5	728	G
6	5	745	U
6	5	752	G
6	5	768	G
6	5	790	U
6	5	791	A
6	5	811	A

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Mol	Chain	Res	Type
6	5	812	A
6	5	814	C
6	5	818	A
6	5	825	A
6	5	829	G
6	5	836	C
6	5	838	A
6	5	839	U
6	5	867	A
6	5	883	A
6	5	885	U
6	5	908	A
6	5	910	C
6	5	911	G
6	5	921	G
6	5	922	G
6	5	929	C
6	5	930	A
6	5	955	U
6	5	964	A
6	5	970	A
6	5	971	A
6	5	972	A
6	5	982	A
6	5	987	U
6	5	988	G
6	5	989	A
6	5	994	C
6	5	995	U
6	5	996	U
6	5	997	G
6	5	998	G
6	5	999	C
6	5	1000	A
6	5	1002	A
6	5	1007	U
6	5	1009	G
6	5	1015	U
6	5	1018	U
6	5	1019	G
6	5	1020	G
6	5	1022	G

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Mol	Chain	Res	Type
6	5	1023	G
6	5	1024	U
6	5	1025	U
6	5	1027	A
6	5	1028	C
6	5	1029	C
6	5	1030	G
6	5	1032	G
6	5	1034	G
6	5	1036	C
6	5	1044	G
6	5	1047	U
6	5	1056	U
6	5	1072	G
6	5	1076	U
6	5	1078	G
6	5	1083	A
6	5	1085	G
6	5	1086	U
6	5	1092	A
6	5	1118	A
6	5	1121	U
6	5	1122	U
6	5	1123	G
6	5	1124	U
6	5	1134	C
6	5	1135	U
6	5	1141	U
6	5	1142	G
6	5	1158	A
6	5	1159	A
6	5	1170	C
6	5	1171	A
6	5	1172	A
6	5	1188	A
6	5	1189	U
6	5	1202	A
6	5	1203	A
6	5	1213	A
6	5	1215	U
6	5	1231	U
6	5	1232	C

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Mol	Chain	Res	Type
6	5	1233	G
6	5	1235	C
6	5	1255	A
6	5	1260	U
6	5	1271	U
6	5	1273	A
6	5	1274	G
6	5	1276	U
6	5	1279	G
6	5	1291	C
6	5	1294	U
6	5	1296	C
6	5	1297	G
6	5	1306	A
6	5	1312	G
6	5	1320	A
6	5	1321	G
6	5	1337	U
6	5	1338	A
6	5	1343	G
6	5	1345	G
6	5	1372	C
6	5	1373	A
6	5	1397	G
6	5	1417	U
6	5	1426	U
6	5	1427	U
6	5	1428	A
6	5	1429	G
6	5	1462	G
6	5	1466	U
6	5	1467	A
6	5	1469	G
6	5	1472	G
6	5	1478	A
6	5	1480	G
6	5	1481	U
6	5	1482	A
6	5	1492	G
6	5	1504	G
6	5	1505	G
6	5	1510	C

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Mol	Chain	Res	Type
6	5	1511	C
7	6	2	G
7	6	6	U
7	6	9	A
7	6	11	C
7	6	13	C
7	6	14	A
7	6	15	A
7	6	16	C
7	6	17	U
7	6	18	G
7	6	19	A
7	6	20	U
7	6	21	A
7	6	22	G
7	6	35	G
7	6	37	A
7	6	44	A
7	6	45	G
7	6	46	G
7	6	47	U
7	6	55	U
7	6	57	G
7	6	59	G
7	6	61	C
7	6	70	U
7	6	71	C
7	6	72	C
7	6	75	C
7	6	76	A
8	7	4	U
8	7	11	U
8	7	13	U
8	7	15	G
8	7	16	U
8	7	17	G
8	7	19	A
8	7	20	U
8	7	21	A
8	7	22	A
8	7	34	G
8	7	44	G

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Mol	Chain	Res	Type
8	7	46	U
8	7	47	U
8	7	48	G
8	7	51	G
8	7	57	A
8	7	71	C
8	7	73	C
8	7	75	A
9	8	3	A
9	8	9	A
9	8	10	G
9	8	15	G
9	8	16	U
9	8	17	U
9	8	18	G
9	8	19	G
9	8	20	U
9	8	21	A
9	8	30	G
9	8	31	A
9	8	41	A
9	8	46	G
9	8	47	U
9	8	48	C
9	8	58	A
9	8	60	C
9	8	71	G
9	8	73	A
9	8	74	C
9	8	75	C
9	8	76	A
31	Y	36	U
31	Y	37	G
31	Y	40	G
31	Y	42	U
31	Y	43	A
31	Y	46	G
31	Y	47	U
31	Y	49	U
31	Y	50	U
31	Y	51	C
31	Y	52	A

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Mol	Chain	Res	Type
31	Y	53	A
31	Y	54	A
31	Y	55	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	315	A
4	3	410	G
4	3	881	A
4	3	901	C
4	3	1124	G
4	3	1209	U
4	3	1352	G
4	3	1583	G
4	3	1618	U
4	3	2116	U
4	3	2117	G
4	3	2129	U
4	3	2130	A
4	3	2152	C
4	3	2165	A
4	3	2169	G
4	3	2182	C
4	3	2183	U
4	3	2184	A
4	3	2194	G
4	3	2764	U
6	5	196	G
6	5	994	C
6	5	995	U
6	5	1024	U
6	5	1123	G
6	5	1158	A
6	5	1273	A
7	6	17	U
7	6	18	G
7	6	46	G
7	6	54	U
7	6	58	A
7	6	71	C
8	7	10	G

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Mol	Chain	Res	Type
8	7	46	U
31	Y	42	U
31	Y	49	U
31	Y	51	C
31	Y	54	A

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

8 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
6	B8T	5	1377	6	19,22,23	3.30	8 (42%)	26,31,34	0.83	1 (3%)
6	5MC	5	1375	6	18,22,23	4.07	7 (38%)	26,32,35	1.02	2 (7%)
6	MA6	5	1493	6	18,26,27	1.07	2 (11%)	19,38,41	3.38	3 (15%)
4	2MA	3	2511	4,62	17,25,26	2.64	5 (29%)	17,37,40	1.32	3 (17%)
4	1MG	3	783	4	18,26,27	2.75	6 (33%)	19,39,42	1.47	3 (15%)
6	MA6	5	1494	6	18,26,27	1.06	2 (11%)	19,38,41	3.39	3 (15%)
4	OMG	3	2259	8,4,62	18,26,27	2.88	8 (44%)	19,38,41	1.60	4 (21%)
6	7MG	5	525	6	22,26,27	3.88	10 (45%)	29,39,42	2.03	9 (31%)

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
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2
6	MA6	5	1493	6	-	0/7/29/30	0/3/3/3
4	2MA	3	2511	4,62	-	2/3/25/26	0/3/3/3
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MA6	5	1494	6	-	3/7/29/30	0/3/3/3
4	OMG	3	2259	8,4,62	-	3/5/27/28	0/3/3/3
6	7MG	5	525	6	-	2/7/37/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1375	5MC	C6-C5	10.02	1.51	1.34
6	5	525	7MG	C8-N9	9.81	1.51	1.46
6	5	525	7MG	C5-N7	8.01	1.44	1.35
4	3	2511	2MA	C2-N3	7.90	1.48	1.31
6	5	1375	5MC	C4-N3	7.54	1.46	1.34
6	5	1377	B8T	C4-N3	7.26	1.45	1.32
4	3	2259	OMG	C2-N2	7.23	1.51	1.34
6	5	1375	5MC	C2-N3	7.04	1.50	1.36
4	3	783	1MG	C2-N3	6.91	1.47	1.34
6	5	1377	B8T	C2-N3	6.48	1.49	1.36
4	3	783	1MG	C2-N2	6.43	1.45	1.34
6	5	1377	B8T	C6-C5	6.07	1.49	1.35
6	5	525	7MG	C2-N3	5.87	1.47	1.33
6	5	525	7MG	C4-N9	5.73	1.44	1.37
6	5	1375	5MC	C4-N4	5.71	1.49	1.34
6	5	1375	5MC	C6-N1	5.60	1.47	1.38
6	5	525	7MG	C4-N3	5.55	1.47	1.34
4	3	2259	OMG	C2-N3	5.27	1.46	1.33
4	3	2511	2MA	C4-N3	5.12	1.49	1.37
4	3	783	1MG	C4-N3	5.11	1.49	1.37
6	5	1377	B8T	C4-N4	4.79	1.45	1.35
6	5	525	7MG	C2-N2	4.77	1.45	1.34
4	3	2259	OMG	C4-N3	4.63	1.48	1.37
6	5	1375	5MC	C2-N1	4.57	1.49	1.40
6	5	1377	B8T	C2-N1	4.31	1.49	1.40
6	5	1377	B8T	C5-C4	3.90	1.49	1.40
6	5	525	7MG	C2-N1	3.84	1.47	1.37
6	5	525	7MG	C5-C6	3.59	1.52	1.43
6	5	525	7MG	C6-N1	3.42	1.45	1.38
4	3	2259	OMG	C2-N1	3.32	1.45	1.37
4	3	2511	2MA	C6-N1	3.18	1.44	1.38
6	5	1377	B8T	C6-N1	3.14	1.45	1.38
4	3	2259	OMG	C6-N1	3.13	1.42	1.37
4	3	2259	OMG	C5-C6	3.10	1.53	1.47
4	3	2511	2MA	C2-N1	2.75	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1493	MA6	C2-N3	2.69	1.36	1.32
6	5	1494	MA6	C2-N3	2.67	1.36	1.32
6	5	1377	B8T	O2-C2	-2.66	1.18	1.23
6	5	525	7MG	O6-C6	-2.45	1.18	1.23
4	3	783	1MG	C6-N1	2.43	1.43	1.39
4	3	2259	OMG	C5-C4	-2.36	1.37	1.43
4	3	783	1MG	C5-C4	-2.35	1.37	1.43
4	3	783	1MG	C5-C6	2.29	1.54	1.47
6	5	1493	MA6	C5-C4	-2.25	1.35	1.40
6	5	1494	MA6	C5-C4	-2.24	1.35	1.40
6	5	1375	5MC	O2-C2	-2.22	1.19	1.23
4	3	2511	2MA	C5-C4	-2.18	1.37	1.43
4	3	2259	OMG	C8-N7	2.11	1.38	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1494	MA6	N1-C6-N6	-12.26	104.16	117.06
6	5	1493	MA6	N1-C6-N6	-12.20	104.22	117.06
6	5	1493	MA6	C1'-N9-C4	5.62	136.51	126.64
6	5	1494	MA6	C1'-N9-C4	5.54	136.38	126.64
6	5	1494	MA6	N3-C2-N1	-5.53	120.03	128.68
6	5	1493	MA6	N3-C2-N1	-5.51	120.07	128.68
6	5	525	7MG	C5-C6-N1	4.98	119.77	110.99
6	5	525	7MG	C2-N3-C4	4.50	120.31	112.30
6	5	525	7MG	C5-C4-N3	-4.08	120.36	128.13
4	3	783	1MG	C5-C6-N1	4.05	119.99	113.90
4	3	2259	OMG	C5-C6-N1	3.48	120.09	113.95
4	3	2511	2MA	C5-C6-N1	3.35	119.81	114.02
6	5	1375	5MC	C5-C6-N1	-3.24	120.01	123.34
6	5	525	7MG	C5-C4-N9	3.08	110.35	106.35
6	5	525	7MG	C4-C5-N7	3.07	109.79	105.53
4	3	2259	OMG	C8-N7-C5	3.00	108.70	102.99
4	3	2259	OMG	C2-N1-C6	-2.97	119.62	125.10
6	5	525	7MG	C2-N1-C6	-2.82	119.96	125.10
6	5	525	7MG	O6-C6-C5	-2.81	120.64	127.54
4	3	783	1MG	C8-N7-C5	2.69	108.11	102.99
4	3	2511	2MA	C8-N7-C5	2.66	108.06	102.99
6	5	525	7MG	N9-C4-N3	2.55	129.28	125.47
6	5	1377	B8T	C6-C5-C4	2.46	119.97	116.96
4	3	783	1MG	O6-C6-C5	-2.33	120.06	124.19
6	5	525	7MG	N9-C8-N7	2.31	106.68	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2511	2MA	CM2-C2-N1	2.14	120.98	116.23
6	5	1375	5MC	CM5-C5-C6	-2.11	120.03	122.85
4	3	2259	OMG	O6-C6-C5	-2.10	120.27	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-C4'-C5'-O5'
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	525	7MG	O4'-C4'-C5'-O5'
6	5	525	7MG	C3'-C4'-C5'-O5'
6	5	1494	MA6	O4'-C4'-C5'-O5'
6	5	1494	MA6	C3'-C4'-C5'-O5'
6	5	1494	MA6	C5-C6-N6-C10
6	5	1377	B8T	O4'-C4'-C5'-O5'
4	3	2511	2MA	O4'-C4'-C5'-O5'
6	5	1377	B8T	C3'-C4'-C5'-O5'
4	3	2511	2MA	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 369 ligands modelled in this entry, 333 are monoatomic - leaving 36 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
67	LYS	8	103	9	7,8,9	0.84	0	3,8,10	0.35	0
64	SPM	3	3251	-	13,13,13	0.36	0	12,12,12	0.90	0
65	SPD	3	3235	-	9,9,9	0.32	0	8,8,8	0.87	0
65	SPD	3	3240	-	9,9,9	0.33	0	8,8,8	0.86	0
64	SPM	3	3229	-	13,13,13	0.36	0	12,12,12	0.90	0
65	SPD	3	3234	-	9,9,9	0.35	0	8,8,8	0.79	0
65	SPD	3	3252	-	9,9,9	0.18	0	8,8,8	0.19	0
65	SPD	3	3242	-	9,9,9	0.32	0	8,8,8	0.86	0
63	PUT	3	3244	-	5,5,5	0.25	0	4,4,4	0.54	0
65	SPD	3	3230	-	9,9,9	0.33	0	8,8,8	0.87	0
65	SPD	3	3232	-	9,9,9	0.33	0	8,8,8	0.83	0
63	PUT	5	1604	-	5,5,5	0.25	0	4,4,4	0.54	0
66	N2P	3	3246	-	6,6,6	0.25	0	5,5,5	0.65	0
64	SPM	3	3243	-	13,13,13	0.34	0	12,12,12	0.91	0
63	PUT	3	3225	-	5,5,5	0.24	0	4,4,4	0.54	0
66	N2P	3	3249	-	6,6,6	0.25	0	5,5,5	0.65	0
63	PUT	3	3233	-	5,5,5	0.25	0	4,4,4	0.53	0
65	SPD	3	3241	-	9,9,9	0.32	0	8,8,8	0.85	0
66	N2P	3	3245	-	6,6,6	0.25	0	5,5,5	0.65	0
65	SPD	5	1601	-	9,9,9	0.41	0	8,8,8	1.41	2 (25%)
63	PUT	3	3227	-	5,5,5	0.25	0	4,4,4	0.53	0
65	SPD	3	3247	-	9,9,9	0.33	0	8,8,8	0.89	0
64	SPM	b	303	-	13,13,13	0.16	0	12,12,12	0.32	0
65	SPD	3	3250	-	9,9,9	0.33	0	8,8,8	0.86	0
65	SPD	5	1603	-	9,9,9	0.32	0	8,8,8	0.74	0
65	SPD	3	3238	-	9,9,9	0.33	0	8,8,8	0.90	0
60	CLM	3	3001	-	19,20,20	2.06	2 (10%)	23,27,27	0.86	1 (4%)
66	N2P	5	1602	-	6,6,6	0.25	0	5,5,5	0.65	0
65	SPD	3	3231	-	9,9,9	0.32	0	8,8,8	0.90	0
65	SPD	3	3248	-	9,9,9	0.32	0	8,8,8	0.87	0
63	PUT	3	3224	-	5,5,5	0.25	0	4,4,4	0.54	0
65	SPD	3	3237	-	9,9,9	0.33	0	8,8,8	0.87	0
63	PUT	3	3226	-	5,5,5	0.25	0	4,4,4	0.54	0
65	SPD	3	3239	-	9,9,9	0.33	0	8,8,8	0.91	0
65	SPD	3	3236	-	9,9,9	0.32	0	8,8,8	0.78	0
63	PUT	3	3228	-	5,5,5	0.26	0	4,4,4	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	LYS	8	103	9	-	3/6/7/9	-
64	SPM	3	3251	-	-	2/11/11/11	-
65	SPD	3	3235	-	-	0/7/7/7	-
65	SPD	3	3240	-	-	0/7/7/7	-
64	SPM	3	3229	-	-	4/11/11/11	-
65	SPD	3	3234	-	-	1/7/7/7	-
65	SPD	3	3252	-	-	0/7/7/7	-
65	SPD	3	3242	-	-	0/7/7/7	-
63	PUT	3	3244	-	-	0/3/3/3	-
65	SPD	3	3230	-	-	0/7/7/7	-
65	SPD	3	3232	-	-	0/7/7/7	-
63	PUT	5	1604	-	-	0/3/3/3	-
66	N2P	3	3246	-	-	2/4/4/4	-
64	SPM	3	3243	-	-	2/11/11/11	-
63	PUT	3	3225	-	-	0/3/3/3	-
66	N2P	3	3249	-	-	1/4/4/4	-
63	PUT	3	3233	-	-	0/3/3/3	-
65	SPD	3	3241	-	-	2/7/7/7	-
66	N2P	3	3245	-	-	1/4/4/4	-
65	SPD	5	1601	-	-	1/7/7/7	-
63	PUT	3	3227	-	-	1/3/3/3	-
65	SPD	3	3247	-	-	0/7/7/7	-
64	SPM	b	303	-	-	2/11/11/11	-
65	SPD	3	3250	-	-	0/7/7/7	-
65	SPD	5	1603	-	-	1/7/7/7	-
65	SPD	3	3238	-	-	0/7/7/7	-
60	CLM	3	3001	-	-	3/20/22/22	0/1/1/1
66	N2P	5	1602	-	-	3/4/4/4	-
65	SPD	3	3231	-	-	1/7/7/7	-
65	SPD	3	3248	-	-	0/7/7/7	-
63	PUT	3	3224	-	-	0/3/3/3	-
65	SPD	3	3237	-	-	0/7/7/7	-
63	PUT	3	3226	-	-	0/3/3/3	-
65	SPD	3	3239	-	-	1/7/7/7	-
65	SPD	3	3236	-	-	1/7/7/7	-
63	PUT	3	3228	-	-	0/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	3	3001	CLM	C2-N2	7.20	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	3	3001	CLM	O9B-N9	-2.68	1.18	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	5	1601	SPD	C4-C3-C2	-2.25	97.82	113.77
65	5	1601	SPD	C4-C5-N6	-2.07	106.56	112.14
60	3	3001	CLM	C3-N2-C2	-2.06	119.42	123.07

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	8	103	LYS	O-C-CA-CB
67	8	103	LYS	N-CA-CB-CG
67	8	103	LYS	C-CA-CB-CG
65	5	1603	SPD	C8-C7-N6-C5
66	3	3245	N2P	C2-C3-C4-C5
66	5	1602	N2P	C2-C3-C4-C5
64	3	3229	SPM	C7-C8-C9-N10
65	3	3231	SPD	N6-C7-C8-C9
64	3	3243	SPM	C7-C6-N5-C4
66	3	3249	N2P	C2-C3-C4-C5
66	3	3246	N2P	C2-C3-C4-C5
64	3	3251	SPM	C6-C7-C8-C9
65	3	3236	SPD	C8-C7-N6-C5
64	3	3229	SPM	C7-C6-N5-C4
66	5	1602	N2P	C3-C4-C5-N1
65	3	3234	SPD	N1-C2-C3-C4
63	3	3227	PUT	C1-C2-C3-C4
60	3	3001	CLM	N2-C3-C4-O4
65	3	3241	SPD	C8-C7-N6-C5
65	5	1601	SPD	N1-C2-C3-C4
65	3	3239	SPD	C8-C7-N6-C5
64	3	3229	SPM	N10-C11-C12-C13
64	3	3243	SPM	N10-C11-C12-C13
64	b	303	SPM	C3-C4-N5-C6
66	3	3246	N2P	C3-C4-C5-N1
66	5	1602	N2P	NE2-C1-C2-C3
65	3	3241	SPD	C2-C3-C4-C5
60	3	3001	CLM	C5-C3-N2-C2
64	b	303	SPM	C7-C6-N5-C4

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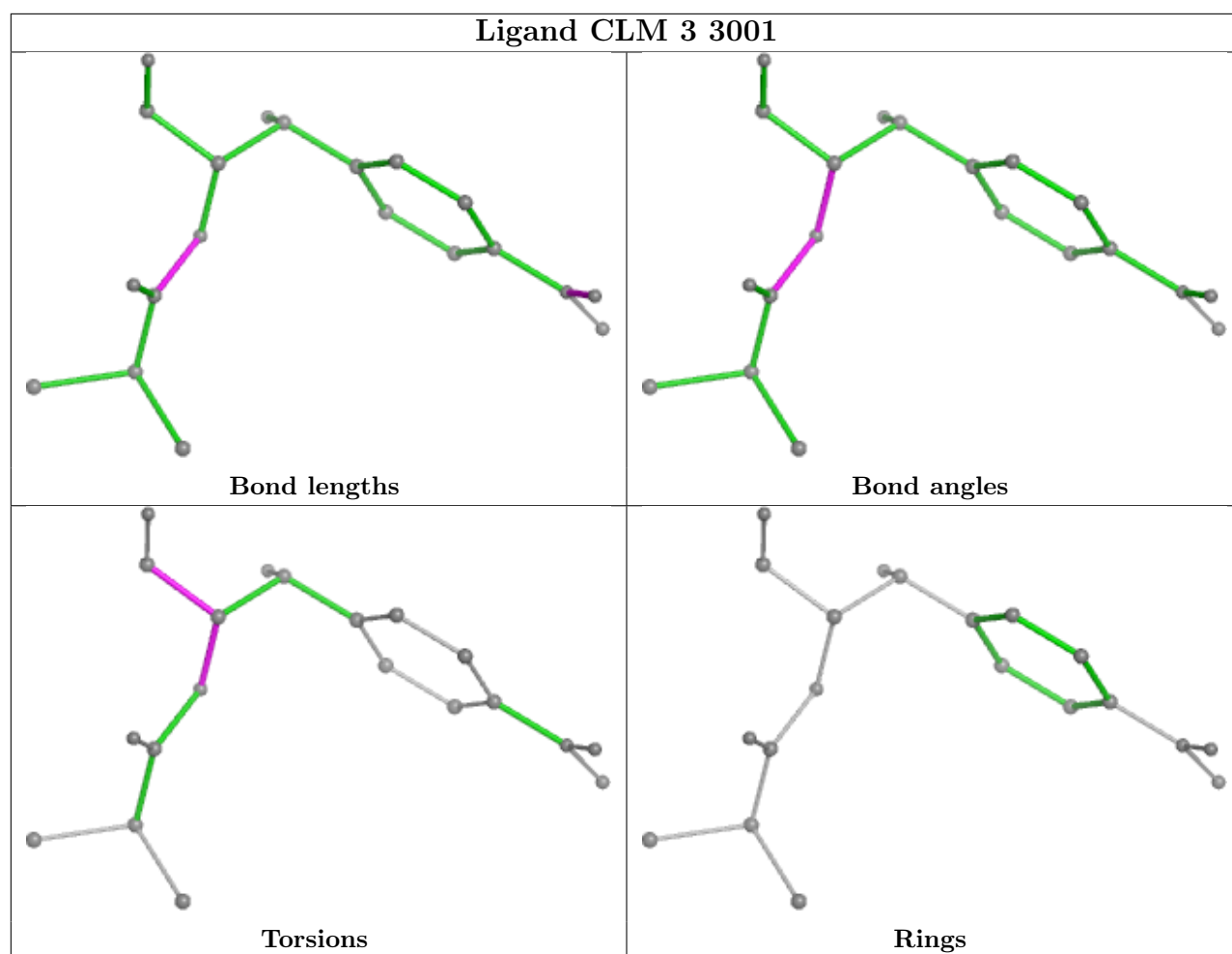
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Mol	Chain	Res	Type	Atoms
64	3	3229	SPM	C6-C7-C8-C9
60	3	3001	CLM	C5-C3-C4-O4
64	3	3251	SPM	C7-C8-C9-N10

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.