



Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:33 pm GMT

PDB ID : 8P8V
EMDB ID : EMD-17145
Title : Mycoplasma pneumoniae di-ribosome in chloramphenicol-treated cells (leading 70S)
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-06-02
Resolution : 8.70 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:

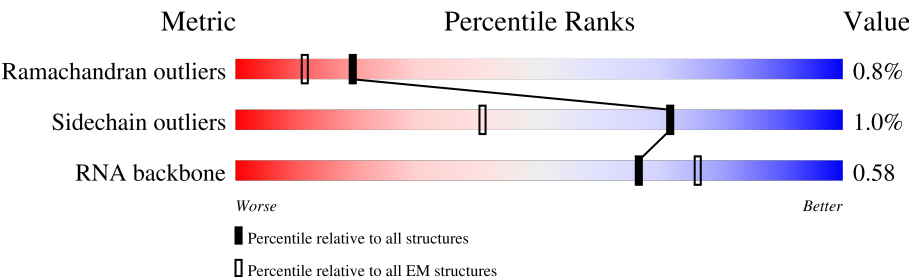
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance i

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

The reported resolution of this entry is 8.70 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.



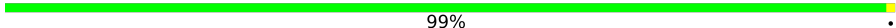


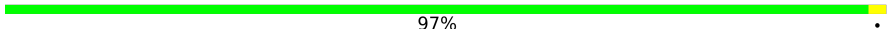


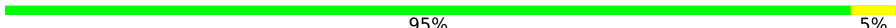
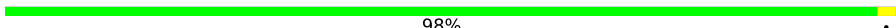

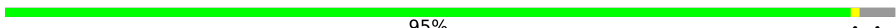

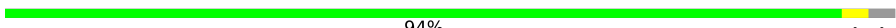
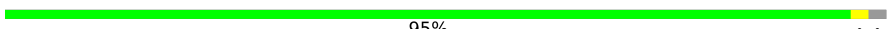
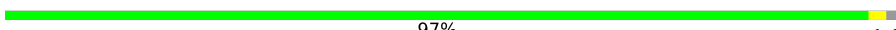
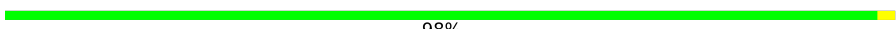

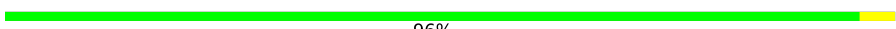

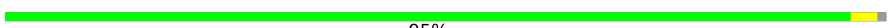

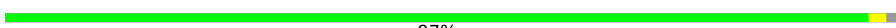

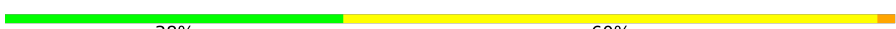


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	


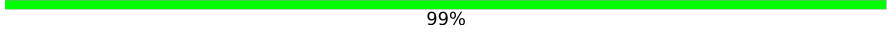
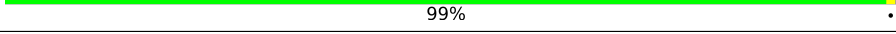
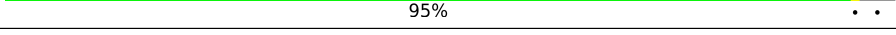
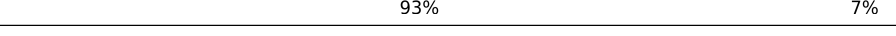
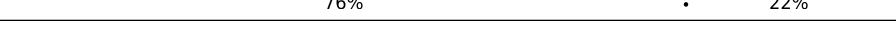
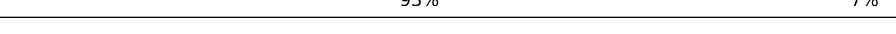
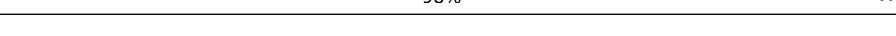
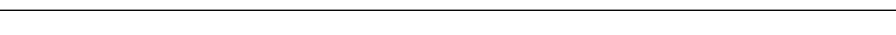

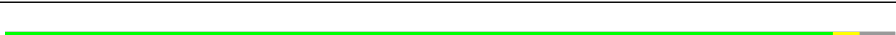



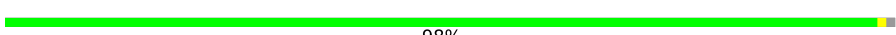


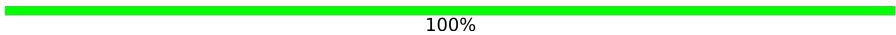

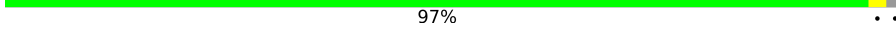
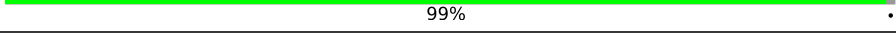

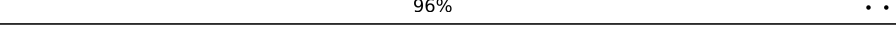
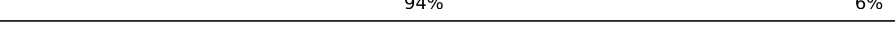

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Mol	Chain	Length	Quality of chain
10	9	226	 99%
11	A	294	 89% 9%
12	B	273	 81% 18%
13	C	205	 97%
14	D	219	 71% 28%
15	E	215	 94% 5%
16	F	155	 95% 5%
17	G	142	 98%
18	H	132	 93% 5%
19	I	108	 95%
20	J	121	 93% 6%
21	K	139	 94%
22	L	124	 95%
23	M	61	 97%
24	N	86	 98%
25	O	94	 87% 7%
26	P	85	 96%
27	Q	104	 67% 30%
28	R	87	 95%
29	S	87	 87% 9%
30	T	60	 97%
31	X	444	 7% 93%
32	Y	40	 38% 60%
33	Z	36	 100%
34	a	287	 97%

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Mol	Chain	Length	Quality of chain
35	b	287	
36	c	212	
37	d	180	
38	e	184	
39	f	149	
40	g	161	
41	h	137	
42	i	146	
43	j	122	
44	k	151	
45	l	139	
46	m	124	
47	n	116	
48	o	119	
49	p	127	
50	q	100	
51	r	159	
52	s	237	
53	t	111	
54	u	104	
55	v	65	
56	w	111	
57	x	97	
58	y	57	
59	z	53	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153622 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	47	Total	C	N	O	S	0	0
			380	236	81	61	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	1506	Total	C	N	O	P	0	0
			32238	14411	5844	10477	1506		

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 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	226	Total	C	N	O	S	0	0
			1711	1095	292	318	6		

- Molecule 11 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	268	Total	C	N	O	S	0	0
			2152	1368	379	396	9		

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	224	Total	C	N	O	S	0	0
			1764	1116	326	317	5		

- Molecule 13 is a protein called 30S ribosomal protein S4.

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

- Molecule 14 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	158	Total	C	N	O	S	0	0
			1217	771	232	211	3		

- Molecule 15 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	215	Total	C	N	O	S	0	0
			1793	1111	341	339	2		

- Molecule 16 is a protein called 30S ribosomal protein S7.

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

- Molecule 17 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	142	Total	C	N	O	S	0	0
			1118	728	194	193	3		

- Molecule 18 is a protein called 30S ribosomal protein S9.

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

- Molecule 19 is a protein called 30S ribosomal protein S10.

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

- Molecule 20 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	120	Total	C	N	O	S	0	0
			878	547	163	162	6		

- Molecule 21 is a protein called 30S ribosomal protein S12.

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

- Molecule 22 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	121	Total	C	N	O		0	0
			975	609	197	169			

- Molecule 23 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 24 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	86	Total	C	N	O	S	0	0
			697	441	131	124	1		

- Molecule 25 is a protein called 30S ribosomal protein S16.

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

- Molecule 26 is a protein called 30S ribosomal protein S17.

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

- Molecule 27 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	73	Total	C	N	O	S	0	0
			605	389	117	95	4		

- Molecule 28 is a protein called 30S ribosomal protein S19.

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

- Molecule 29 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 31 is a protein called Trigger factor.

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

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	40	Total	C	N	O	P	0	0
			862	388	170	264	40		

- Molecule 33 is a protein called Nascent chain.

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

- Molecule 34 is a protein called 50S ribosomal protein L2.

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

- Molecule 35 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	229	Total	C	N	O	S	0	0
			1762	1119	318	318	7		

- Molecule 36 is a protein called 50S ribosomal protein L4.

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

- Molecule 37 is a protein called 50S ribosomal protein L5.

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

- Molecule 38 is a protein called 50S ribosomal protein L6.

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

- Molecule 39 is a protein called 50S ribosomal protein L9.

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

- Molecule 40 is a protein called 50S ribosomal protein L10.

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

- Molecule 41 is a protein called 50S ribosomal protein L11.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

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

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L27.

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

- Molecule 55 is a protein called 50S ribosomal protein L28.

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

- Molecule 56 is a protein called 50S ribosomal protein L29.

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

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	89	Total	C	N	O	S	0	0
			708	449	124	131	4		

- Molecule 58 is a protein called 50S ribosomal protein L32.

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

- Molecule 59 is a protein called 50S ribosomal protein L33 1.

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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

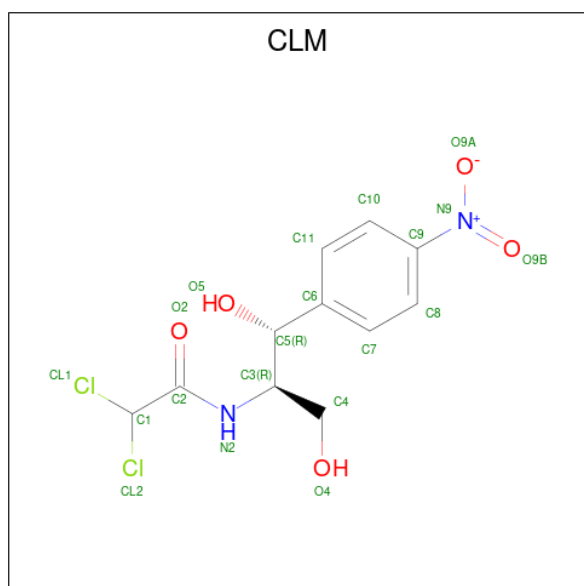
Mol	Chain	Residues	Atoms		AltConf
60	2	1	Total	Zn	0
			1	1	
60	M	1	Total	Zn	0
			1	1	
60	Q	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
60	x	1	Total	Zn	0
			1	1	
60	y	1	Total	Zn	0
			1	1	
60	z	1	Total	Zn	0
			1	1	

- Molecule 61 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
61	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
62	3	1	Total	K	0
			1	1	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

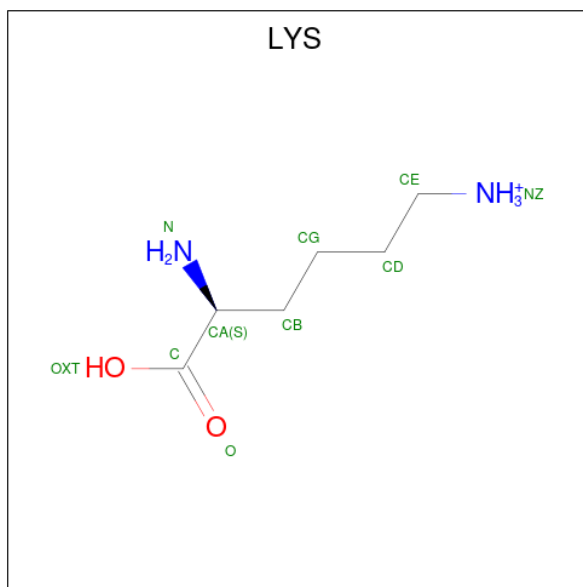
Mol	Chain	Residues	Atoms		AltConf
63	3	209	Total	Mg	0
			209	209	

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Mol	Chain	Residues	Atoms		AltConf
63	4	1	Total 1	Mg 1	0
63	5	87	Total 87	Mg 87	0
63	6	1	Total 1	Mg 1	0
63	8	1	Total 1	Mg 1	0
63	E	1	Total 1	Mg 1	0
63	K	1	Total 1	Mg 1	0
63	L	1	Total 1	Mg 1	0
63	P	1	Total 1	Mg 1	0
63	Y	2	Total 2	Mg 2	0
63	a	1	Total 1	Mg 1	0
63	b	1	Total 1	Mg 1	0
63	f	12	Total 12	Mg 12	0
63	i	1	Total 1	Mg 1	0
63	y	2	Total 2	Mg 2	0

- Molecule 64 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
64	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:  96% 



- Molecule 2: 50S ribosomal protein L35

Chain 1:  98% 




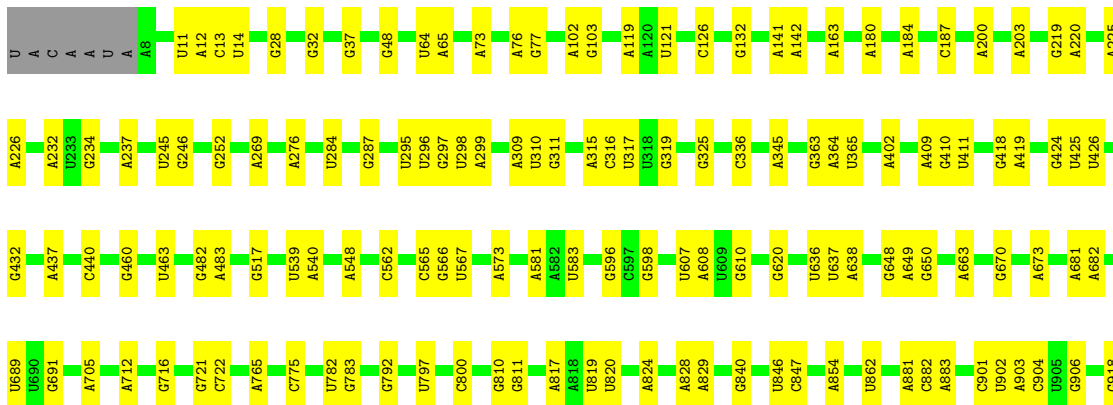
- Molecule 3: 50S ribosomal protein L36

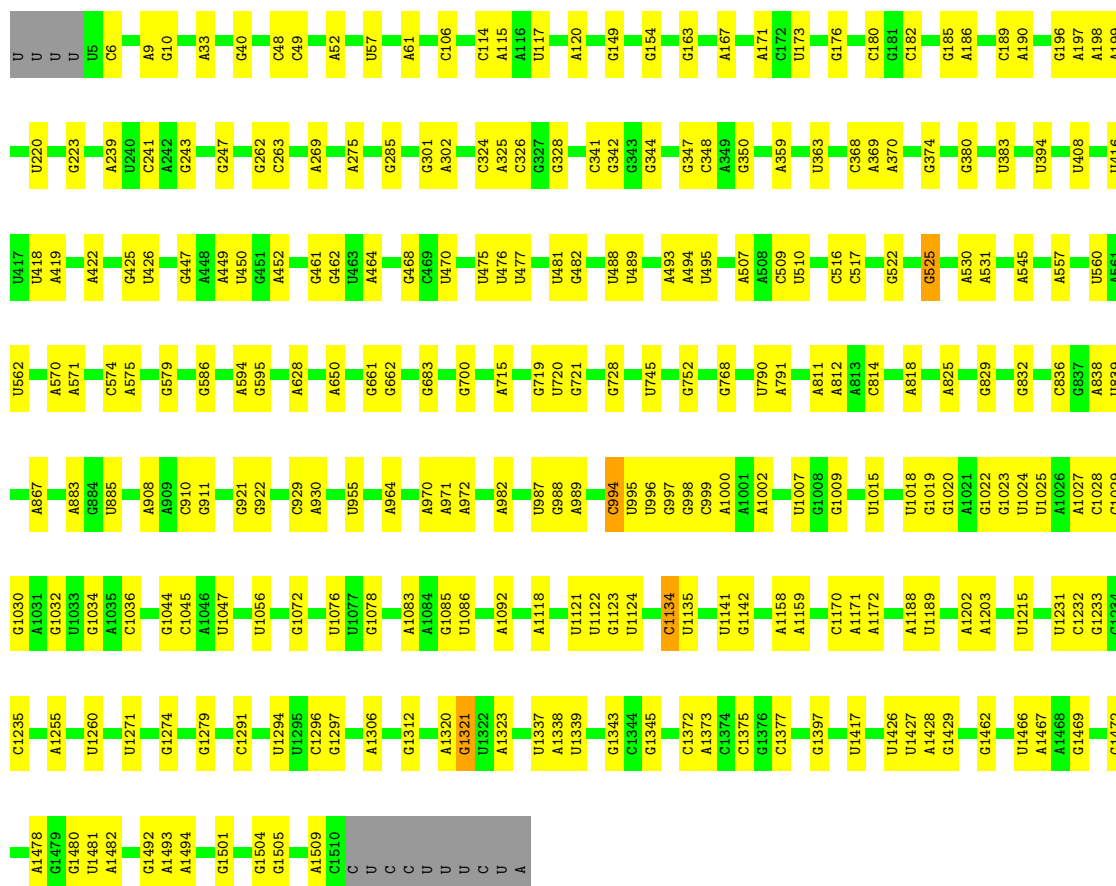
Chain 2:  97% 



- Molecule 4: 23S ribosomal RNA

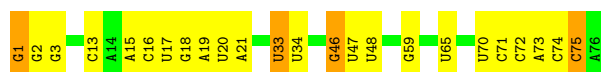
Chain 3:  81% 19%





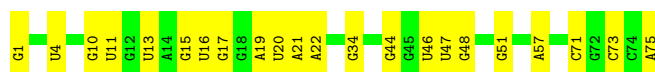
• Molecule 7: tRNA-Ala (E-site)

Chain 6: 68% 26% 5%



• Molecule 8: tRNA-Asp (P-site)

Chain 7: 71% 29%



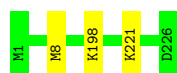
• Molecule 9: tRNA-Lys (A-site)

Chain 8: 70% 29%



• Molecule 10: 50S ribosomal protein L1

Chain 9: 99%



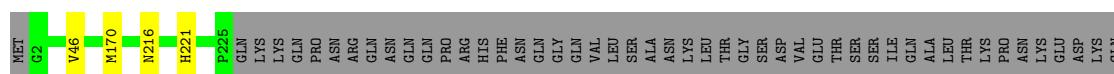
- Molecule 11: 30S ribosomal protein S2

Chain A: 89% 9%



- Molecule 12: 30S ribosomal protein S3

Chain B: 81% 18%



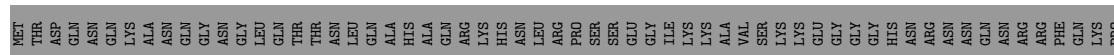
- Molecule 13: 30S ribosomal protein S4

Chain C: 97% 0%



- Molecule 14: 30S ribosomal protein S5

Chain D: 71% 28%



- Molecule 15: 30S ribosomal protein S6

Chain E: 94% 5%



- Molecule 16: 30S ribosomal protein S7

Chain F: 95% 5%



- Molecule 17: 30S ribosomal protein S8

Chain G:  98% .



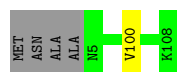
- Molecule 18: 30S ribosomal protein S9

Chain H:  93% 5% .



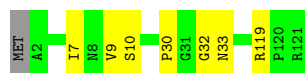
- Molecule 19: 30S ribosomal protein S10

Chain I:  95% . .



- Molecule 20: 30S ribosomal protein S11

Chain J:  93% 6% .



- Molecule 21: 30S ribosomal protein S12

Chain K:  94% . .



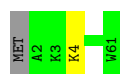
- Molecule 22: 30S ribosomal protein S13

Chain L:  95% . .



- Molecule 23: 30S ribosomal protein S14 type Z

Chain M:  97% . .




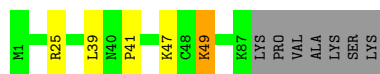
- Molecule 24: 30S ribosomal protein S15

Chain N:  98% .



- Molecule 25: 30S ribosomal protein S16

Chain O:  87% . . 7%



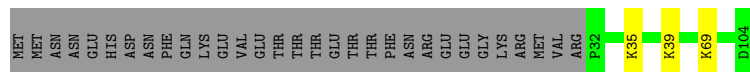
- Molecule 26: 30S ribosomal protein S17

Chain P:  96% .



- Molecule 27: 30S ribosomal protein S18

Chain Q:  67% . 30%




- Molecule 28: 30S ribosomal protein S19

Chain R:  95% . .



- Molecule 29: 30S ribosomal protein S20

Chain S:  87% . 9%



- Molecule 30: 30S ribosomal protein S21

Chain T:  97% . .



- Molecule 31: Trigger factor

Chain c:  99%



- Molecule 37: 50S ribosomal protein L5

Chain d:  99%



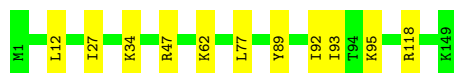
- Molecule 38: 50S ribosomal protein L6

Chain e:  95%




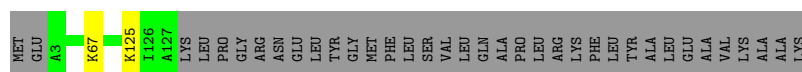
- Molecule 39: 50S ribosomal protein L9

Chain f:  93%



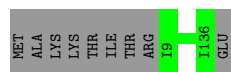
- Molecule 40: 50S ribosomal protein L10

Chain g:  76%



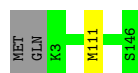
- Molecule 41: 50S ribosomal protein L11

Chain h:  93%



- Molecule 42: 50S ribosomal protein L13

Chain i:  98%



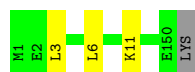
- Molecule 43: 50S ribosomal protein L14

Chain j:  97% ..



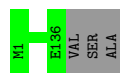
- Molecule 44: 50S ribosomal protein L15

Chain k:  97% ..



- Molecule 45: 50S ribosomal protein L16

Chain l:  98% .



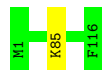
- Molecule 46: 50S ribosomal protein L17

Chain m:  93% . .



- Molecule 47: 50S ribosomal protein L18

Chain n:  99% .




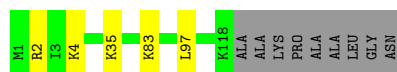
- Molecule 48: 50S ribosomal protein L19

Chain o:  97% ..



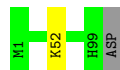
- Molecule 49: 50S ribosomal protein L20

Chain p:  89% . 7%




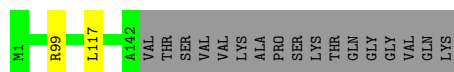
- Molecule 50: 50S ribosomal protein L21

Chain q:  98% ..



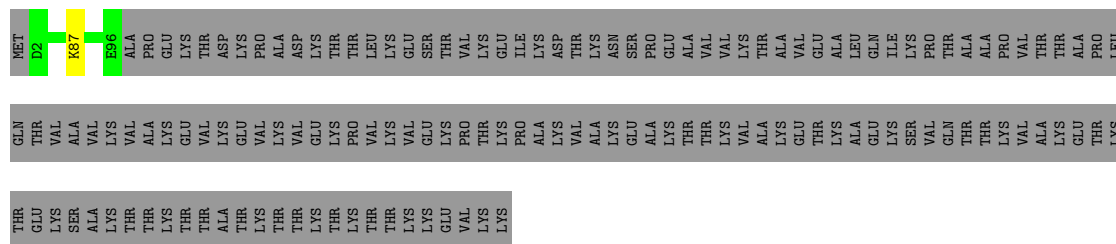
- Molecule 51: 50S ribosomal protein L22

Chain r:  88% • 11%



- Molecule 52: 50S ribosomal protein L23

Chain s:  40% 60%




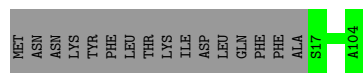
- Molecule 53: 50S ribosomal protein L24

Chain t:  100%

There are no outlier residues recorded for this chain.

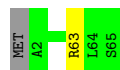
- Molecule 54: 50S ribosomal protein L27

Chain u:  85% 15%



- Molecule 55: 50S ribosomal protein L28

Chain v:  97% • •




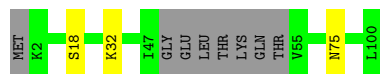
- Molecule 56: 50S ribosomal protein L29

Chain w:  99% •



- Molecule 57: 50S ribosomal protein L31

Chain x:  89% • 8%



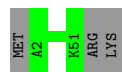
- Molecule 58: 50S ribosomal protein L32

Chain y:  96% • •



- Molecule 59: 50S ribosomal protein L33 1

Chain z:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	963	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: B8T, MA6, K, ZN, 2MA, 7MG, 1MG, 5MC, OMG, CLM, MG

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	0.26	0/383	0.67	0/504
2	1	0.27	0/484	0.68	1/637 (0.2%)
3	2	0.25	0/306	0.65	0/401
4	3	0.20	1/69363 (0.0%)	0.73	10/108161 (0.0%)
5	4	0.17	0/2578	0.72	0/4016
6	5	0.20	0/35970	0.73	14/56077 (0.0%)
7	6	0.34	1/1810 (0.1%)	0.84	4/2817 (0.1%)
8	7	0.35	1/1785 (0.1%)	0.79	0/2779
9	8	0.49	3/1804 (0.2%)	1.03	8/2807 (0.3%)
10	9	0.28	0/1735	0.61	2/2337 (0.1%)
11	A	0.32	0/2186	0.65	0/2952
12	B	0.27	0/1791	0.64	1/2421 (0.0%)
13	C	0.32	0/1700	0.71	0/2278
14	D	0.27	0/1233	0.65	0/1651
15	E	0.36	0/1824	0.77	3/2454 (0.1%)
16	F	0.33	0/1274	0.77	2/1710 (0.1%)
17	G	0.32	0/1134	0.74	2/1527 (0.1%)
18	H	0.33	0/1056	0.75	2/1409 (0.1%)
19	I	0.27	0/843	0.67	0/1132
20	J	0.30	0/893	0.68	1/1198 (0.1%)
21	K	0.27	0/1089	0.66	0/1461
22	L	0.30	0/986	0.70	0/1321
23	M	0.30	0/483	0.67	0/643
24	N	0.26	0/703	0.64	0/936
25	O	0.28	0/718	0.75	2/962 (0.2%)
26	P	0.29	0/702	0.76	1/934 (0.1%)
27	Q	0.37	0/617	0.81	1/823 (0.1%)
28	R	0.33	0/716	0.73	2/958 (0.2%)
29	S	0.27	0/645	0.68	1/857 (0.1%)
30	T	0.36	0/524	0.82	1/685 (0.1%)
31	X	0.31	0/245	0.74	0/325
32	Y	0.31	0/969	0.91	1/1508 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.75	0/26	1.33	0/33
34	a	0.29	0/2267	0.67	3/3044 (0.1%)
35	b	0.30	0/1795	0.69	0/2412
36	c	0.29	0/1681	0.64	2/2257 (0.1%)
37	d	0.30	0/1437	0.67	1/1931 (0.1%)
38	e	0.29	0/1420	0.64	0/1912
39	f	0.44	0/1233	0.64	0/1653
40	g	0.27	0/960	0.57	0/1284
41	h	0.26	0/968	0.54	0/1298
42	i	0.27	0/1186	0.62	1/1592 (0.1%)
43	j	0.70	2/953 (0.2%)	1.26	8/1275 (0.6%)
44	k	0.31	0/1187	0.73	2/1581 (0.1%)
45	l	0.30	0/1104	0.66	0/1481
46	m	0.31	0/973	0.72	1/1309 (0.1%)
47	n	0.31	0/927	0.66	0/1239
48	o	0.36	0/976	0.74	0/1296
49	p	0.29	0/996	0.69	1/1325 (0.1%)
50	q	0.31	0/828	0.66	0/1111
51	r	0.27	0/1100	0.64	1/1471 (0.1%)
52	s	0.31	0/752	0.61	0/1015
53	t	0.31	0/878	0.62	0/1165
54	u	0.30	0/678	0.66	0/902
55	v	0.26	0/526	0.72	0/703
56	w	0.27	0/916	0.66	0/1222
57	x	0.28	0/722	0.59	0/959
58	y	0.30	0/457	0.81	1/601 (0.2%)
59	z	0.26	0/412	0.64	0/547
All	All	0.25	8/165907 (0.0%)	0.73	80/247299 (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
34	a	0	1
39	f	0	1
55	v	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	76	A	C6-N6	15.01	1.46	1.33
43	j	93	PRO	CB-CG	14.81	2.23	1.50
43	j	93	PRO	CG-CD	-11.35	1.13	1.50
7	6	1	G	OP3-P	-10.61	1.48	1.61
8	7	1	G	OP3-P	-10.59	1.48	1.61
9	8	76	A	N7-C5	-6.67	1.35	1.39
9	8	76	A	N9-C8	-6.21	1.32	1.37
4	3	2259	OMG	O3'-P	-5.78	1.54	1.61

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	76	A	C2-N3-C4	22.23	121.71	110.60
43	j	93	PRO	CA-N-CD	-22.00	80.69	111.50
43	j	93	PRO	CB-CG-CD	-19.32	31.15	106.50
9	8	76	A	N1-C2-N3	-15.24	121.68	129.30
43	j	92	SER	C-N-CD	13.36	156.45	128.40
43	j	93	PRO	N-CD-CG	13.17	122.96	103.20
9	8	76	A	N3-C4-C5	-12.79	117.84	126.80
9	8	76	A	N3-C4-N9	10.23	135.58	127.40
9	8	76	A	N7-C8-N9	-9.52	109.04	113.80
44	k	6	LEU	CA-CB-CG	9.37	136.86	115.30
9	8	76	A	C5-N7-C8	9.23	108.52	103.90
37	d	16	LEU	CA-CB-CG	8.31	134.41	115.30
16	F	69	MET	CA-CB-CG	8.07	127.02	113.30
9	8	76	A	C8-N9-C4	7.70	108.88	105.80
49	p	97	LEU	CA-CB-CG	7.67	132.94	115.30
6	5	1323	A	C5-C6-N1	7.62	121.51	117.70
4	3	32	G	O5'-P-OP1	-7.58	98.88	105.70
9	8	76	A	C4-C5-N7	-7.42	106.99	110.70
10	9	198	LYS	CB-CG-CD	7.41	130.87	111.60
6	5	1323	A	O4'-C1'-N9	-7.25	102.40	108.20
4	3	1486	U	C2-N1-C1'	7.23	126.37	117.70
17	G	54	LEU	CA-CB-CG	7.16	131.76	115.30
4	3	2268	C	C5-C6-N1	7.01	124.51	121.00
6	5	9	A	N9-C4-C5	-6.92	103.03	105.80
43	j	5	MET	CA-CB-CG	6.78	124.83	113.30
6	5	1323	A	C4-C5-C6	-6.70	113.65	117.00
15	E	121	ARG	CA-CB-CG	6.66	128.05	113.40
42	i	111	MET	CB-CG-SD	-6.54	92.77	112.40
4	3	482	G	P-O3'-C3'	-6.52	111.87	119.70
4	3	1486	U	N1-C2-O2	6.51	127.36	122.80
18	H	125	ARG	CB-CG-CD	-6.41	94.95	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Q	69	LYS	CA-CB-CG	6.36	127.39	113.40
4	3	1486	U	N3-C2-O2	-6.34	117.76	122.20
34	a	132	PRO	CA-N-CD	-6.29	102.69	111.50
20	J	119	ARG	CA-CB-CG	6.28	127.21	113.40
7	6	46	G	P-O3'-C3'	6.27	127.23	119.70
46	m	91	GLU	CA-CB-CG	6.13	126.89	113.40
30	T	33	GLU	N-CA-CB	6.10	121.58	110.60
34	a	207	ASP	CB-CG-OD1	6.09	123.78	118.30
15	E	45	LEU	CA-CB-CG	6.08	129.28	115.30
25	O	41	PRO	CA-N-CD	-6.04	103.05	111.50
36	c	97	ARG	CA-CB-CG	5.96	126.52	113.40
6	5	1323	A	C5-C6-N6	-5.94	118.95	123.70
6	5	1321	G	O4'-C1'-N9	5.90	112.92	108.20
28	R	76	PRO	CA-N-CD	-5.87	103.29	111.50
32	Y	61	A	O5'-P-OP2	-5.85	100.44	105.70
7	6	75	C	O5'-P-OP1	-5.76	100.51	105.70
6	5	9	A	O4'-C1'-N9	-5.75	103.60	108.20
4	3	1341	U	C2-N1-C1'	5.74	124.58	117.70
28	R	40	ILE	C-N-CA	5.71	135.98	121.70
36	c	97	ARG	CB-CG-CD	5.66	126.32	111.60
7	6	33	U	C5'-C4'-O4'	-5.66	102.31	109.10
4	3	2259	OMG	OP2-P-O3'	5.66	117.64	105.20
4	3	2268	C	C2-N1-C1'	5.59	124.95	118.80
43	j	93	PRO	N-CA-CB	-5.58	96.46	102.60
2	1	13	LEU	CA-CB-CG	5.55	128.06	115.30
6	5	9	A	N1-C6-N6	5.53	121.92	118.60
4	3	1303	U	C2-N1-C1'	5.53	124.34	117.70
6	5	1501	G	O5'-P-OP2	5.53	117.34	110.70
7	6	33	U	P-O3'-C3'	5.52	126.32	119.70
26	P	29	ARG	CA-CB-CG	5.50	125.50	113.40
29	S	53	ARG	CA-CB-CG	5.48	125.46	113.40
6	5	9	A	C4-C5-N7	5.48	113.44	110.70
18	H	90	LEU	CA-CB-CG	5.47	127.88	115.30
15	E	121	ARG	CB-CG-CD	5.46	125.78	111.60
6	5	832	G	O5'-P-OP1	-5.38	100.85	105.70
44	k	3	LEU	CA-CB-CG	5.38	127.68	115.30
6	5	994	C	N1-C2-O2	5.37	122.12	118.90
25	O	39	LEU	CA-CB-CG	5.36	127.63	115.30
17	G	95	LEU	CA-CB-CG	5.31	127.51	115.30
34	a	132	PRO	N-CD-CG	-5.25	95.33	103.20
10	9	8	MET	CA-CB-CG	-5.21	104.45	113.30
6	5	1323	A	C5-N7-C8	-5.15	101.32	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	170	MET	CA-CB-CG	5.13	122.01	113.30
16	F	115	MET	CG-SD-CE	-5.10	92.04	100.20
51	r	117	LEU	CA-CB-CG	5.09	127.01	115.30
43	j	5	MET	CB-CG-SD	-5.08	97.14	112.40
58	y	52	ARG	CA-CB-CG	5.08	124.58	113.40
43	j	29	ARG	CA-CB-CG	5.04	124.48	113.40
6	5	1134	C	C2-N1-C1'	5.03	124.33	118.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	a	225	ARG	Sidechain
39	f	118	ARG	Sidechain
55	v	63	ARG	Sidechain

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	45/48 (94%)	45 (100%)	0	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	9	224/226 (99%)	218 (97%)	5 (2%)	1 (0%)	30	68
11	A	264/294 (90%)	233 (88%)	28 (11%)	3 (1%)	12	47
12	B	222/273 (81%)	198 (89%)	21 (10%)	3 (1%)	9	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	C	202/205 (98%)	168 (83%)	33 (16%)	1 (0%)	25	64
14	D	156/219 (71%)	147 (94%)	7 (4%)	2 (1%)	10	43
15	E	213/215 (99%)	171 (80%)	33 (16%)	9 (4%)	2	17
16	F	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	4	26
17	G	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
18	H	127/132 (96%)	115 (91%)	10 (8%)	2 (2%)	8	38
19	I	102/108 (94%)	89 (87%)	12 (12%)	1 (1%)	13	49
20	J	118/121 (98%)	103 (87%)	9 (8%)	6 (5%)	1	15
21	K	133/139 (96%)	113 (85%)	16 (12%)	4 (3%)	3	23
22	L	119/124 (96%)	109 (92%)	10 (8%)	0	100	100
23	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
24	N	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
25	O	85/94 (90%)	78 (92%)	5 (6%)	2 (2%)	5	27
26	P	83/85 (98%)	71 (86%)	11 (13%)	1 (1%)	11	44
27	Q	71/104 (68%)	63 (89%)	6 (8%)	2 (3%)	4	24
28	R	84/87 (97%)	79 (94%)	5 (6%)	0	100	100
29	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	10	43
30	T	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
31	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
33	Z	3/36 (8%)	3 (100%)	0	0	100	100
34	a	283/287 (99%)	268 (95%)	14 (5%)	1 (0%)	30	68
35	b	227/287 (79%)	220 (97%)	7 (3%)	0	100	100
36	c	209/212 (99%)	199 (95%)	10 (5%)	0	100	100
37	d	177/180 (98%)	168 (95%)	9 (5%)	0	100	100
38	e	174/184 (95%)	162 (93%)	12 (7%)	0	100	100
39	f	147/149 (99%)	113 (77%)	29 (20%)	5 (3%)	3	21
40	g	123/161 (76%)	115 (94%)	8 (6%)	0	100	100
41	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
42	i	142/146 (97%)	133 (94%)	9 (6%)	0	100	100
43	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	k	148/151 (98%)	137 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	l	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
46	m	117/124 (94%)	111 (95%)	6 (5%)	0	100	100
47	n	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
48	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
49	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
50	q	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
51	r	140/159 (88%)	137 (98%)	3 (2%)	0	100	100
52	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
53	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
54	u	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
55	v	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
56	w	108/111 (97%)	103 (95%)	5 (5%)	0	100	100
57	x	85/97 (88%)	63 (74%)	21 (25%)	1 (1%)	11	44
58	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
59	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6295/7376 (85%)	5799 (92%)	447 (7%)	49 (1%)	19	55

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	D	216	LEU
15	E	121	ARG
15	E	143	LEU
18	H	102	SER
20	J	32	GLY
26	P	54	LEU
39	f	34	LYS
13	C	81	GLN
16	F	9	ARG
16	F	15	PRO
20	J	9	VAL
20	J	33	ASN
27	Q	39	LYS
29	S	37	LYS
39	f	27	ILE
39	f	95	LYS
10	9	221	LYS

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Mol	Chain	Res	Type
11	A	52	ASN
11	A	219	ASN
12	B	221	HIS
16	F	12	LEU
16	F	79	ILE
21	K	56	LYS
11	A	17	LEU
14	D	66	PHE
15	E	133	THR
15	E	182	ASN
19	I	100	VAL
20	J	10	SER
25	O	47	LYS
25	O	49	LYS
27	Q	35	LYS
34	a	128	ILE
39	f	12	LEU
15	E	42	LEU
15	E	139	THR
15	E	169	VAL
15	E	185	HIS
18	H	93	ASN
21	K	72	ASN
12	B	216	ASN
15	E	163	MET
57	x	18	SER
12	B	46	VAL
20	J	7	ILE
21	K	57	LYS
20	J	30	PRO
39	f	93	ILE
21	K	55	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	40/41 (98%)	39 (98%)	1 (2%)	42	61
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	34 (97%)	1 (3%)	37	56
10	9	186/186 (100%)	186 (100%)	0	100	100
11	A	239/262 (91%)	237 (99%)	2 (1%)	79	85
12	B	187/232 (81%)	187 (100%)	0	100	100
13	C	182/183 (100%)	178 (98%)	4 (2%)	47	65
14	D	128/178 (72%)	127 (99%)	1 (1%)	79	85
15	E	196/196 (100%)	194 (99%)	2 (1%)	73	82
16	F	132/132 (100%)	130 (98%)	2 (2%)	60	75
17	G	124/124 (100%)	123 (99%)	1 (1%)	79	85
18	H	112/115 (97%)	110 (98%)	2 (2%)	54	71
19	I	97/99 (98%)	97 (100%)	0	100	100
20	J	96/97 (99%)	96 (100%)	0	100	100
21	K	117/120 (98%)	117 (100%)	0	100	100
22	L	102/105 (97%)	99 (97%)	3 (3%)	37	56
23	M	47/48 (98%)	46 (98%)	1 (2%)	48	66
24	N	78/78 (100%)	76 (97%)	2 (3%)	41	59
25	O	76/82 (93%)	74 (97%)	2 (3%)	41	59
26	P	75/75 (100%)	74 (99%)	1 (1%)	65	77
27	Q	64/94 (68%)	64 (100%)	0	100	100
28	R	76/77 (99%)	75 (99%)	1 (1%)	65	77
29	S	71/77 (92%)	70 (99%)	1 (1%)	62	75
30	T	55/56 (98%)	55 (100%)	0	100	100
31	X	27/406 (7%)	27 (100%)	0	100	100
33	Z	2/2 (100%)	2 (100%)	0	100	100
34	a	241/243 (99%)	238 (99%)	3 (1%)	67	78
35	b	186/233 (80%)	184 (99%)	2 (1%)	70	80
36	c	183/184 (100%)	183 (100%)	0	100	100
37	d	153/154 (99%)	153 (100%)	0	100	100
38	e	153/159 (96%)	152 (99%)	1 (1%)	81	87
39	f	134/134 (100%)	129 (96%)	5 (4%)	29	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	g	100/129 (78%)	98 (98%)	2 (2%)	50	68
41	h	102/110 (93%)	102 (100%)	0	100	100
42	i	126/128 (98%)	126 (100%)	0	100	100
43	j	103/103 (100%)	102 (99%)	1 (1%)	73	82
44	k	125/126 (99%)	124 (99%)	1 (1%)	79	85
45	l	113/115 (98%)	113 (100%)	0	100	100
46	m	105/109 (96%)	102 (97%)	3 (3%)	37	56
47	n	99/99 (100%)	98 (99%)	1 (1%)	73	82
48	o	104/105 (99%)	102 (98%)	2 (2%)	52	69
49	p	104/108 (96%)	100 (96%)	4 (4%)	28	49
50	q	90/91 (99%)	89 (99%)	1 (1%)	70	80
51	r	118/132 (89%)	117 (99%)	1 (1%)	79	85
52	s	84/208 (40%)	83 (99%)	1 (1%)	67	78
53	t	96/96 (100%)	96 (100%)	0	100	100
54	u	70/85 (82%)	70 (100%)	0	100	100
55	v	59/60 (98%)	59 (100%)	0	100	100
56	w	97/98 (99%)	97 (100%)	0	100	100
57	x	79/86 (92%)	77 (98%)	2 (2%)	42	61
58	y	48/49 (98%)	48 (100%)	0	100	100
59	z	47/50 (94%)	47 (100%)	0	100	100
All	All	5514/6345 (87%)	5457 (99%)	57 (1%)	71	82

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	9	LYS
3	2	21	GLN
11	A	14	LYS
11	A	49	ARG
13	C	27	LYS
13	C	43	ARG
13	C	72	ARG
13	C	111	ARG
14	D	212	ARG
15	E	43	LYS

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Mol	Chain	Res	Type
15	E	114	LYS
16	F	63	ARG
16	F	67	ASN
17	G	9	LYS
18	H	11	ARG
18	H	124	ARG
22	L	70	ARG
22	L	71	ARG
22	L	120	LYS
23	M	4	LYS
24	N	10	LYS
24	N	85	ARG
25	O	25	ARG
25	O	49	LYS
26	P	17	LYS
28	R	29	ARG
29	S	22	LYS
34	a	24	LYS
34	a	29	ASN
34	a	56	ARG
35	b	46	LYS
35	b	218	LYS
38	e	51	ASN
39	f	47	ARG
39	f	62	LYS
39	f	77	LEU
39	f	89	TYR
39	f	92	ILE
40	g	67	LYS
40	g	125	LYS
43	j	29	ARG
44	k	11	LYS
46	m	30	LYS
46	m	102	LYS
46	m	107	ARG
47	n	85	LYS
48	o	68	LYS
48	o	117	ARG
49	p	2	ARG
49	p	4	LYS
49	p	35	LYS
49	p	83	LYS

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Mol	Chain	Res	Type
50	q	52	LYS
51	r	99	ARG
52	s	87	LYS
57	x	32	LYS
57	x	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	32	HIS
3	2	34	GLN
11	A	51	HIS
11	A	55	HIS
11	A	174	ASN
12	B	6	ASN
12	B	86	GLN
12	B	216	ASN
13	C	81	GLN
13	C	88	ASN
14	D	123	HIS
14	D	132	HIS
15	E	25	GLN
15	E	101	ASN
16	F	18	ASN
16	F	83	ASN
18	H	52	GLN
20	J	8	ASN
21	K	29	ASN
24	N	15	HIS
26	P	25	GLN
26	P	42	HIS
26	P	46	GLN
26	P	49	ASN
26	P	62	GLN
30	T	30	GLN
35	b	21	ASN
35	b	34	ASN
35	b	157	GLN
37	d	37	ASN
37	d	63	GLN
39	f	61	ASN
39	f	100	GLN

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Mol	Chain	Res	Type
41	h	13	ASN
41	h	38	GLN
42	i	80	HIS
43	j	56	GLN
44	k	39	GLN
44	k	75	GLN
46	m	62	GLN
47	n	49	ASN
47	n	69	ASN
48	o	85	ASN
51	r	15	GLN
54	u	90	GLN
55	v	6	GLN
56	w	35	HIS
56	w	46	GLN
57	x	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	Y	39/40 (97%)	25 (64%)	6 (15%)
4	3	2891/2907 (99%)	533 (18%)	20 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	1502/1520 (98%)	251 (16%)	8 (0%)
7	6	76/76 (100%)	22 (28%)	6 (7%)
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	4764/4802 (99%)	903 (18%)	42 (0%)

All (903) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G
4	3	37	G
4	3	48	G
4	3	64	U
4	3	65	A

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Mol	Chain	Res	Type
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
4	3	309	A
4	3	310	U
4	3	311	G
4	3	315	A
4	3	316	C
4	3	317	U

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Mol	Chain	Res	Type
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	463	U
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
4	3	610	G
4	3	620	G
4	3	636	U
4	3	637	U
4	3	638	A

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Mol	Chain	Res	Type
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
4	3	901	C
4	3	902	U
4	3	903	A
4	3	904	C
4	3	906	G

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Mol	Chain	Res	Type
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	933	A
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
4	3	1084	C
4	3	1096	U
4	3	1097	G

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Mol	Chain	Res	Type
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	1144	C
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
4	3	1242	G
4	3	1246	U
4	3	1250	A

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Mol	Chain	Res	Type
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
4	3	1483	G
4	3	1486	U
4	3	1487	U

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Mol	Chain	Res	Type
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	1589	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
4	3	1688	A
4	3	1694	A

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Mol	Chain	Res	Type
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
4	3	2028	G

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Mol	Chain	Res	Type
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	2107	A
4	3	2108	C
4	3	2109	A
4	3	2110	U
4	3	2111	U
4	3	2112	A
4	3	2114	C
4	3	2118	U
4	3	2119	A
4	3	2122	G
4	3	2123	A
4	3	2124	A
4	3	2125	U
4	3	2126	A
4	3	2128	G
4	3	2129	U
4	3	2131	G
4	3	2135	C
4	3	2139	C
4	3	2140	G
4	3	2151	G
4	3	2152	C
4	3	2153	U
4	3	2156	G
4	3	2158	C

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Mol	Chain	Res	Type
4	3	2159	U
4	3	2160	U
4	3	2161	G
4	3	2165	A
4	3	2166	U
4	3	2167	G
4	3	2168	C
4	3	2169	G
4	3	2170	A
4	3	2171	A
4	3	2175	U
4	3	2178	A
4	3	2179	A
4	3	2180	U
4	3	2181	A
4	3	2184	A
4	3	2185	C
4	3	2187	C
4	3	2188	U
4	3	2193	U
4	3	2194	G
4	3	2195	U
4	3	2196	G
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

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Mol	Chain	Res	Type
4	3	2287	G
4	3	2291	U
4	3	2295	A
4	3	2298	G
4	3	2305	C
4	3	2311	G
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

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Mol	Chain	Res	Type
4	3	2499	U
4	3	2510	G
4	3	2512	U
4	3	2513	G
4	3	2521	A
4	3	2526	A
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	2611	G
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	1045	C
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

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Mol	Chain	Res	Type
6	5	1188	A
6	5	1189	U
6	5	1202	A
6	5	1203	A
6	5	1215	U
6	5	1231	U
6	5	1232	C
6	5	1233	G
6	5	1235	C
6	5	1255	A
6	5	1260	U
6	5	1271	U
6	5	1274	G
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	1339	U
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

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Mol	Chain	Res	Type
6	5	1481	U
6	5	1482	A
6	5	1492	G
6	5	1504	G
6	5	1505	G
6	5	1509	A
7	6	2	G
7	6	3	G
7	6	13	C
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	33	U
7	6	34	U
7	6	46	G
7	6	47	U
7	6	48	U
7	6	59	G
7	6	65	U
7	6	70	U
7	6	71	C
7	6	72	C
7	6	73	A
7	6	75	C
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
8	7	46	U
8	7	47	U

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Mol	Chain	Res	Type
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
32	Y	58	A
32	Y	59	A
32	Y	61	A
32	Y	62	A
32	Y	64	A
32	Y	65	C
32	Y	66	U
32	Y	67	G
32	Y	70	G
32	Y	77	U
32	Y	79	U
32	Y	80	U
32	Y	81	C

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Mol	Chain	Res	Type
32	Y	82	A
32	Y	83	A
32	Y	84	A
32	Y	86	A
32	Y	87	A
32	Y	88	A
32	Y	89	A
32	Y	91	A
32	Y	92	A
32	Y	94	A
32	Y	95	C
32	Y	96	U

All (42) 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	902	U
4	3	1124	G
4	3	1209	U
4	3	1583	G
4	3	1618	U
4	3	2106	G
4	3	2118	U
4	3	2139	C
4	3	2152	C
4	3	2164	G
4	3	2167	G
4	3	2169	G
4	3	2180	U
4	3	2194	G
4	3	2410	C
4	3	2764	U
6	5	196	G
6	5	571	A
6	5	994	C
6	5	995	U
6	5	1024	U
6	5	1123	G

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Mol	Chain	Res	Type
6	5	1158	A
6	5	1338	A
7	6	1	G
7	6	15	A
7	6	17	U
7	6	33	U
7	6	46	G
7	6	74	C
8	7	10	G
8	7	46	U
32	Y	64	A
32	Y	65	C
32	Y	79	U
32	Y	81	C
32	Y	94	A
32	Y	95	C

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

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
4	OMG	3	2259	4,8	18,26,27	2.83	7 (38%)	19,38,41	1.56	4 (21%)
4	1MG	3	783	4	18,26,27	0.95	1 (5%)	19,39,42	0.83	0
6	7MG	5	525	6	22,26,27	3.90	10 (45%)	29,39,42	2.02	9 (31%)
6	MA6	5	1494	6	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
6	5MC	5	1375	6	18,22,23	4.06	7 (38%)	26,32,35	1.03	2 (7%)
6	MA6	5	1493	6	18,26,27	1.07	2 (11%)	19,38,41	3.25	3 (15%)
6	B8T	5	1377	6	19,22,23	3.29	8 (42%)	26,31,34	0.84	1 (3%)
4	2MA	3	2511	4,63	17,25,26	2.64	5 (29%)	17,37,40	1.34	3 (17%)

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
4	OMG	3	2259	4,8	-	3/5/27/28	0/3/3/3
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3
6	7MG	5	525	6	-	2/7/37/38	0/3/3/3
6	MA6	5	1494	6	-	2/7/29/30	0/3/3/3
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
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
4	2MA	3	2511	4,63	-	2/3/25/26	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	525	7MG	C8-N9	9.95	1.51	1.46
6	5	1375	5MC	C6-C5	9.93	1.50	1.34
6	5	525	7MG	C5-N7	7.98	1.44	1.35
4	3	2511	2MA	C2-N3	7.88	1.47	1.31
6	5	1375	5MC	C4-N3	7.57	1.46	1.34
6	5	1377	B8T	C4-N3	7.19	1.45	1.32
4	3	2259	OMG	C2-N2	7.16	1.51	1.34
6	5	1375	5MC	C2-N3	7.00	1.50	1.36
6	5	1377	B8T	C2-N3	6.50	1.49	1.36
6	5	1377	B8T	C6-C5	6.10	1.49	1.35
6	5	525	7MG	C2-N3	5.88	1.47	1.33
6	5	525	7MG	C4-N9	5.74	1.44	1.37
6	5	1375	5MC	C4-N4	5.69	1.48	1.34
6	5	525	7MG	C4-N3	5.59	1.47	1.34
6	5	1375	5MC	C6-N1	5.59	1.47	1.38
4	3	2259	OMG	C2-N3	5.11	1.45	1.33
4	3	2511	2MA	C4-N3	5.10	1.49	1.37
6	5	525	7MG	C2-N2	4.78	1.45	1.34
6	5	1377	B8T	C4-N4	4.78	1.45	1.35
6	5	1375	5MC	C2-N1	4.66	1.50	1.40
4	3	2259	OMG	C4-N3	4.56	1.48	1.37
6	5	1377	B8T	C2-N1	4.28	1.49	1.40
6	5	1377	B8T	C5-C4	3.87	1.49	1.40
6	5	525	7MG	C2-N1	3.87	1.47	1.37
6	5	525	7MG	C5-C6	3.60	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	2511	2MA	C6-N1	3.22	1.45	1.38
4	3	2259	OMG	C6-N1	3.13	1.42	1.37
6	5	1377	B8T	C6-N1	3.12	1.45	1.38
4	3	2259	OMG	C5-C6	2.83	1.53	1.47
4	3	2511	2MA	C2-N1	2.75	1.45	1.36
6	5	1493	MA6	C2-N3	2.69	1.36	1.32
6	5	1377	B8T	O2-C2	-2.68	1.18	1.23
6	5	1494	MA6	C2-N3	2.65	1.36	1.32
4	3	2259	OMG	C5-C4	-2.45	1.36	1.43
6	5	525	7MG	O6-C6	-2.42	1.19	1.23
6	5	1494	MA6	C5-C4	-2.31	1.34	1.40
6	5	1493	MA6	C5-C4	-2.25	1.35	1.40
4	3	2511	2MA	C5-C4	-2.22	1.37	1.43
4	3	783	1MG	C5-C4	-2.17	1.37	1.43
6	5	1375	5MC	O2-C2	-2.15	1.19	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1494	MA6	N1-C6-N6	-12.27	104.15	117.06
6	5	1493	MA6	N1-C6-N6	-11.50	104.95	117.06
6	5	1493	MA6	C1'-N9-C4	5.71	136.68	126.64
6	5	1494	MA6	N3-C2-N1	-5.64	119.87	128.68
6	5	1493	MA6	N3-C2-N1	-5.45	120.15	128.68
6	5	1494	MA6	C1'-N9-C4	5.14	135.66	126.64
6	5	525	7MG	C5-C6-N1	4.94	119.70	110.99
6	5	525	7MG	C2-N3-C4	4.47	120.25	112.30
6	5	525	7MG	C5-C4-N3	-4.11	120.30	128.13
4	3	2259	OMG	C5-C6-N1	3.45	120.04	113.95
4	3	2511	2MA	C5-C6-N1	3.39	119.88	114.02
6	5	525	7MG	C5-C4-N9	3.14	110.42	106.35
6	5	1375	5MC	C5-C6-N1	-3.07	120.18	123.34
6	5	525	7MG	C4-C5-N7	3.02	109.72	105.53
4	3	2259	OMG	C2-N1-C6	-2.93	119.70	125.10
4	3	2259	OMG	C8-N7-C5	2.83	108.39	102.99
6	5	525	7MG	C2-N1-C6	-2.82	119.95	125.10
4	3	2511	2MA	C8-N7-C5	2.76	108.25	102.99
6	5	525	7MG	O6-C6-C5	-2.75	120.80	127.54
6	5	525	7MG	N9-C4-N3	2.55	129.28	125.47
6	5	1377	B8T	C6-C5-C4	2.53	120.06	116.96
6	5	525	7MG	N9-C8-N7	2.26	106.61	103.38
6	5	1375	5MC	CM5-C5-C6	-2.20	119.91	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2511	2MA	CM2-C2-N1	2.18	121.09	116.23
4	3	2259	OMG	O6-C6-C5	-2.17	120.14	124.37

There are no chirality outliers.

All (11) 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	1377	B8T	O4'-C4'-C5'-O5'
6	5	1377	B8T	C3'-C4'-C5'-O5'
4	3	2511	2MA	O4'-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 331 ligands modelled in this entry, 329 are monoatomic - leaving 2 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	$\# Z > 2$
64	LYS	8	102	9	7,8,9	0.86	0	3,8,10	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	CLM	3	3001	-	19,20,20	2.08	2 (10%)	23,27,27	0.86	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
64	LYS	8	102	9	-	3/6/7/9	-
61	CLM	3	3001	-	-	2/20/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	3	3001	CLM	C2-N2	7.22	1.49	1.34
61	3	3001	CLM	O9B-N9	-2.71	1.18	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

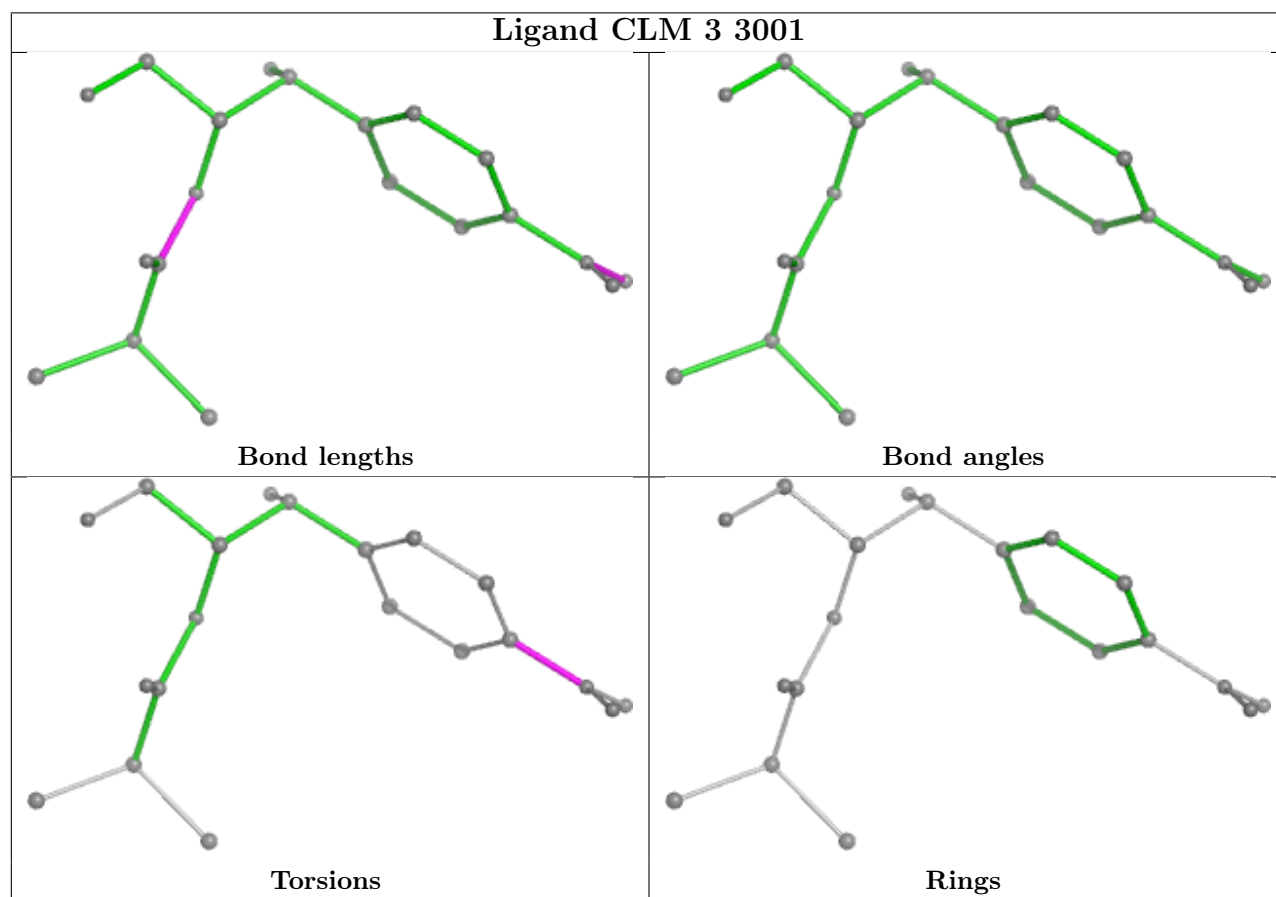
Mol	Chain	Res	Type	Atoms
61	3	3001	CLM	C8-C9-N9-O9B
64	8	102	LYS	O-C-CA-CB
64	8	102	LYS	N-CA-CB-CG
64	8	102	LYS	C-CA-CB-CG
61	3	3001	CLM	C10-C9-N9-O9B

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.