



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 05:47 pm BST

PDB ID : 7BL5 / pdb\_00007bl5  
EMDB ID : EMD-12218  
Title : pre-50S-ObgE particle  
Authors : Hilal, T.; Nikolay, R.; Spahn, C.M.T.; Schmidt, S.  
Deposited on : 2021-01-18  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
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) : 2.42

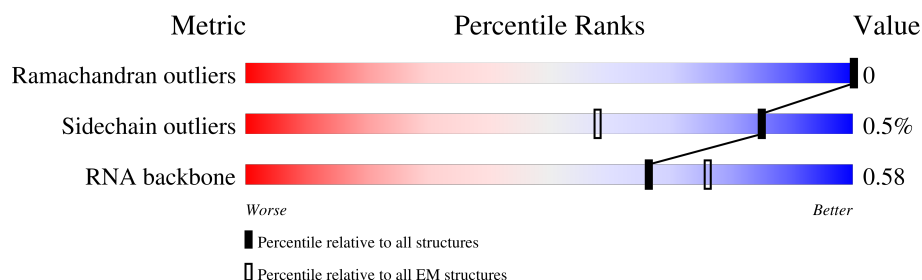
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.


















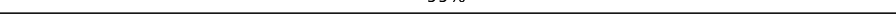
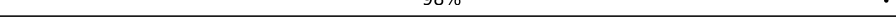
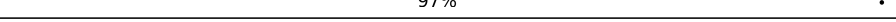
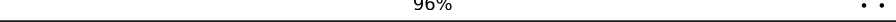


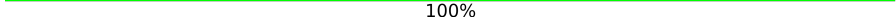

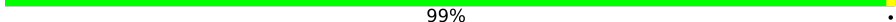

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	C	273	99% .
2	D	209	100%
3	E	201	99% .
4	G	177	97% .
5	J	142	99% .
6	L	144	99% .
7	N	127	94% 6%
8	O	117	99% .
9	Q	118	99% .


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Mol	Chain	Length	Quality of chain
10	R	103	 100%
11	S	110	 100%
12	T	100	 93% 7%
13	U	104	 98% .
14	V	94	 100%
15	W	85	 89% 11%
16	X	78	 97% ..
17	Y	63	 100%
18	Z	59	 98% .
19	0	57	 98% .
20	1	55	 91% 9%
21	2	46	 98% .
22	B	120	 84% 15% .
23	I	142	 98% ..
24	K	123	 99% .
25	P	115	 98% .
26	6	105	 97% .
27	7	326	 96% ..
28	8	183	 85% . 14%
29	9	390	 86% . 13%
30	M	136	 100%
31	A	2919	 83% 17%
32	H	149	 99% .
33	e	165	 79% 21%
34	F	179	 98% ..

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Mol	Chain	Length	Quality of chain
35	b	70	 67% 33%

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 98927 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 L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	171	Total	C	N	O	S	0	0
			1281	806	235	238	2		

- Molecule 5 is a protein called 50S ribosomal protein L13.

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

- Molecule 6 is a protein called 50S ribosomal protein L15.

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

- Molecule 7 is a protein called 50S ribosomal protein L17.

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

- Molecule 8 is a protein called 50S ribosomal protein L18.

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

- Molecule 9 is a protein called 50S ribosomal protein L20.

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

- Molecule 10 is a protein called 50S ribosomal protein L21.

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

- Molecule 11 is a protein called 50S ribosomal protein L22.

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

- Molecule 12 is a protein called 50S ribosomal protein L23.

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

- Molecule 13 is a protein called 50S ribosomal protein L24.

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

- Molecule 14 is a protein called 50S ribosomal protein L25.

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

- Molecule 15 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 16 is a protein called 50S ribosomal protein L28.

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

- Molecule 17 is a protein called 50S ribosomal protein L29.

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

- Molecule 18 is a protein called 50S ribosomal protein L30.

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

- Molecule 19 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 20 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 21 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 23 is a protein called 50S ribosomal protein L11.

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

- Molecule 24 is a protein called 50S ribosomal protein L14.

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

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

- Molecule 26 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	102	Total	C	N	O	S	0	0
			780	485	133	157	5		

- Molecule 27 is a protein called Ribosomal large subunit pseudouridine synthase D.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	317	Total	C	N	O	S	0	0
			2533	1593	471	457	12		

- Molecule 28 is a protein called UPF0307 protein YjgA.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	8	157	Total	C	N	O	S	0	0
			1281	792	251	237	1		

- Molecule 29 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 30 is a protein called 50S ribosomal protein L16.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	2913	Total	C	N	O	P	0	0
			62534	27897	11506	20218	2913		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 33 is a protein called 50S ribosomal protein L10.

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

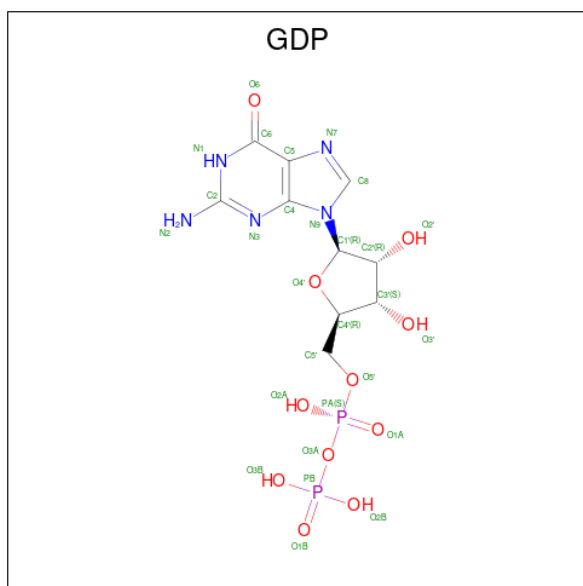
- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 36 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
36	9	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	9	1	Total	Mg	0
			1	1	
37	A	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	b	1	Total	Zn	0
			1	1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	C	3	Total 3	O 3	0
39	D	1	Total 1	O 1	0
39	N	2	Total 2	O 2	0
39	S	1	Total 1	O 1	0
39	2	1	Total 1	O 1	0
39	B	1	Total 1	O 1	0
39	A	17	Total 17	O 17	0
39	F	1	Total 1	O 1	0

### 3 Residue-property plots [i](#)

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 L2

Chain C:  99%



- Molecule 2: 50S ribosomal protein L3

Chain D:  100%



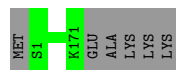
- Molecule 3: 50S ribosomal protein L4

Chain E:  99%



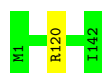
- Molecule 4: 50S ribosomal protein L6

Chain G:  97%



- Molecule 5: 50S ribosomal protein L13

Chain J:  99%



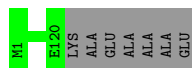
- Molecule 6: 50S ribosomal protein L15

Chain L:  99%



- Molecule 7: 50S ribosomal protein L17

Chain N: 94% 6%



- Molecule 8: 50S ribosomal protein L18

Chain O: 99% .



- Molecule 9: 50S ribosomal protein L20

Chain Q: 99% .



- Molecule 10: 50S ribosomal protein L21

Chain R: 100%

There are no outlier residues recorded for this chain.

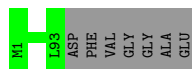
- Molecule 11: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

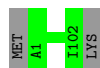
- Molecule 12: 50S ribosomal protein L23

Chain T: 93% 7%



- Molecule 13: 50S ribosomal protein L24

Chain U: 98% .




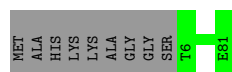
- Molecule 14: 50S ribosomal protein L25

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 50S ribosomal protein L27

Chain W:  89%  11%



- Molecule 16: 50S ribosomal protein L28

Chain X:  97%  ..



- Molecule 17: 50S ribosomal protein L29

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L30

Chain Z:  98%  .





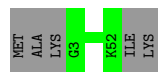
- Molecule 19: 50S ribosomal protein L32

Chain 0:  98%  .



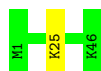
- Molecule 20: 50S ribosomal protein L33

Chain 1:  91%  9%



- Molecule 21: 50S ribosomal protein L34

Chain 2:  98%  .



- Molecule 22: 5S ribosomal RNA

Chain B: 84% 15%



- Molecule 23: 50S ribosomal protein L11

Chain I: 98%



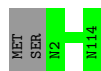
- Molecule 24: 50S ribosomal protein L14

Chain K: 99%



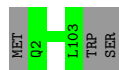
- Molecule 25: 50S ribosomal protein L19

Chain P: 98%



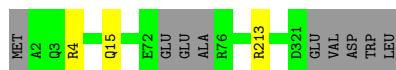
- Molecule 26: Ribosomal silencing factor RsfS

Chain 6: 97%



- Molecule 27: Ribosomal large subunit pseudouridine synthase D

Chain 7: 96%

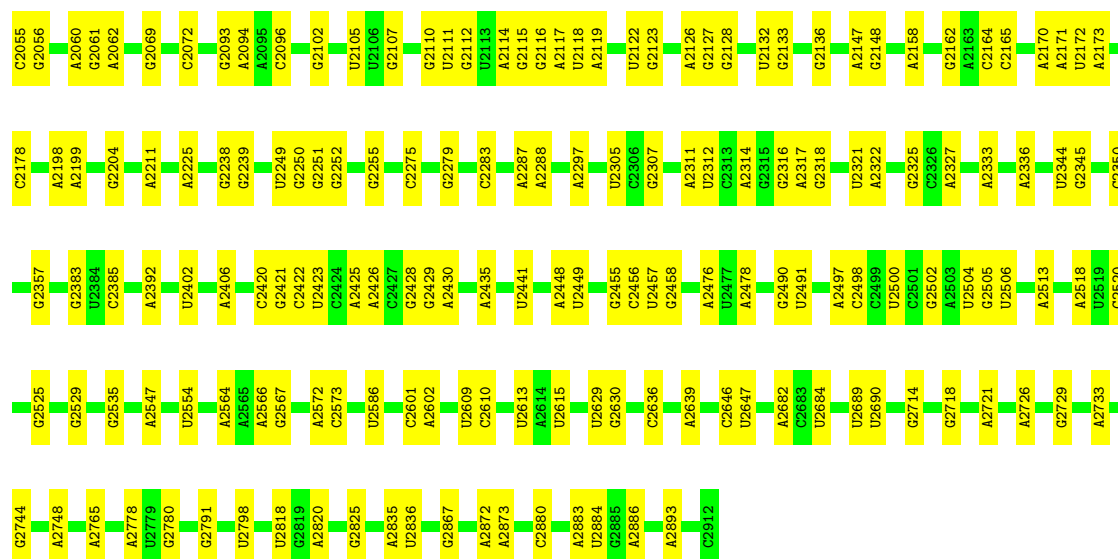


- Molecule 28: UPF0307 protein YjgA

Chain 8: 85% 14%







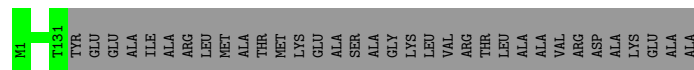
• Molecule 32: 50S ribosomal protein L9

Chain H: 99%



• Molecule 33: 50S ribosomal protein L10

Chain e: 79%



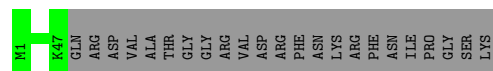
• Molecule 34: 50S ribosomal protein L5

Chain F: 98%



• Molecule 35: 50S ribosomal protein L31

Chain b: 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GDP, 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	C	0.24	0/2121	0.44	0/2852
2	D	0.25	0/1586	0.48	0/2134
3	E	0.24	0/1571	0.42	0/2113
4	G	0.24	0/1301	0.45	0/1764
5	J	0.24	0/1152	0.42	0/1551
6	L	0.26	0/1054	0.55	0/1403
7	N	0.24	0/973	0.44	0/1301
8	O	0.25	0/902	0.42	0/1209
9	Q	0.24	0/960	0.36	0/1278
10	R	0.27	0/829	0.53	0/1107
11	S	0.23	0/864	0.44	0/1156
12	T	0.23	0/744	0.43	0/994
13	U	0.25	0/787	0.46	0/1051
14	V	0.24	0/766	0.48	0/1025
15	W	0.26	0/582	0.46	0/769
16	X	0.23	0/635	0.42	0/848
17	Y	0.24	0/510	0.50	0/677
18	Z	0.23	0/453	0.47	0/605
19	0	0.23	0/450	0.45	0/599
20	1	0.24	0/416	0.46	0/554
21	2	0.23	0/380	0.39	0/498
22	B	0.15	0/2847	0.71	0/4440
23	I	0.25	0/1046	0.47	0/1410
24	K	0.25	0/947	0.47	0/1268
25	P	0.25	0/923	0.45	0/1234
26	6	0.24	0/787	0.47	0/1062
27	7	0.23	0/2590	0.43	0/3513
28	8	0.23	0/1292	0.41	0/1727
29	9	0.25	0/2626	0.45	0/3542
30	M	0.24	0/1093	0.44	0/1460
31	A	0.17	0/70038	0.73	12/109262 (0.0%)
32	H	0.24	0/1121	0.45	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	e	0.25	0/1001	0.47	0/1350
34	F	0.25	0/1434	0.44	0/1926
35	b	0.23	0/371	0.43	0/496
All	All	0.20	0/107152	0.66	12/159693 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	1313	U	C2-N1-C1'	7.05	126.17	117.70
31	A	106	C	N3-C2-O2	-6.91	117.07	121.90
31	A	1075	C	N3-C2-O2	-6.88	117.08	121.90
31	A	1075	C	N1-C2-O2	6.46	122.77	118.90
31	A	1939	U	C2-N1-C1'	6.37	125.34	117.70
31	A	1939	U	N1-C2-O2	6.29	127.20	122.80
31	A	1313	U	N3-C2-O2	-5.93	118.05	122.20
31	A	1313	U	N1-C2-O2	5.87	126.91	122.80
31	A	1939	U	N3-C2-O2	-5.79	118.14	122.20
31	A	274	C	N1-C2-O2	5.43	122.16	118.90
31	A	106	C	C6-N1-C2	-5.22	118.21	120.30
31	A	274	C	N3-C2-O2	-5.16	118.29	121.90

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
2	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
3	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
4	G	169/177 (96%)	163 (96%)	6 (4%)	0	100	100
5	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
6	L	141/144 (98%)	119 (84%)	22 (16%)	0	100	100
7	N	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
8	O	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
9	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
10	R	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
11	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
12	T	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
13	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
14	V	92/94 (98%)	92 (100%)	0	0	100	100
15	W	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
16	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
17	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
18	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
19	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
20	1	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
21	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
23	I	139/142 (98%)	116 (84%)	23 (16%)	0	100	100
24	K	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
25	P	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
26	6	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
27	7	313/326 (96%)	304 (97%)	9 (3%)	0	100	100
28	8	155/183 (85%)	152 (98%)	3 (2%)	0	100	100
29	9	336/390 (86%)	312 (93%)	24 (7%)	0	100	100
30	M	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
32	H	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
33	e	129/165 (78%)	113 (88%)	16 (12%)	0	100	100
34	F	175/179 (98%)	168 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	b	45/70 (64%)	41 (91%)	4 (9%)	0	100	100
All	All	4280/4545 (94%)	4035 (94%)	245 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	C	216/218 (99%)	216 (100%)	0	100	100
2	D	164/164 (100%)	163 (99%)	1 (1%)	84	90
3	E	165/165 (100%)	163 (99%)	2 (1%)	67	80
4	G	133/138 (96%)	133 (100%)	0	100	100
5	J	116/116 (100%)	115 (99%)	1 (1%)	75	85
6	L	102/103 (99%)	102 (100%)	0	100	100
7	N	100/103 (97%)	100 (100%)	0	100	100
8	O	86/87 (99%)	86 (100%)	0	100	100
9	Q	89/90 (99%)	89 (100%)	0	100	100
10	R	84/84 (100%)	84 (100%)	0	100	100
11	S	93/93 (100%)	93 (100%)	0	100	100
12	T	80/84 (95%)	80 (100%)	0	100	100
13	U	83/85 (98%)	83 (100%)	0	100	100
14	V	78/78 (100%)	78 (100%)	0	100	100
15	W	56/63 (89%)	56 (100%)	0	100	100
16	X	67/68 (98%)	66 (98%)	1 (2%)	60	77
17	Y	55/55 (100%)	55 (100%)	0	100	100
18	Z	48/49 (98%)	48 (100%)	0	100	100
19	0	47/48 (98%)	47 (100%)	0	100	100
20	1	45/49 (92%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	2	38/38 (100%)	37 (97%)	1 (3%)	41	66
23	I	109/110 (99%)	107 (98%)	2 (2%)	54	74
24	K	103/104 (99%)	103 (100%)	0	100	100
25	P	98/100 (98%)	98 (100%)	0	100	100
26	6	88/91 (97%)	88 (100%)	0	100	100
27	7	274/282 (97%)	271 (99%)	3 (1%)	70	82
28	8	135/161 (84%)	133 (98%)	2 (2%)	60	77
29	9	273/321 (85%)	271 (99%)	2 (1%)	81	88
30	M	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	113 (99%)	1 (1%)	75	85
33	e	100/123 (81%)	100 (100%)	0	100	100
34	F	148/150 (99%)	147 (99%)	1 (1%)	81	88
35	b	43/62 (69%)	43 (100%)	0	100	100
All	All	3539/3705 (96%)	3522 (100%)	17 (0%)	85	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	36	GLN
3	E	21	ARG
3	E	102	ARG
5	J	120	ARG
16	X	22	ASN
21	2	25	LYS
23	I	81	LYS
23	I	133	ARG
27	7	4	ARG
27	7	15	GLN
27	7	213	ARG
28	8	99	GLN
28	8	117	LYS
29	9	24	ARG
29	9	143	ASN
32	H	68	ARG
34	F	32	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	52	HIS
4	G	127	GLN
7	N	11	ASN
10	R	11	GLN
10	R	18	GLN
27	7	18	GLN
27	7	22	GLN
27	7	117	ASN
27	7	239	HIS
27	7	245	HIS
29	9	113	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	B	118/120 (98%)	18 (15%)	0
31	A	2911/2919 (99%)	474 (16%)	17 (0%)
All	All	3029/3039 (99%)	492 (16%)	17 (0%)

All (492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	B	15	A
22	B	16	G
22	B	30	C
22	B	35	C
22	B	36	C
22	B	41	G
22	B	43	C
22	B	44	G
22	B	45	A
22	B	46	A
22	B	52	A
22	B	53	A
22	B	56	G
22	B	87	U
22	B	89	U
22	B	90	C
22	B	99	A
22	B	109	A
31	A	10	A
31	A	12	U

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Mol	Chain	Res	Type
31	A	14	A
31	A	27	G
31	A	35	G
31	A	46	G
31	A	51	G
31	A	63	A
31	A	74	A
31	A	75	G
31	A	118	A
31	A	120	U
31	A	125	A
31	A	138	U
31	A	139	U
31	A	140	C
31	A	141	G
31	A	142	A
31	A	160	A
31	A	181	A
31	A	196	A
31	A	199	A
31	A	215	G
31	A	216	A
31	A	222	A
31	A	224	U
31	A	230	G
31	A	233	A
31	A	248	G
31	A	255	A
31	A	266	G
31	A	267	C
31	A	272	A
31	A	277	G
31	A	278	A
31	A	302	C
31	A	311	A
31	A	329	G
31	A	330	A
31	A	331	C
31	A	343	C
31	A	352	A
31	A	353	C
31	A	370	G

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Mol	Chain	Res	Type
31	A	371	A
31	A	372	G
31	A	384	A
31	A	385	C
31	A	386	G
31	A	396	G
31	A	401	A
31	A	404	A
31	A	405	U
31	A	411	G
31	A	424	G
31	A	430	A
31	A	451	U
31	A	452	G
31	A	456	C
31	A	466	A
31	A	480	A
31	A	481	G
31	A	491	G
31	A	496	G
31	A	504	A
31	A	505	A
31	A	508	A
31	A	532	A
31	A	533	G
31	A	543	G
31	A	544	C
31	A	546	U
31	A	547	A
31	A	548	G
31	A	550	C
31	A	563	A
31	A	568	U
31	A	573	U
31	A	575	A
31	A	586	A
31	A	588	U
31	A	603	A
31	A	614	A
31	A	615	U
31	A	621	A
31	A	627	A

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Mol	Chain	Res	Type
31	A	631	A
31	A	637	A
31	A	643	A
31	A	644	A
31	A	645	C
31	A	646	U
31	A	647	G
31	A	654	A
31	A	655	A
31	A	686	U
31	A	722	A
31	A	726	G
31	A	730	A
31	A	747	U
31	A	748	G
31	A	752	A
31	A	764	A
31	A	765	C
31	A	775	G
31	A	776	G
31	A	782	A
31	A	784	G
31	A	785	G
31	A	789	A
31	A	792	A
31	A	805	G
31	A	812	C
31	A	819	A
31	A	827	U
31	A	828	U
31	A	830	G
31	A	845	A
31	A	846	U
31	A	847	U
31	A	857	G
31	A	859	G
31	A	860	U
31	A	878	A
31	A	879	G
31	A	885	C
31	A	896	A
31	A	907	G

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Mol	Chain	Res	Type
31	A	910	A
31	A	915	C
31	A	931	U
31	A	941	A
31	A	946	C
31	A	959	A
31	A	961	C
31	A	973	A
31	A	974	G
31	A	983	A
31	A	985	C
31	A	995	C
31	A	996	A
31	A	1009	A
31	A	1010	A
31	A	1012	U
31	A	1013	C
31	A	1020	A
31	A	1022	G
31	A	1026	G
31	A	1033	U
31	A	1040	A
31	A	1046	A
31	A	1047	G
31	A	1056	G
31	A	1059	G
31	A	1060	U
31	A	1061	U
31	A	1062	G
31	A	1063	G
31	A	1065	U
31	A	1066	U
31	A	1068	G
31	A	1070	A
31	A	1071	G
31	A	1073	A
31	A	1075	C
31	A	1077	A
31	A	1078	U
31	A	1080	A
31	A	1081	U
31	A	1082	U

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Mol	Chain	Res	Type
31	A	1083	U
31	A	1084	A
31	A	1085	A
31	A	1088	A
31	A	1093	G
31	A	1097	U
31	A	1098	A
31	A	1101	U
31	A	1112	G
31	A	1132	U
31	A	1133	A
31	A	1135	C
31	A	1136	G
31	A	1142	A
31	A	1157	G
31	A	1168	G
31	A	1172	C
31	A	1173	U
31	A	1174	U
31	A	1175	A
31	A	1179	G
31	A	1180	U
31	A	1182	G
31	A	1212	G
31	A	1225	G
31	A	1236	G
31	A	1238	G
31	A	1253	A
31	A	1255	U
31	A	1256	G
31	A	1266	G
31	A	1272	A
31	A	1300	G
31	A	1301	A
31	A	1302	A
31	A	1314	C
31	A	1325	U
31	A	1329	U
31	A	1345	C
31	A	1365	A
31	A	1368	G
31	A	1378	A

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Mol	Chain	Res	Type
31	A	1383	A
31	A	1386	C
31	A	1395	A
31	A	1416	G
31	A	1419	A
31	A	1428	C
31	A	1452	G
31	A	1458	U
31	A	1476	U
31	A	1482	G
31	A	1504	A
31	A	1510	G
31	A	1515	A
31	A	1523	U
31	A	1534	U
31	A	1535	A
31	A	1555	G
31	A	1569	A
31	A	1578	U
31	A	1583	A
31	A	1585	C
31	A	1603	A
31	A	1607	C
31	A	1613	G
31	A	1634	A
31	A	1646	C
31	A	1647	U
31	A	1648	U
31	A	1654	A
31	A	1665	A
31	A	1667	G
31	A	1674	G
31	A	1715	G
31	A	1730	C
31	A	1732	C
31	A	1736	U
31	A	1737	G
31	A	1738	G
31	A	1764	C
31	A	1773	A
31	A	1781	U
31	A	1800	C

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Mol	Chain	Res	Type
31	A	1801	A
31	A	1808	A
31	A	1816	C
31	A	1829	A
31	A	1847	A
31	A	1870	C
31	A	1907	G
31	A	1909	C
31	A	1911	U
31	A	1912	A
31	A	1914	C
31	A	1915	U
31	A	1916	A
31	A	1917	U
31	A	1918	A
31	A	1919	A
31	A	1921	G
31	A	1922	G
31	A	1923	U
31	A	1925	C
31	A	1929	G
31	A	1930	G
31	A	1931	U
31	A	1934	C
31	A	1935	G
31	A	1936	A
31	A	1937	A
31	A	1938	A
31	A	1940	U
31	A	1941	C
31	A	1942	C
31	A	1945	G
31	A	1946	U
31	A	1955	U
31	A	1959	G
31	A	1961	C
31	A	1962	C
31	A	1964	G
31	A	1965	C
31	A	1966	A
31	A	1967	C
31	A	1968	G

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Mol	Chain	Res	Type
31	A	1970	A
31	A	1971	U
31	A	1972	G
31	A	1991	U
31	A	1992	G
31	A	1993	U
31	A	1997	C
31	A	2021	C
31	A	2022	U
31	A	2023	C
31	A	2030	A
31	A	2031	A
31	A	2033	A
31	A	2043	C
31	A	2050	C
31	A	2055	C
31	A	2056	G
31	A	2060	A
31	A	2061	G
31	A	2062	A
31	A	2069	G
31	A	2072	C
31	A	2093	G
31	A	2094	A
31	A	2096	C
31	A	2102	G
31	A	2105	U
31	A	2107	G
31	A	2110	G
31	A	2111	U
31	A	2112	G
31	A	2114	A
31	A	2115	G
31	A	2116	G
31	A	2117	A
31	A	2118	U
31	A	2119	A
31	A	2122	U
31	A	2123	G
31	A	2126	A
31	A	2128	G
31	A	2132	U

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Mol	Chain	Res	Type
31	A	2133	G
31	A	2136	G
31	A	2147	A
31	A	2148	G
31	A	2158	A
31	A	2162	G
31	A	2164	C
31	A	2165	C
31	A	2170	A
31	A	2171	A
31	A	2172	U
31	A	2173	A
31	A	2178	C
31	A	2198	A
31	A	2199	A
31	A	2204	G
31	A	2211	A
31	A	2225	A
31	A	2238	G
31	A	2239	G
31	A	2250	G
31	A	2251	G
31	A	2252	G
31	A	2255	G
31	A	2275	C
31	A	2279	G
31	A	2283	C
31	A	2287	A
31	A	2288	A
31	A	2297	A
31	A	2305	U
31	A	2307	G
31	A	2312	U
31	A	2314	A
31	A	2316	G
31	A	2317	A
31	A	2318	G
31	A	2321	U
31	A	2322	A
31	A	2325	G
31	A	2327	A
31	A	2333	A

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Mol	Chain	Res	Type
31	A	2336	A
31	A	2344	U
31	A	2345	G
31	A	2350	C
31	A	2357	G
31	A	2383	G
31	A	2385	C
31	A	2392	A
31	A	2402	U
31	A	2406	A
31	A	2420	C
31	A	2421	G
31	A	2422	C
31	A	2423	U
31	A	2425	A
31	A	2426	A
31	A	2428	G
31	A	2429	G
31	A	2430	A
31	A	2435	A
31	A	2441	U
31	A	2448	A
31	A	2449	U
31	A	2455	G
31	A	2456	C
31	A	2457	U
31	A	2458	G
31	A	2476	A
31	A	2478	A
31	A	2490	G
31	A	2491	U
31	A	2497	A
31	A	2498	C
31	A	2500	U
31	A	2502	G
31	A	2504	U
31	A	2505	G
31	A	2506	U
31	A	2513	A
31	A	2518	A
31	A	2520	C
31	A	2525	G

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Mol	Chain	Res	Type
31	A	2529	G
31	A	2535	G
31	A	2547	A
31	A	2554	U
31	A	2564	A
31	A	2566	A
31	A	2567	G
31	A	2572	A
31	A	2573	C
31	A	2586	U
31	A	2601	C
31	A	2602	A
31	A	2609	U
31	A	2610	C
31	A	2613	U
31	A	2615	U
31	A	2629	U
31	A	2630	G
31	A	2636	C
31	A	2639	A
31	A	2646	C
31	A	2647	U
31	A	2682	A
31	A	2684	U
31	A	2689	U
31	A	2690	U
31	A	2714	G
31	A	2718	G
31	A	2721	A
31	A	2726	A
31	A	2729	G
31	A	2733	A
31	A	2744	G
31	A	2748	A
31	A	2765	A
31	A	2778	A
31	A	2780	G
31	A	2791	G
31	A	2798	U
31	A	2818	U
31	A	2820	A
31	A	2825	G

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Mol	Chain	Res	Type
31	A	2835	A
31	A	2836	U
31	A	2867	G
31	A	2872	A
31	A	2873	A
31	A	2880	C
31	A	2883	A
31	A	2884	U
31	A	2886	A
31	A	2893	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	271	G
31	A	404	A
31	A	479	A
31	A	995	C
31	A	1070	A
31	A	1076	C
31	A	1080	A
31	A	1224	U
31	A	1606	C
31	A	1666	G
31	A	1736	U
31	A	1914	C
31	A	1936	A
31	A	2127	G
31	A	2249	U
31	A	2311	A
31	A	2425	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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
36	GDP	9	1001	29,37	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)

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
36	GDP	9	1001	29,37	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	9	1001	GDP	C6-N1	-2.38	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	9	1001	GDP	PA-O3A-PB	-3.64	120.34	132.83
36	9	1001	GDP	C3'-C2'-C1'	2.92	105.37	100.98
36	9	1001	GDP	C8-N7-C5	2.36	107.50	102.99
36	9	1001	GDP	C5-C6-N1	2.26	117.95	113.95

There are no chirality outliers.

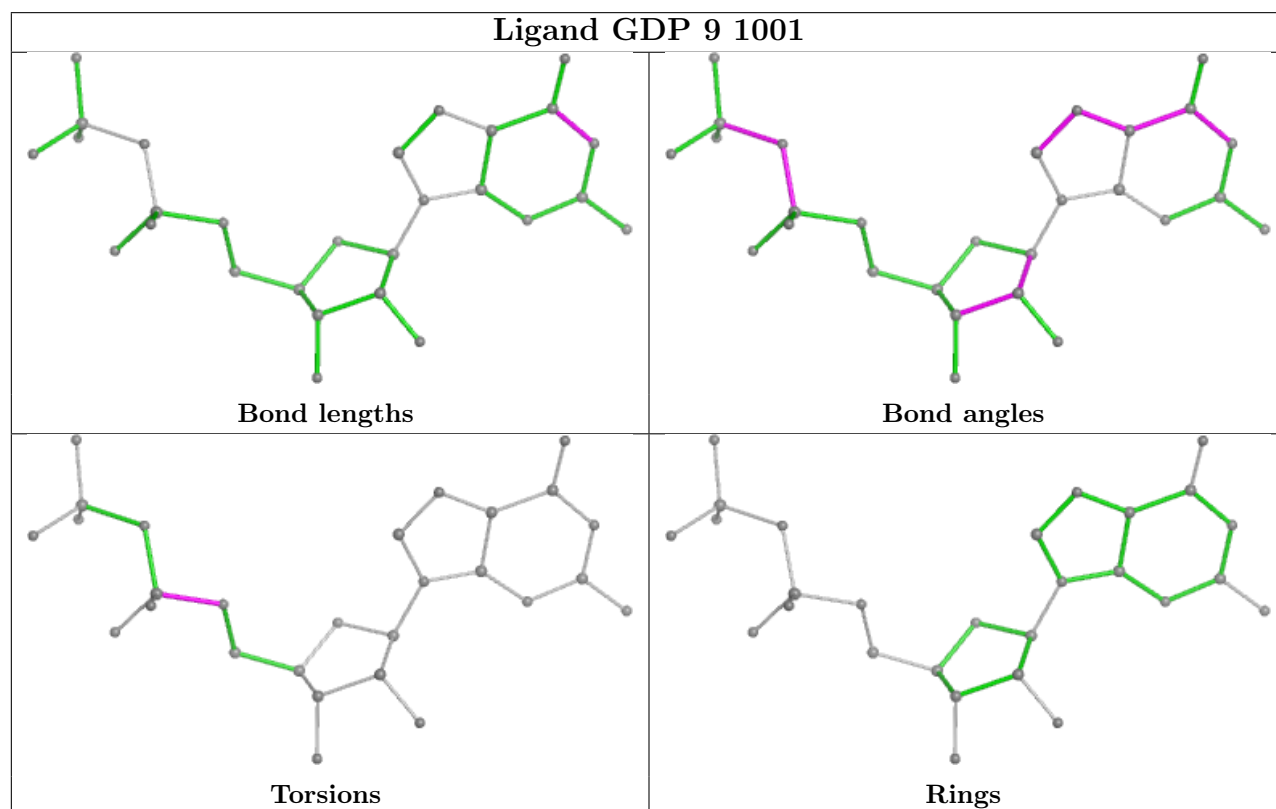
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	9	1001	GDP	C5'-O5'-PA-O1A
36	9	1001	GDP	C5'-O5'-PA-O2A
36	9	1001	GDP	C5'-O5'-PA-O3A

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.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12218. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.