



## wwPDB EM Validation Summary Report ⓘ

May 13, 2024 – 10:17 pm BST

PDB ID : 6SG9  
EMDB ID : EMD-10175  
Title : Head domain of the mt-SSU assemblosome from Trypanosoma brucei  
Authors : Saurer, M.; Ramrath, D.J.F.; Niemann, M.; Calderaro, S.; Prange, C.; Mattei, S.; Scaiola, A.; Leitner, A.; Bieri, P.; Horn, E.K.; Leibundgut, M.; Boehringer, D.; Schneider, A.; Ban, N.  
Deposited on : 2019-08-03  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary 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.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 3.10 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 104694 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 uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CE	23	Total	C	N	O	S	0	0
			200	132	35	31	2		

- Molecule 2 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CK	40	Total	C	N	O	S	0	0
			337	209	65	62	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7

- Molecule 3 is a protein called mS38.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Cn	18	Total	C	N	O	0	0
			154	103	28	23		

- Molecule 4 is a protein called mt-SAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	FJ	41	Total	C	N	O	S	0	0
			338	208	61	67	2		

- Molecule 5 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	FY	92	Total	C	N	O	S	0	0
			723	463	123	131	6		

- Molecule 6 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fa	39	Total	C	N	O	S	0	0
			297	192	55	49	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fa	73	ALA	VAL	conflict	UNP Q57VU7

- Molecule 7 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CA	146	Total	C	N	O	P	0	0
			2501	1098	308	949	146		

- Molecule 8 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CC	74	Total	C	N	O	S	0	0
			646	451	96	98	1		

- Molecule 9 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CI	423	Total	C	N	O	S	0	0
			3357	2108	601	631	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 10 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CJ	701	Total	C	N	O	S	0	0
			5709	3605	1017	1064	23		

- Molecule 11 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CN	153	Total	C	N	O	S	0	0
			1285	820	242	216	7		

- Molecule 12 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CS	85	Total	C	N	O	S	0	0
			708	463	121	121	3		

- Molecule 13 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Cg	484	Total	C	N	O	S	0	0
			3922	2511	688	703	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	MET	conflict	UNP Q585C2

- Molecule 14 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ci	147	Total	C	N	O	S	0	0
			1222	770	226	218	8		

- Molecule 15 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ck	638	Total	C	N	O	S	0	0
			5123	3220	927	953	23		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 16 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	DB	679	Total	C	N	O	S	0	0
			5688	3558	1062	1047	21		

- Molecule 17 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	DC	1028	Total	C	N	O	S	0	0
			8223	5194	1453	1546	30		

- Molecule 18 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DE	590	Total	C	N	O	S	0	0
			4639	2957	832	834	16		

- Molecule 19 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DF	491	Total	C	N	O	S	0	0
			3967	2496	745	703	23		

- Molecule 20 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DG	566	Total	C	N	O	S	0	0
			4575	2875	835	834	31		

- Molecule 21 is a protein called mS55 (KRIPP8).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DH	472	Total	C	N	O	S	0	0
			3849	2417	720	693	19		

- Molecule 22 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DJ	308	Total	C	N	O	S	0	0
			2521	1612	446	450	13		

- Molecule 23 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DK	245	Total	C	N	O	S	0	0
			1929	1213	349	362	5		

- Molecule 24 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DT	221	Total	C	N	O	S	0	0
			1912	1231	334	337	10		

- Molecule 25 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DV	157	Total	C	N	O	S	0	0
			1323	840	248	231	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 26 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DW	133	Total	C	N	O	S	0	0
			1140	730	216	190	4		

- Molecule 27 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DX	115	Total	C	N	O	S	0	0
			967	612	182	166	7		

- Molecule 28 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	DY	154	Total	C	N	O	S	0	0
			1295	829	247	214	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DY	34	HIS	ASP	conflict	UNP Q57YD4

- Molecule 29 is a protein called mt-SAF1 (RSM22).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F1	833	Total	C	N	O	S	0	0
			6729	4212	1265	1213	39		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	707	SER	GLY	conflict	UNP Q385R2
F1	973	THR	MET	conflict	UNP Q385R2

- Molecule 30 is a protein called mt-SAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F4	541	Total	C	N	O	S	0	0
			4382	2783	775	802	22		

- Molecule 31 is a protein called mt-SAF12 (KRIPP18).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	FD	394	Total	C	N	O	S	0	0
			3135	2004	546	566	19		

- Molecule 32 is a protein called mt-SAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FF	408	Total	C	N	O	S	0	0
			3265	2052	586	603	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	70	ALA	PRO	conflict	UNP Q57W60
FF	179	PHE	LEU	conflict	UNP Q57W60

- Molecule 33 is a protein called mt-SAF15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	FG	169	Total	C	N	O	S	0	0
			1359	852	260	240	7		

- Molecule 34 is a protein called mt-SAF16.



Mol	Chain	Residues	Atoms					AltConf	Trace
34	FH	317	Total	C	N	O	S	0	0
			2486	1555	440	471	20		

- Molecule 35 is a protein called mt-SAF17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	FI	348	Total	C	N	O	S	0	0
			2786	1726	510	537	13		

- Molecule 36 is a protein called mt-SAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	FK	208	Total	C	N	O	S	0	0
			1699	1084	284	325	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FK	38	HIS	ARG	conflict	UNP Q57XS8

- Molecule 37 is a protein called mt-SAF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	FL	320	Total	C	N	O	S	0	0
			2555	1609	470	459	17		

- Molecule 38 is a protein called mt-SAF25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	FV	210	Total	C	N	O	S	0	0
			1636	1039	283	303	11		

- Molecule 39 is a protein called mt-SAF34.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Fe	122	Total	C	N	O	S	0	0
			1033	642	200	184	7		

- Molecule 40 is a protein called UNK-a.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	Ua	47	Total	C	N	O	0	0
			282	188	47	47		

- Molecule 41 is a protein called UNK-b.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Ub	42	Total	C	N	O	0	0
			252	168	42	42		

- Molecule 42 is a protein called UNK-c.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Uc	12	Total	C	N	O	0	0
			72	48	12	12		

- Molecule 43 is a protein called UNK-d.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Ud	59	Total	C	N	O	0	0
			354	236	59	59		

- Molecule 44 is a protein called UNK-e.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Ue	29	Total	C	N	O	0	0
			174	116	29	29		

- Molecule 45 is a protein called UNK-f.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Uf	9	Total	C	N	O	0	0
			54	36	9	9		

- Molecule 46 is a protein called UNK-g.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Ug	167	Total	C	N	O	0	0
			1002	668	167	167		

- Molecule 47 is a protein called UNK-h.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Uh	255	Total	C	N	O	0	0
			1530	1020	255	255		

- Molecule 48 is a protein called UNK-i.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Ui	32	Total	C	N	O	0	0
			192	128	32	32		

- Molecule 49 is a protein called UNK-j.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	Uj	19	Total	C	N	O	0	0
			114	76	19	19		

- Molecule 50 is a protein called UNK-k.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Uk	27	Total	C	N	O	0	0
			162	108	27	27		

- Molecule 51 is a protein called UNK-l.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ul	14	Total	C	N	O	0	0
			84	56	14	14		

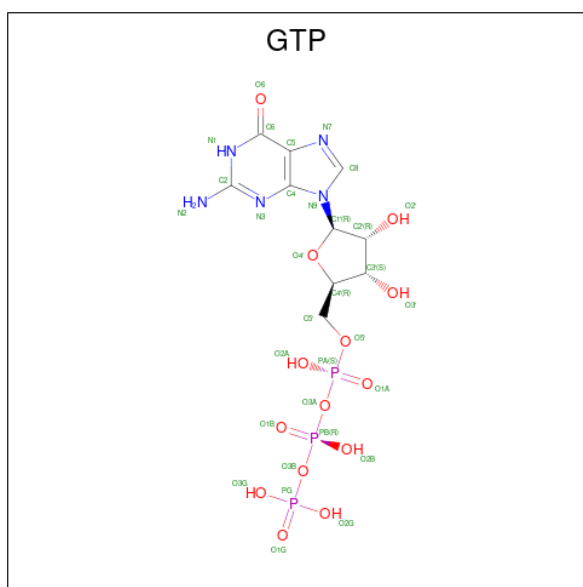
- Molecule 52 is a protein called UNK-m.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Um	11	Total	C	N	O	0	0
			66	44	11	11		

- Molecule 53 is a protein called UNK-x.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Ux	108	Total	C	N	O	0	0
			648	432	108	108		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
54	CgA	1	Total	C	N	O	P	0
			32	10	5	14	3	

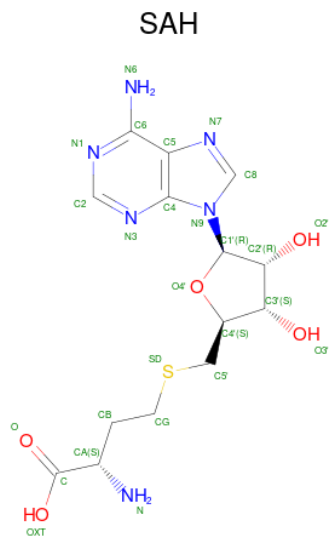
- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	CgB	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	F1A	1	Total	Zn	0
			1	1	
56	FGA	1	Total	Zn	0
			1	1	
56	FLA	1	Total	Zn	0
			1	1	
56	FLB	1	Total	Zn	0
			1	1	
56	FeA	1	Total	Zn	0
			1	1	

- Molecule 57 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					AltConf
57	F1B	1	Total 26	C 14	N 6	O 5	S 1	0
57	FFA	1	Total 26	C 14	N 6	O 5	S 1	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms	AltConf
58	CgC	3	Total O 3 3	0

MolProbity failed to run properly - this section is therefore empty.

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; On the fly in RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z  > 2$
54	GTP	CgA	1	-	26,34,34	1.13	1 (3%)	32,54,54	1.66	8 (25%)
57	SAH	FFA	1	-	24,28,28	1.22	3 (12%)	25,40,40	1.75	5 (20%)
57	SAH	F1B	1	-	24,28,28	1.19	3 (12%)	25,40,40	1.71	5 (20%)

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
54	GTP	CgA	1	-	-	5/18/38/38	0/3/3/3
57	SAH	FFA	1	-	-	1/11/31/31	0/3/3/3
57	SAH	F1B	1	-	-	3/11/31/31	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CgA	1	GTP	C5-C6	-4.04	1.39	1.47
57	FFA	1	SAH	C2-N3	4.00	1.38	1.32
57	F1B	1	SAH	C2-N3	3.84	1.38	1.32
57	FFA	1	SAH	C2-N1	2.45	1.38	1.33
57	F1B	1	SAH	C2-N1	2.38	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	F1B	1	SAH	N3-C2-N1	-5.42	120.21	128.68
57	FFA	1	SAH	N3-C2-N1	-5.36	120.30	128.68
57	FFA	1	SAH	C5'-SD-CG	-4.21	89.64	102.27
57	F1B	1	SAH	C5'-SD-CG	-3.94	90.45	102.27
54	CgA	1	GTP	C3'-C2'-C1'	3.67	106.50	100.98

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	CgA	1	GTP	C5'-O5'-PA-O3A

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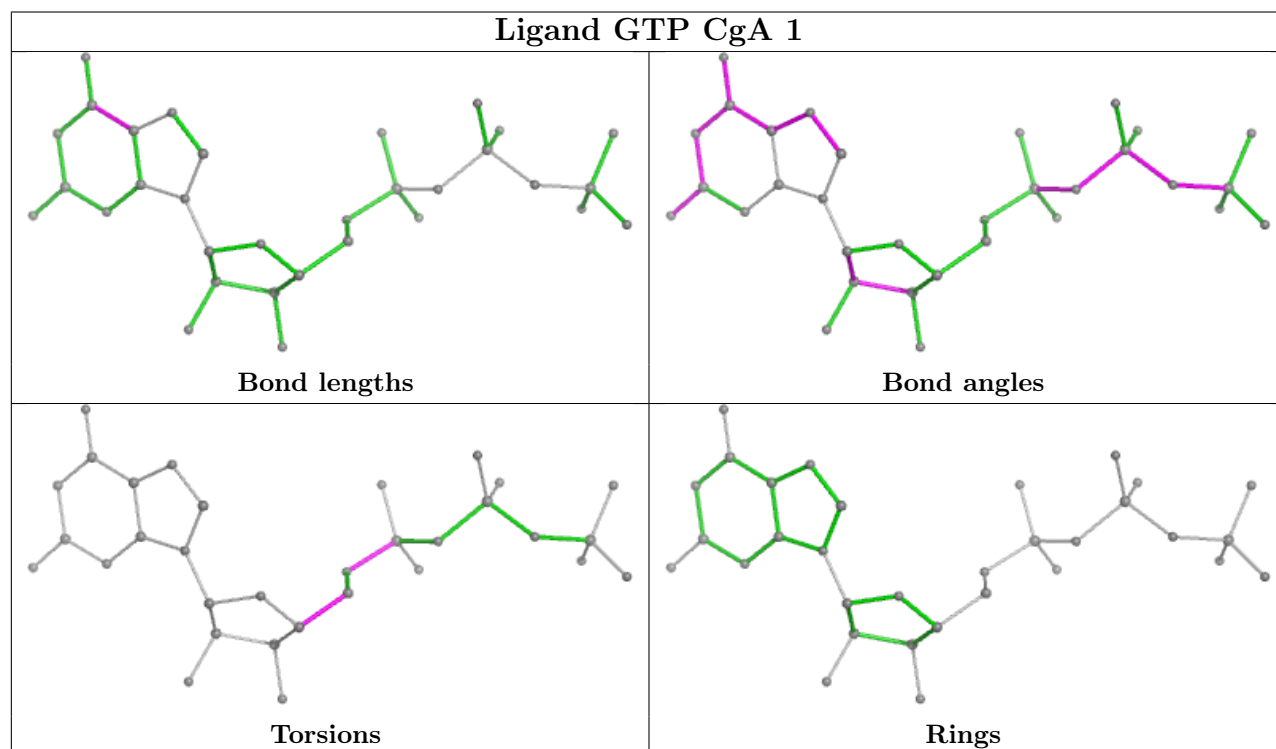
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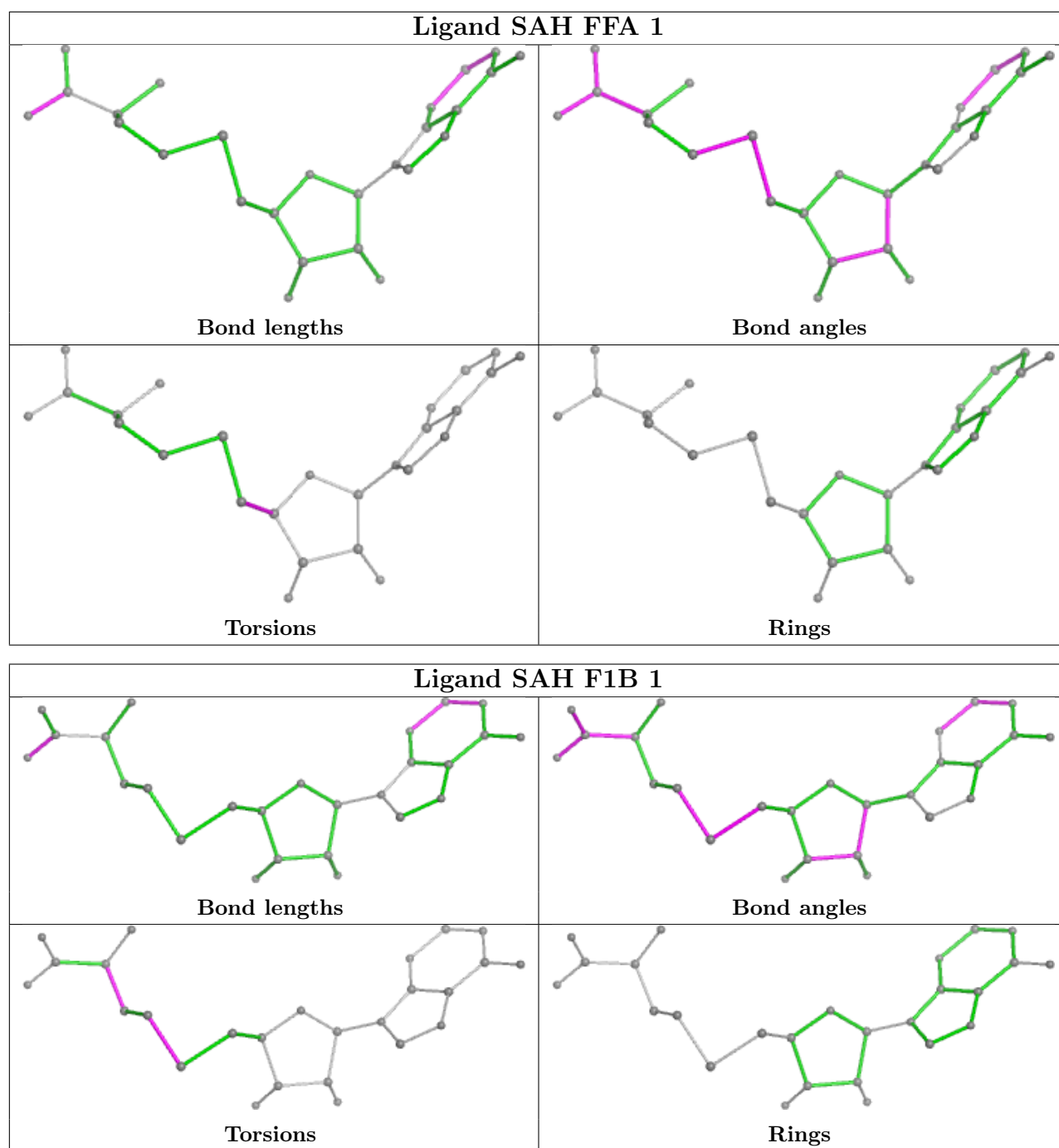
Mol	Chain	Res	Type	Atoms
54	CgA	1	GTP	C5'-O5'-PA-O1A
54	CgA	1	GTP	C5'-O5'-PA-O2A
57	F1B	1	SAH	N-CA-CB-CG
57	F1B	1	SAH	C-CA-CB-CG

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.





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	Uh	11
46	Ug	10
53	Ux	3

The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Uh	219:UNK	C	267:UNK	N	51.70
1	Uh	13:UNK	C	14:UNK	N	49.42
1	Uh	88:UNK	C	98:UNK	N	42.41
1	Uh	124:UNK	C	125:UNK	N	39.54
1	Uh	199:UNK	C	200:UNK	N	38.31

## 5 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10175. 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.

### 5.1 Orthogonal projections ⓘ

This section was not generated.

### 5.2 Central slices ⓘ

This section was not generated.

### 5.3 Largest variance slices ⓘ

This section was not generated.

### 5.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

### 5.5 Orthogonal surface views ⓘ

This section was not generated.

### 5.6 Mask visualisation ⓘ

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

## 6 Map analysis ⓘ

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

### 6.1 Map-value distribution ⓘ

This section was not generated.

### 6.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 6.3 Rotationally averaged power spectrum ⓘ

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

## 7 Fourier-Shell correlation ⓘ

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

## 8 Map-model fit

This section was not generated.