



## wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 04:27 AM UTC

PDB ID : 9HIP / pdb\_00009hip  
EMDB ID : EMD-52197  
Title : MnmE-MnmG a2b2 complex  
Authors : Maes, L.; Galicia, C.; Fislage, M.; Versees, W.  
Deposited on : 2024-11-27  
Resolution : 3.31 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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

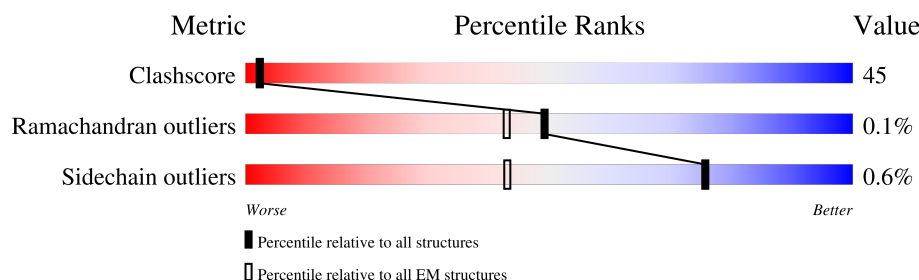
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.31 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	A	454	33% 67%
1	B	454	39% 60% .
2	C	649	46% 49% . .
2	D	649	33% 46% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GNP	A	501	-	-	X	-
3	GNP	B	501	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15846 atoms, of which 26 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 tRNA modification GTPase MnmE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3458	2164	618	668	8		
1	B	451	Total	C	N	O	S	0	0
			3418	2141	611	658	8		

- Molecule 2 is a protein called tRNA uridine 5-carboxymethylaminomethyl modification enzyme MnmG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	624	Total	C	N	O	S	0	0
			4846	3035	872	917	22		
2	D	514	Total	C	N	O	S	0	0
			3981	2499	710	754	18		

There are 40 discrepancies between the modelled and reference sequences:

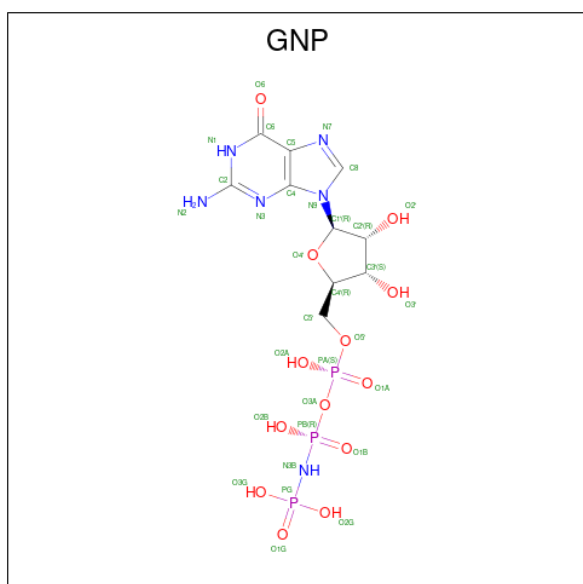
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP P0A6U3
C	-18	GLY	-	expression tag	UNP P0A6U3
C	-17	SER	-	expression tag	UNP P0A6U3
C	-16	SER	-	expression tag	UNP P0A6U3
C	-15	HIS	-	expression tag	UNP P0A6U3
C	-14	HIS	-	expression tag	UNP P0A6U3
C	-13	HIS	-	expression tag	UNP P0A6U3
C	-12	HIS	-	expression tag	UNP P0A6U3
C	-11	HIS	-	expression tag	UNP P0A6U3
C	-10	HIS	-	expression tag	UNP P0A6U3
C	-9	SER	-	expression tag	UNP P0A6U3
C	-8	SER	-	expression tag	UNP P0A6U3
C	-7	GLY	-	expression tag	UNP P0A6U3
C	-6	GLU	-	expression tag	UNP P0A6U3
C	-5	ASN	-	expression tag	UNP P0A6U3
C	-4	LEU	-	expression tag	UNP P0A6U3

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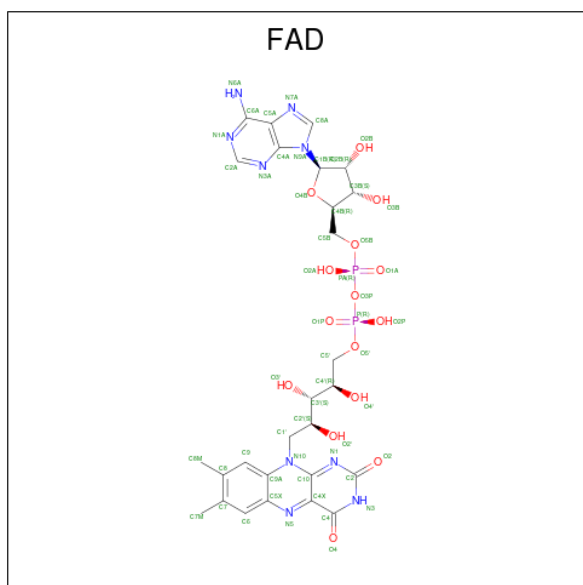
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	expression tag	UNP P0A6U3
C	-2	PHE	-	expression tag	UNP P0A6U3
C	-1	GLN	-	expression tag	UNP P0A6U3
C	0	GLY	-	expression tag	UNP P0A6U3
D	-19	MET	-	initiating methionine	UNP P0A6U3
D	-18	GLY	-	expression tag	UNP P0A6U3
D	-17	SER	-	expression tag	UNP P0A6U3
D	-16	SER	-	expression tag	UNP P0A6U3
D	-15	HIS	-	expression tag	UNP P0A6U3
D	-14	HIS	-	expression tag	UNP P0A6U3
D	-13	HIS	-	expression tag	UNP P0A6U3
D	-12	HIS	-	expression tag	UNP P0A6U3
D	-11	HIS	-	expression tag	UNP P0A6U3
D	-10	HIS	-	expression tag	UNP P0A6U3
D	-9	SER	-	expression tag	UNP P0A6U3
D	-8	SER	-	expression tag	UNP P0A6U3
D	-7	GLY	-	expression tag	UNP P0A6U3
D	-6	GLU	-	expression tag	UNP P0A6U3
D	-5	ASN	-	expression tag	UNP P0A6U3
D	-4	LEU	-	expression tag	UNP P0A6U3
D	-3	TYR	-	expression tag	UNP P0A6U3
D	-2	PHE	-	expression tag	UNP P0A6U3
D	-1	GLN	-	expression tag	UNP P0A6U3
D	0	GLY	-	expression tag	UNP P0A6U3

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
3	A	1	Total 45	C 10	H 13	N 6	O 13	P 3	0
3	B	1	Total 45	C 10	H 13	N 6	O 13	P 3	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).

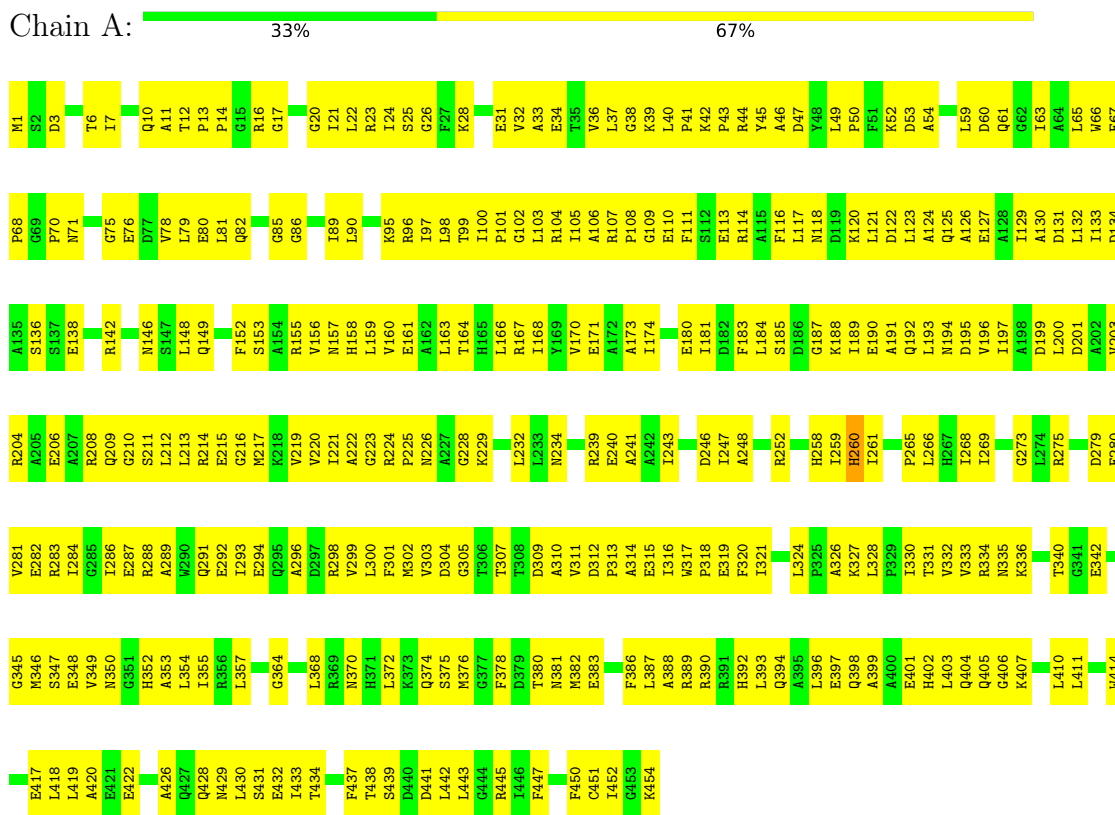


Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			53	27	9	15	2	

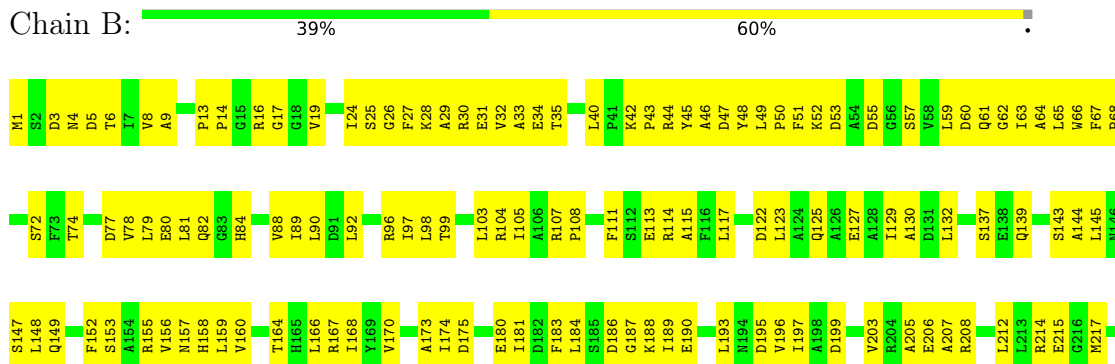
### 3 Residue-property plots

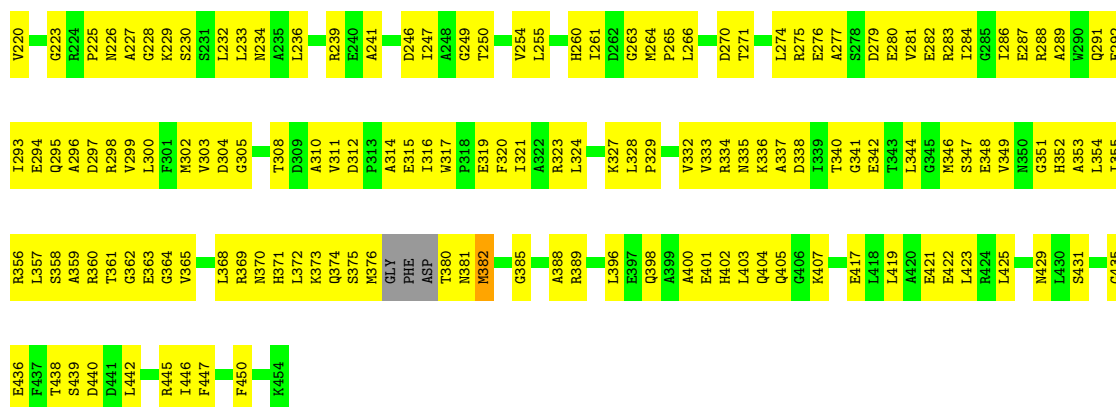
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: tRNA modification GTPase MnME



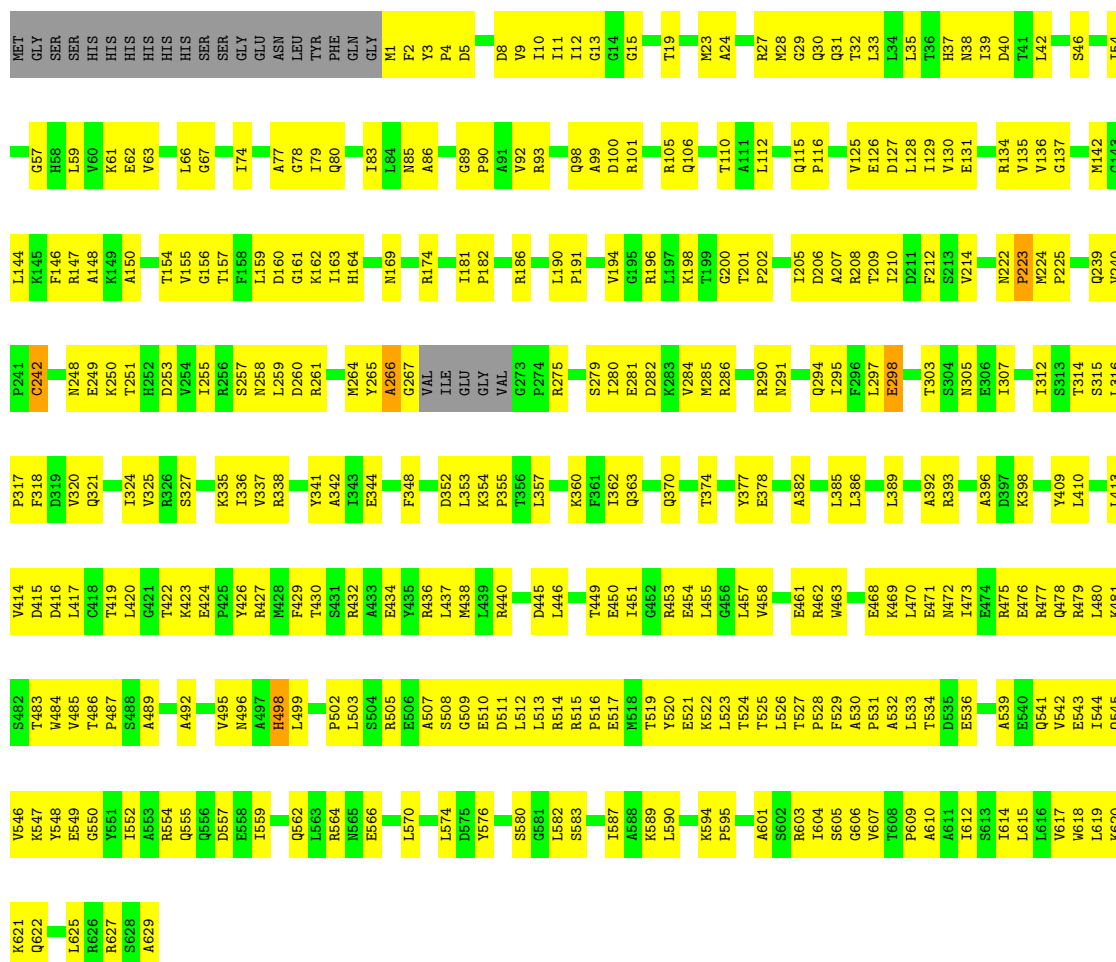
#### • Molecule 1: tRNA modification GTPase MnME





• Molecule 2: tRNA uridine 5-carboxymethylaminomethyl modification enzyme MnmG

Chain C: 46% 49%



• Molecule 2: tRNA uridine 5-carboxymethylaminomethyl modification enzyme MnmG

Chain D: 33% 46% 21%

GLN	GLY	MET	GLN	GLY	MET
LEU	ARG	GLY	LEU	GLY	GLY
ASN	ASN	SER	ASN	SER	SER
GLU	GLU	HIS	GLU	HIS	HIS
ASN	ASN	HIS	ASN	HIS	HIS
THR	THR	HIS	THR	HIS	HIS
LEU	LEU	HIS	LEU	HIS	HIS
PRO	PRO	HIS	PRO	HIS	HIS
ALA	ALA	SER	ALA	SER	SER
THR	THR	SER	THR	SER	SER
LEU	LEU	GLY	LEU	GLY	GLY
ASP	ASP	GLU	ASP	GLU	GLU
TYR	TYR	ASN	TYR	ASN	ASN
ARG	ARG	LEU	ARG	LEU	LEU
GLN	GLN	TYR	GLN	TYR	TYR
R514	R514	R82	R514	R82	R82
R515	R515	R96	R515	R96	R96
R516	R516	R104	R516	R104	R104
R517	R517	R109	R517	R109	R109
R518	R518	R112	R518	R112	R112
R519	R519	R113	R519	R113	R113
R520	R520	R114	R520	R114	R114
R521	R521	R115	R521	R115	R115
R522	R522	R116	R522	R116	R116
R523	R523	R117	R523	R117	R117
R524	R524	R118	R524	R118	R118
R525	R525	R119	R525	R119	R119
R526	R526	R120	R526	R120	R120
R527	R527	R121	R527	R121	R121
R528	R528	R122	R528	R122	R122
R529	R529	R123	R529	R123	R123
R530	R530	R124	R530	R124	R124
R531	R531	R125	R531	R125	R125
R532	R532	R126	R532	R126	R126
R533	R533	R127	R533	R127	R127
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R535	R535	R129	R535	R129	R129
R536	R536	R130	R536	R130	R130
R537	R537	R131	R537	R131	R131
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R539	R539	R133	R539	R133	R133
R540	R540	R134	R540	R134	R134
R541	R541	R135	R541	R135	R135
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R552	R552	R146	R552	R146	R146
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R575	R575	R169	R575	R169	R169
R576	R576	R170	R576	R170	R170
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R578	R578	R172	R578	R172	R172
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R682	R682	R276	R682	R276	R276
R683	R683	R277	R683	R277	R277
R684	R684	R278	R684	R278	R278
R685	R685	R279	R685	R279	R279
R686	R686	R280	R686	R280	R280
R687	R687	R281	R687	R281	R281
R688	R688	R282	R688	R282	R282
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R690	R690	R284	R690	R284	R284
R691	R691	R285	R691	R285	R285
R692	R692	R286	R692	R286	R286
R693	R693	R287	R693	R287	R287
R694	R694	R288	R694	R288	R288
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R699	R699	R293	R699	R293	R293
R700	R700	R294	R700	R294	R294
R701	R701	R295	R701	R295	R295
R702	R702	R296	R702	R296	R296
R703	R703	R297	R703	R297	R297
R704	R704	R298	R704	R298	R298
R705	R705	R299	R705	R299	R299
R706	R706	R300	R706	R300	R300
R707	R707	R301	R707	R301	R301
R708	R708	R302	R708	R302	R302
R709	R709	R303	R709	R303	R303
R710	R710	R304	R710	R304	R304
R711	R711	R305	R711	R305	R305
R712	R712	R306	R712	R306	R306
R713	R713	R307	R713	R307	R307
R714	R714	R308	R714	R308	R308
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R721	R721	R315	R721	R315	R315
R722	R722	R316	R722	R316	R316
R723	R723	R317	R723	R317	R317
R724	R724	R318	R724	R318	R318
R725	R725	R319	R725	R319	R319
R726	R726	R320	R726	R320	R320
R727	R727	R321	R727	R321	R321
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R731	R731	R325	R731	R325	R325
R732	R732	R326	R732	R326	R326
R733	R733	R327	R733	R327	R327
R734	R734	R328	R734	R328	R328
R735	R735	R329	R735	R329	R329
R736	R736	R330	R736	R330	R330
R737	R737	R331	R737	R331	R331
R738	R738</				



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116023	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, GNP

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	A	0.06	0/3511	0.20	0/4752
1	B	0.07	0/3469	0.21	0/4698
2	C	0.09	0/4934	0.25	0/6678
2	D	0.08	0/4055	0.25	1/5492 (0.0%)
All	All	0.08	0/15969	0.23	1/21620 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	312	ILE	N-CA-C	-5.47	107.95	113.20

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3452	436	0
1	B	3418	0	3409	346	0
2	C	4846	0	4847	340	0
2	D	3981	0	3966	334	0
3	A	32	13	13	14	0
3	B	32	13	13	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	53	0	31	2	0
All	All	15820	26	15731	1409	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

The worst 5 of 1409 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:ALA:HB3	2:C:492:ALA:HB2	1.38	1.05
1:B:358:SER:HB3	1:B:363:GLU:HB2	1.33	1.04
2:D:156:GLY:HA2	2:D:370:GLN:HB2	1.38	1.03
2:D:472:ASN:HB3	2:D:533:LEU:HD11	1.41	1.02
2:D:28:MET:HE1	2:D:389:LEU:HA	1.40	0.99

There are no symmetry-related clashes.

## 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	A	452/454 (100%)	435 (96%)	17 (4%)	0	100	100
1	B	447/454 (98%)	414 (93%)	33 (7%)	0	100	100
2	C	620/649 (96%)	579 (93%)	39 (6%)	2 (0%)	36	66
2	D	510/649 (79%)	478 (94%)	32 (6%)	0	100	100
All	All	2029/2206 (92%)	1906 (94%)	121 (6%)	2 (0%)	49	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	223	PRO

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Mol	Chain	Res	Type
2	C	266	ALA

### 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	A	356/359 (99%)	355 (100%)	1 (0%)	86	85
1	B	350/359 (98%)	348 (99%)	2 (1%)	78	80
2	C	511/533 (96%)	506 (99%)	5 (1%)	68	75
2	D	417/533 (78%)	416 (100%)	1 (0%)	87	87
All	All	1634/1784 (92%)	1625 (99%)	9 (1%)	76	80

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	529	PHE
2	D	37	HIS
2	C	37	HIS
2	C	242	CYS
2	C	298	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	218	GLN
2	C	555	GLN
2	C	238	GLN
2	D	218	GLN
2	C	390	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 [i](#)

3 ligands 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$
3	GNP	B	501	-	34,34,34	1.67	6 (17%)	47,54,54	1.78	10 (21%)
4	FAD	C	701	-	58,58,58	1.29	3 (5%)	85,89,89	0.71	1 (1%)
3	GNP	A	501	-	34,34,34	1.53	6 (17%)	47,54,54	2.02	12 (25%)

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
3	GNP	B	501	-	-	9/18/38/38	0/3/3/3
4	FAD	C	701	-	-	12/34/50/50	0/6/6/6
3	GNP	A	501	-	-	11/18/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	FAD	P-O3P	6.55	1.66	1.59
3	B	501	GNP	PG-N3B	4.46	1.75	1.63
3	B	501	GNP	PB-N3B	4.21	1.74	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GNP	PG-N3B	4.11	1.74	1.63
4	C	701	FAD	PA-O3P	3.98	1.63	1.59

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GNP	C5-C4-N3	-5.96	118.91	128.39
3	B	501	GNP	C5-C4-N3	-5.92	118.97	128.39
3	B	501	GNP	N9-C4-N3	4.64	135.24	125.95
3	A	501	GNP	C2-N3-C4	4.50	120.05	112.30
3	B	501	GNP	C2-N3-C4	4.27	119.65	112.30

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

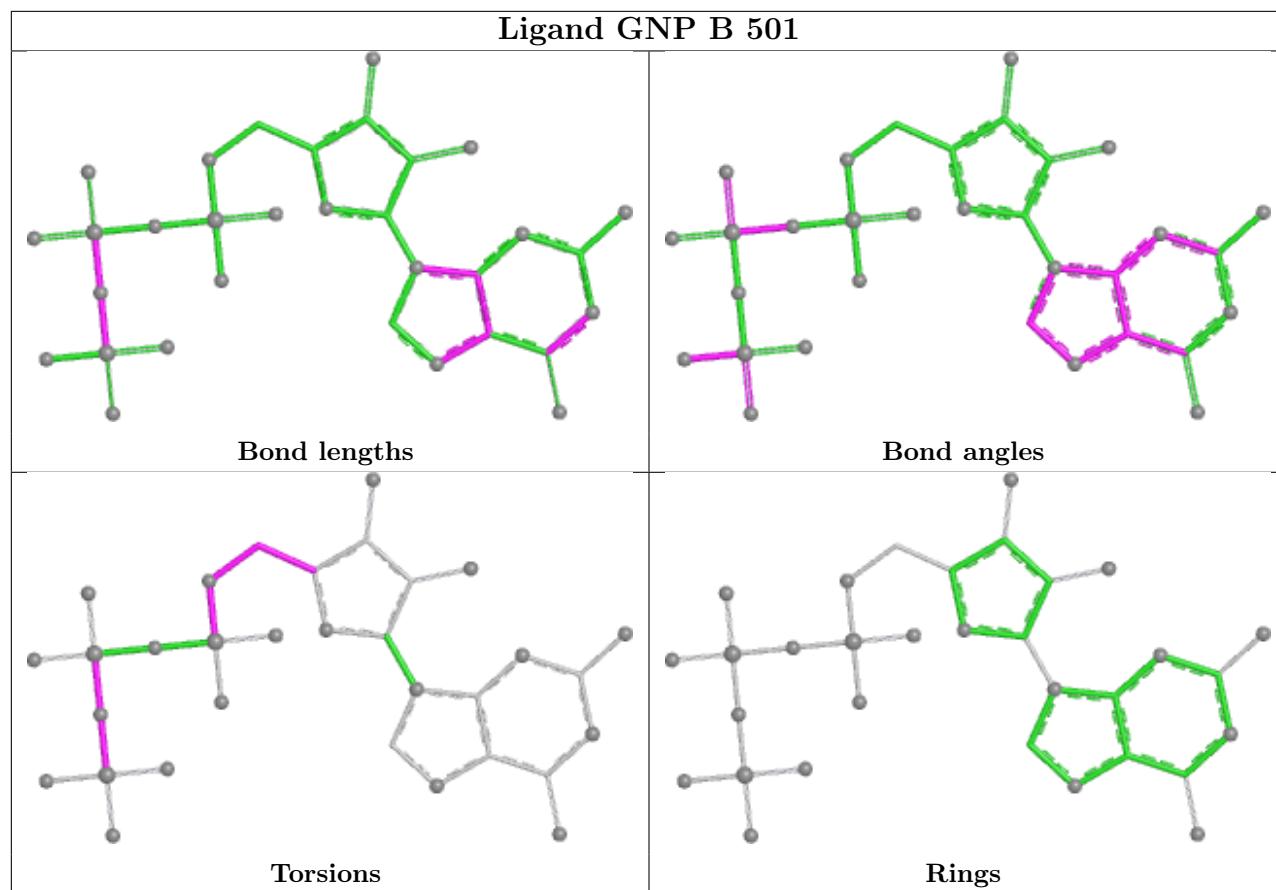
Mol	Chain	Res	Type	Atoms
3	A	501	GNP	PG-N3B-PB-O1B
3	A	501	GNP	PG-N3B-PB-O3A
3	A	501	GNP	PA-O3A-PB-O2B
3	A	501	GNP	C5'-O5'-PA-O1A
3	A	501	GNP	C5'-O5'-PA-O2A

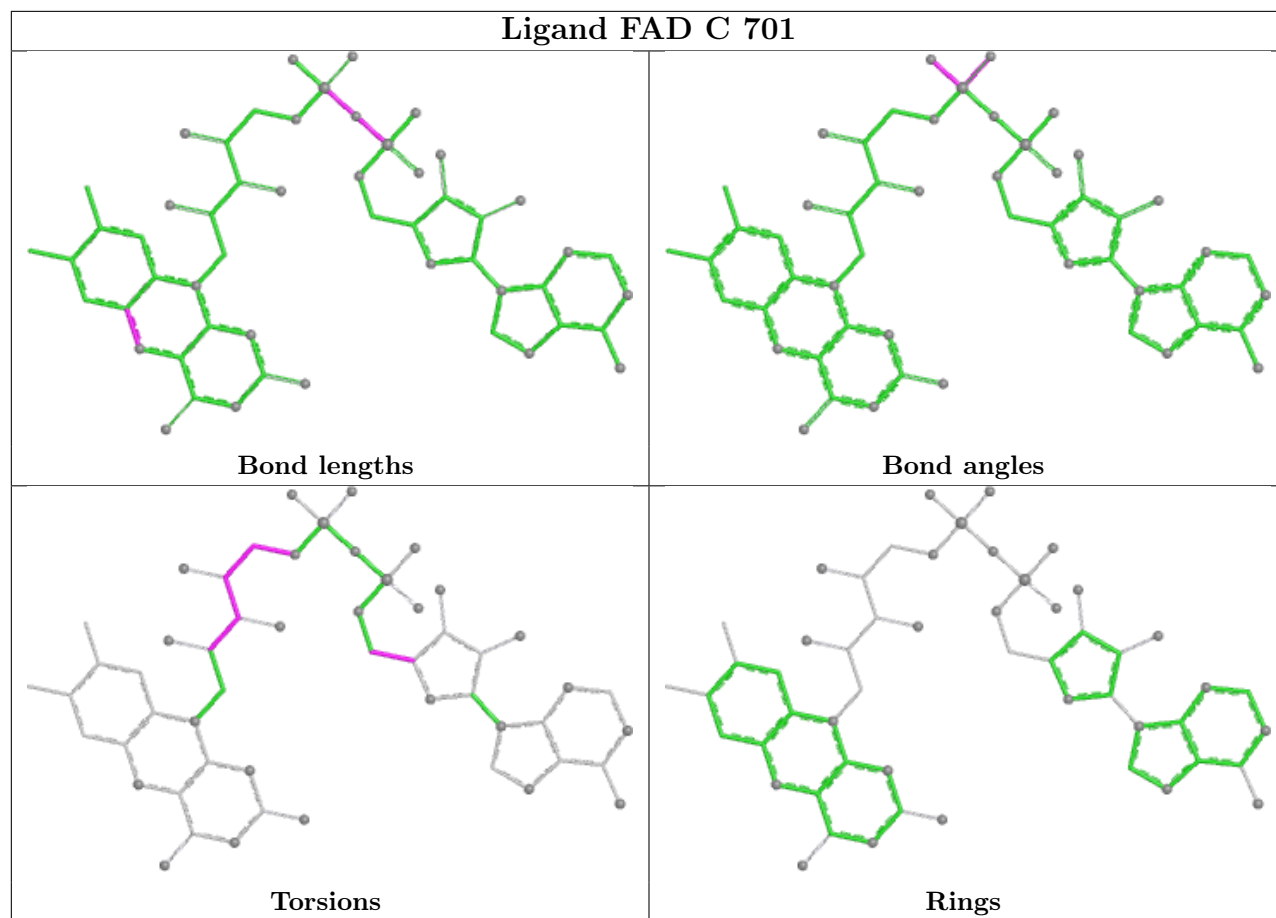
There are no ring outliers.

3 monomers are involved in 31 short contacts:

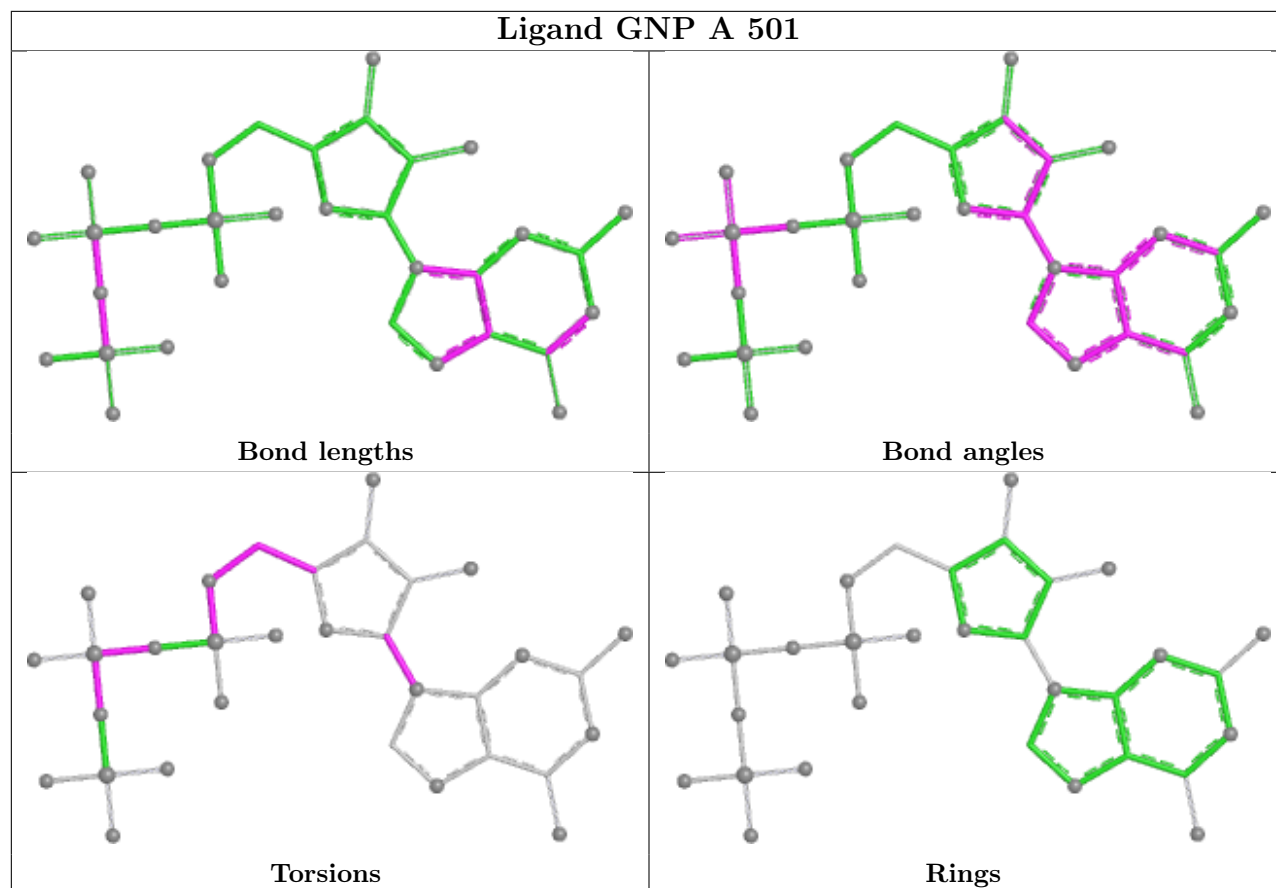
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	GNP	15	0
4	C	701	FAD	2	0
3	A	501	GNP	14	0

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-52197. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 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.