



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 12:20 pm GMT

PDB ID : 7Z2B  
EMDB ID : EMD-14460  
Title : P. berghei kinesin-8B motor domain in AMPPNP state bound to tubulin dimer  
Authors : Liu, T.; Shilliday, F.; Cook, A.D.; Moores, C.A.  
Deposited on : 2022-02-26  
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.

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

EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

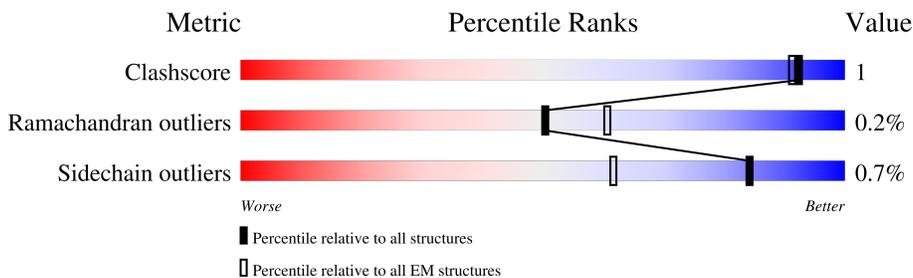
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

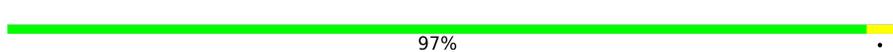
The reported resolution of this entry is 3.30 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	K	341	85% 
2	A	428	97% 
3	H	426	96% 

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17947 atoms, of which 8823 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 Kinesin-8, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	K	308	4772	1493	2390	417	456	16	0	0

- Molecule 2 is a protein called Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	428	6569	2116	3238	571	624	20	0	0

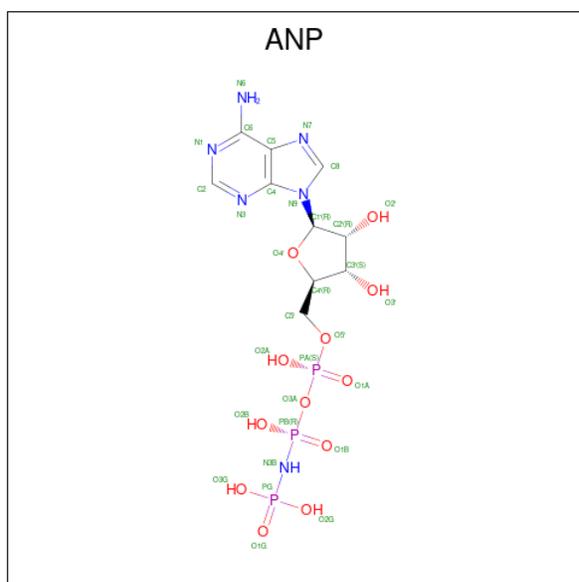
There are 9 discrepancies between the modelled and reference sequences:

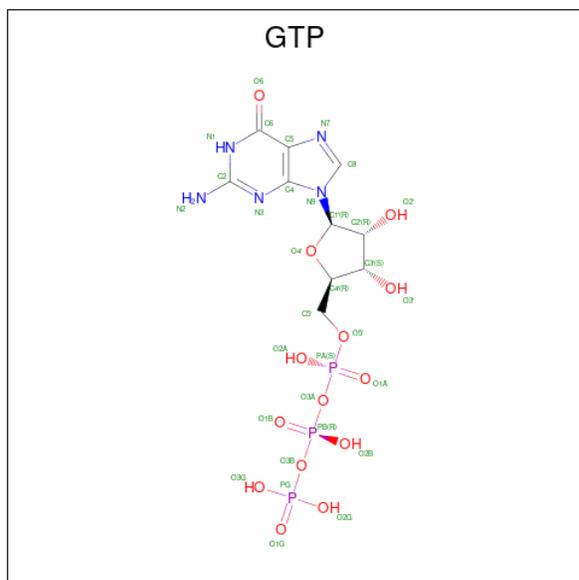
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q2XVP4
A	?	-	ASP	deletion	UNP Q2XVP4
A	?	-	LYS	deletion	UNP Q2XVP4
A	?	-	THR	deletion	UNP Q2XVP4
A	?	-	ILE	deletion	UNP Q2XVP4
A	?	-	GLY	deletion	UNP Q2XVP4
A	?	-	GLY	deletion	UNP Q2XVP4
A	?	-	GLY	deletion	UNP Q2XVP4
A	?	-	ASP	deletion	UNP Q2XVP4

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	H	426	6482	2083	3169	571	635	24	0	0

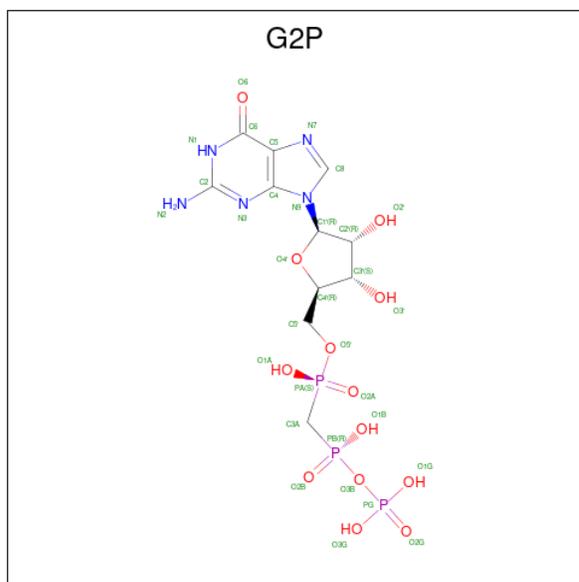
- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).





Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
6	A	1	44	10	12	5	14	3	0

- Molecule 7 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

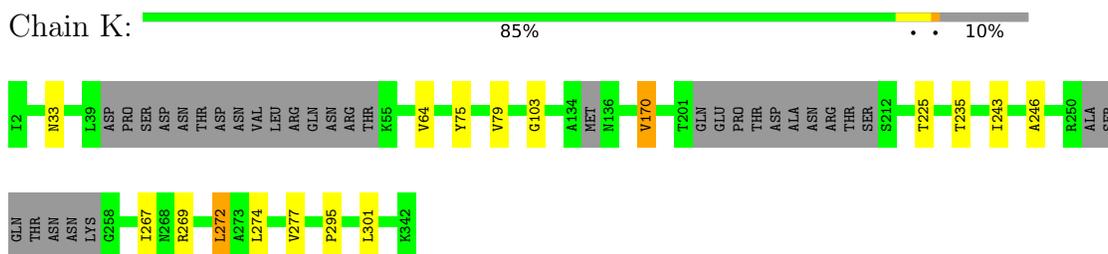


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
7	H	1	46	11	14	5	13	3	0

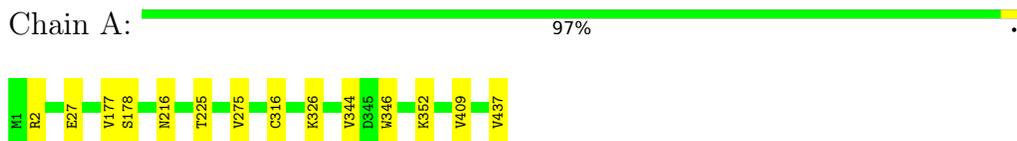
### 3 Residue-property plots

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.

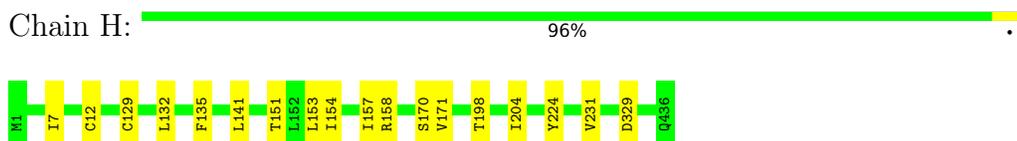
- Molecule 1: Kinesin-8, putative



- Molecule 2: Detyrosinated tubulin alpha-1B chain



- Molecule 3: Tubulin beta chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87907	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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: ANP, MG, G2P, GTP

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	K	0.85	1/2409 (0.0%)	0.87	1/3236 (0.0%)
2	A	0.47	0/3408	0.71	0/4630
3	H	0.46	0/3387	0.70	0/4592
All	All	0.59	1/9204 (0.0%)	0.75	1/12458 (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
1	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	79	VAL	CB-CG2	-5.17	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	75	TYR	CB-CG-CD1	-6.65	117.01	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	170	VAL	Peptide

## 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	K	2382	2390	2389	10	0
2	A	3331	3238	3237	5	0
3	H	3313	3169	3169	11	0
4	K	31	0	13	2	0
5	A	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	A	32	12	12	0	0
7	H	32	14	14	0	0
All	All	9124	8823	8834	25	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 1.

All (25) 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)
1:K:272:LEU:HD22	2:A:409:VAL:HG21	1.83	0.60
3:H:12:CYS:SG	3:H:171:VAL:HG21	2.44	0.57
3:H:135:PHE:CZ	3:H:157:ILE:HG23	2.45	0.52
1:K:277:VAL:HG22	1:K:295:PRO:HG2	1.92	0.51
2:A:177:VAL:HG13	3:H:329:ASP:HB3	1.93	0.50
1:K:274:LEU:HD22	1:K:301:LEU:HD21	1.94	0.48
3:H:141:LEU:HD13	3:H:170:SER:HB3	1.96	0.47
1:K:274:LEU:HD22	1:K:301:LEU:CD2	2.45	0.47
1:K:269:ARG:HA	1:K:272:LEU:HD23	2.00	0.43
1:K:246:ALA:HB3	1:K:267:ILE:HG23	2.01	0.43
4:K:401:ANP:H8	4:K:401:ANP:O2A	2.19	0.42
3:H:151:THR:O	3:H:154:ILE:HG22	2.20	0.42
1:K:33:ASN:O	1:K:64:VAL:N	2.52	0.42
1:K:103:GLY:HA2	4:K:401:ANP:O2A	2.20	0.42
2:A:216:ASN:HB3	2:A:275:VAL:O	2.21	0.41
1:K:225:THR:HA	1:K:235:THR:HG22	2.02	0.41
3:H:204:ILE:HD13	3:H:231:VAL:HG13	2.03	0.41
3:H:154:ILE:CD1	3:H:198:THR:CG2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:ILE:O	3:H:158:ARG:HG2	2.22	0.40
3:H:154:ILE:HD12	3:H:198:THR:HG22	2.02	0.40
3:H:7:ILE:HG21	3:H:153:LEU:HD23	2.02	0.40
2:A:316:CYS:HA	2:A:352:LYS:O	2.21	0.40
2:A:344:VAL:HG11	2:A:346:TRP:NE1	2.36	0.40
1:K:243:ILE:HD12	1:K:243:ILE:N	2.36	0.40
3:H:129:CYS:SG	3:H:132:LEU:HB3	2.61	0.40

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	K	298/341 (87%)	287 (96%)	10 (3%)	1 (0%)	41 71
2	A	424/428 (99%)	409 (96%)	14 (3%)	1 (0%)	47 77
3	H	424/426 (100%)	412 (97%)	12 (3%)	0	100 100
All	All	1146/1195 (96%)	1108 (97%)	36 (3%)	2 (0%)	50 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	2	ARG
1	K	170	VAL

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

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	K	263/306 (86%)	262 (100%)	1 (0%)	91	95
2	A	354/362 (98%)	349 (99%)	5 (1%)	67	82
3	H	356/367 (97%)	355 (100%)	1 (0%)	92	96
All	All	973/1035 (94%)	966 (99%)	7 (1%)	84	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	272	LEU
2	A	27	GLU
2	A	178	SER
2	A	225	THR
2	A	326	LYS
2	A	437	VAL
3	H	224	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 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
6	GTP	A	501	5	26,34,34	1.15	2 (7%)	33,54,54	2.02	9 (27%)
7	G2P	H	501	5	26,34,34	2.86	9 (34%)	30,54,54	1.83	9 (30%)
4	ANP	K	401	5	29,33,33	1.81	6 (20%)	31,52,52	3.21	18 (58%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	A	501	5	-	5/18/38/38	0/3/3/3
7	G2P	H	501	5	-	3/18/38/38	0/3/3/3
4	ANP	K	401	5	-	3/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	501	G2P	C4-N9	-10.91	1.33	1.47
4	K	401	ANP	PG-O1G	4.67	1.53	1.46
7	H	501	G2P	PB-O2B	4.16	1.61	1.51
7	H	501	G2P	PA-O2A	4.10	1.61	1.51
6	A	501	GTP	C5-C6	4.03	1.48	1.41
4	K	401	ANP	O4'-C1'	3.91	1.46	1.41
4	K	401	ANP	PA-O5'	3.88	1.75	1.59
7	H	501	G2P	PB-O1B	-3.53	1.48	1.56
7	H	501	G2P	PA-O1A	-3.39	1.48	1.56
4	K	401	ANP	O5'-C5'	-3.20	1.32	1.44
7	H	501	G2P	C8-N9	-3.01	1.35	1.45
7	H	501	G2P	PA-O5'	2.49	1.61	1.57
4	K	401	ANP	PB-N3B	2.38	1.69	1.63
4	K	401	ANP	PG-O3G	-2.36	1.50	1.56
7	H	501	G2P	PB-O3B	2.27	1.60	1.58
6	A	501	GTP	C5-C4	2.20	1.46	1.40
7	H	501	G2P	C5-C6	-2.07	1.49	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	401	ANP	C5'-C4'-C3'	-7.21	88.17	115.18
4	K	401	ANP	PB-O3A-PA	-6.45	109.90	132.62
4	K	401	ANP	O5'-C5'-C4'	5.96	129.49	108.99
4	K	401	ANP	O3A-PB-N3B	-5.21	92.14	106.59
4	K	401	ANP	N3-C2-N1	-5.11	120.69	128.68
6	A	501	GTP	C2-N3-C4	4.91	120.96	115.36
4	K	401	ANP	O5'-PA-O1A	-4.84	90.17	109.07
4	K	401	ANP	O2A-PA-O5'	-4.75	85.68	107.75
6	A	501	GTP	C4-C5-C6	-4.33	116.67	120.80
7	H	501	G2P	O4'-C4'-C3'	-4.22	96.76	105.11
6	A	501	GTP	C2-N1-C6	4.00	122.28	115.93
6	A	501	GTP	C5-C6-N1	-3.84	118.18	123.43
6	A	501	GTP	N3-C2-N1	-3.46	122.61	127.22
6	A	501	GTP	C4-C5-N7	-3.45	105.80	109.40
4	K	401	ANP	O2B-PB-O3A	3.39	115.97	104.64
7	H	501	G2P	PB-O3B-PG	-3.19	121.39	132.62
7	H	501	G2P	O2'-C2'-C1'	3.13	120.50	110.02
4	K	401	ANP	PA-O5'-C5'	-3.10	103.52	121.68
6	A	501	GTP	PB-O3B-PG	-3.03	122.43	132.83
7	H	501	G2P	O2'-C2'-C3'	-2.96	102.25	111.82
4	K	401	ANP	O1G-PG-N3B	2.85	115.97	111.77
6	A	501	GTP	C1'-N9-C4	-2.75	121.80	126.64
4	K	401	ANP	C2'-C3'-C4'	2.68	107.85	102.64
7	H	501	G2P	O1B-PB-O2B	2.67	118.97	110.07
7	H	501	G2P	C3'-C2'-C1'	-2.66	96.38	101.43
7	H	501	G2P	O5'-C5'-C4'	-2.63	99.94	108.99
4	K	401	ANP	O4'-C4'-C5'	-2.60	100.81	109.37
4	K	401	ANP	O4'-C1'-C2'	2.55	110.66	106.93
4	K	401	ANP	O2A-PA-O1A	2.49	124.57	112.24
4	K	401	ANP	O2G-PG-O1G	-2.46	107.27	113.45
6	A	501	GTP	PA-O3A-PB	-2.45	124.41	132.83
7	H	501	G2P	C4-C5-N7	2.38	105.61	102.46
4	K	401	ANP	C1'-N9-C4	-2.26	122.66	126.64
4	K	401	ANP	C2-N1-C6	2.10	122.34	118.75
4	K	401	ANP	O4'-C4'-C3'	2.00	109.08	105.11
7	H	501	G2P	O4'-C1'-N9	2.00	112.02	109.04

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	401	ANP	PB-N3B-PG-O1G
4	K	401	ANP	PG-N3B-PB-O1B

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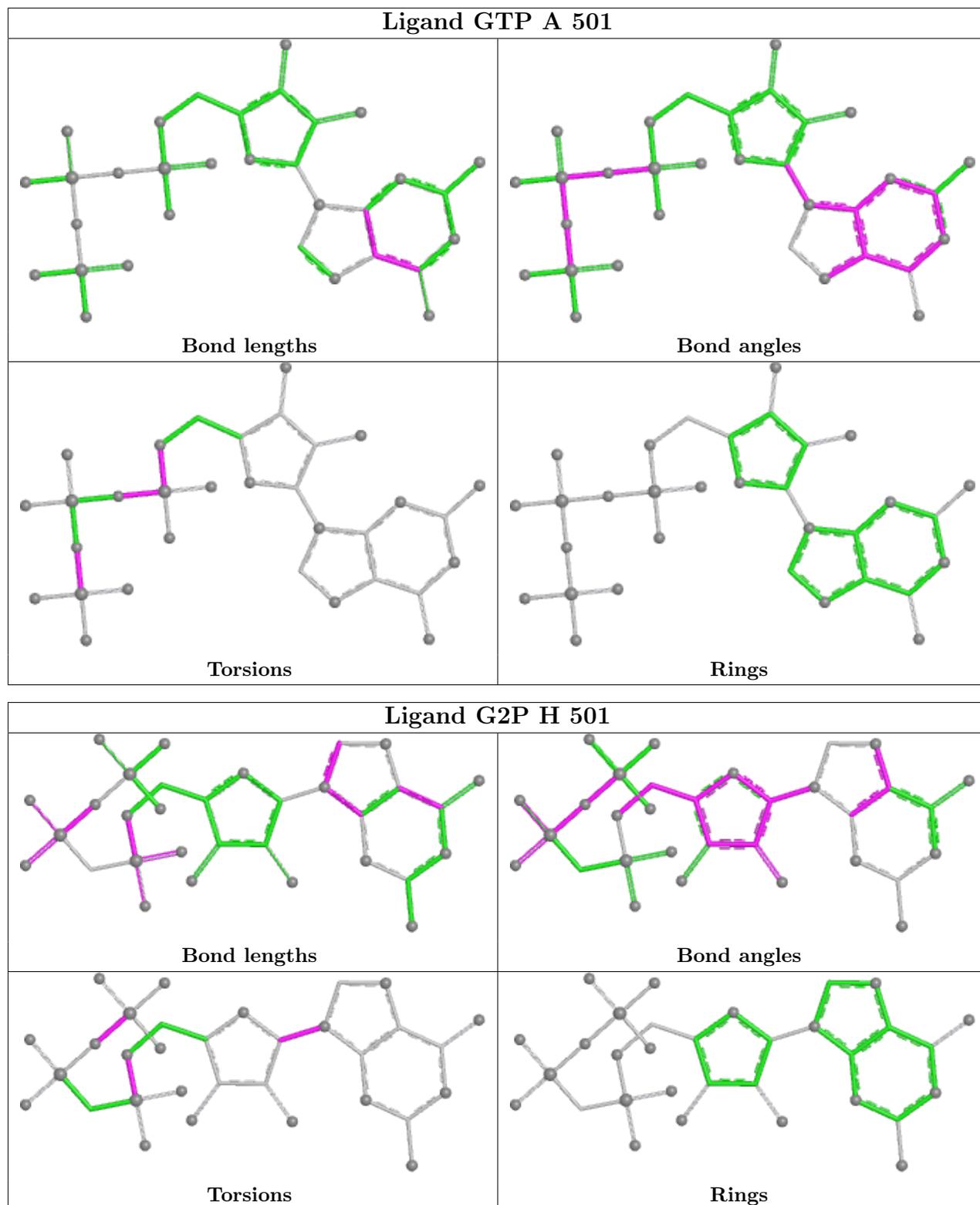
Mol	Chain	Res	Type	Atoms
6	A	501	GTP	PB-O3B-PG-O3G
6	A	501	GTP	C5'-O5'-PA-O1A
6	A	501	GTP	C5'-O5'-PA-O2A
7	H	501	G2P	C2'-C1'-N9-C4
4	K	401	ANP	PG-N3B-PB-O3A
7	H	501	G2P	C5'-O5'-PA-O1A
7	H	501	G2P	PB-O3B-PG-O1G
6	A	501	GTP	C5'-O5'-PA-O3A
6	A	501	GTP	PB-O3A-PA-O1A

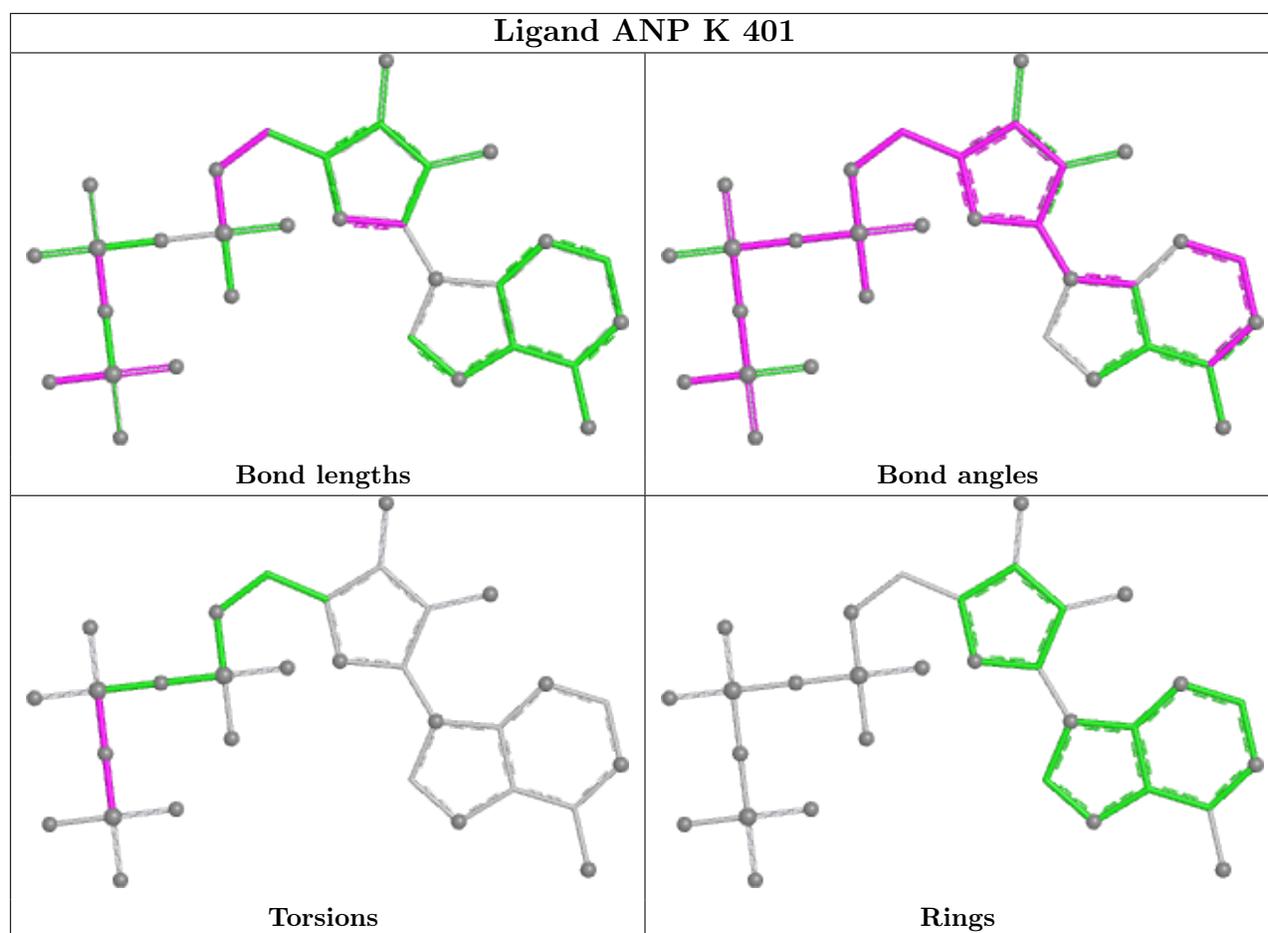
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	401	ANP	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	37:PRO	C	47:ASP	N	14.01

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14460. 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 surface views

This section was not generated.

### 6.5 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.