



wwPDB/EMDataBank EM Map/Model Validation Summary Report

Jul 11, 2018 – 03:13 PM EDT


PDB ID : 2P4N
EMDB ID: : EMD-1340
Title : Human Monomeric Kinesin (1BG2) and Bovine Tubulin (1JFF) Docked into the 9-Angstrom Cryo-EM Map of Nucleotide-Free Kinesin Complexed to the Microtubule
Authors : Sindelar, C.V.; Downing, K.H.
Deposited on : 2007-03-12
Resolution : 9.00 Å (reported)
Based on PDB ID : 1BG2, 1JFF

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the  symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

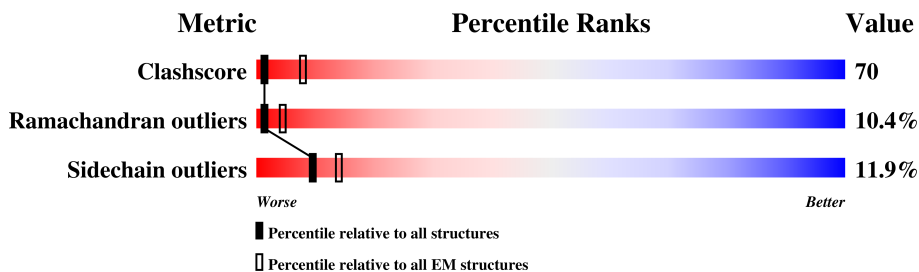
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	325	75% 22% ...
2	A	451	15% 57% 17% • 9%
3	B	445	20% 55% 18% • •

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9264 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 Kinesin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	K	323	2534	1578	434	507	15	0	0

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	412	3227	2043	551	613	20	0	0

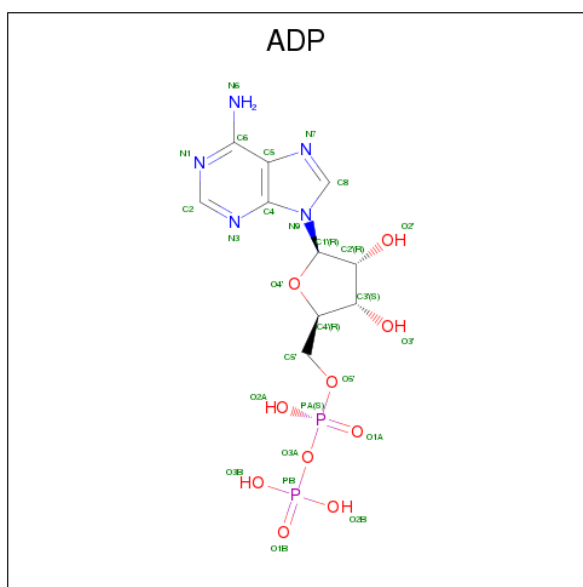
- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	426	3351	2105	575	646	25	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	K	1	1	1	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

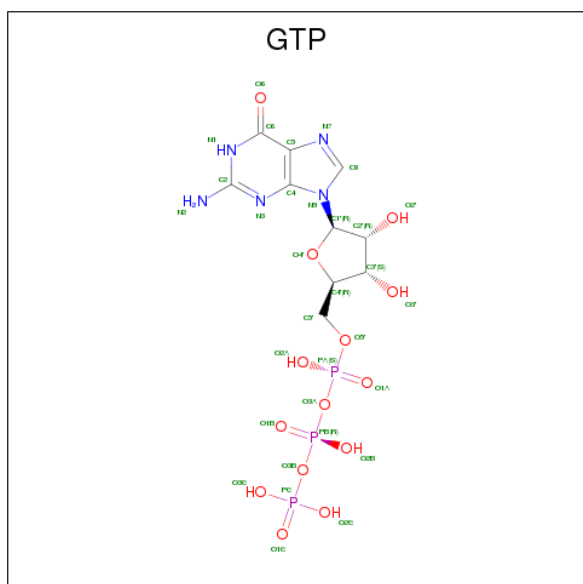


Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

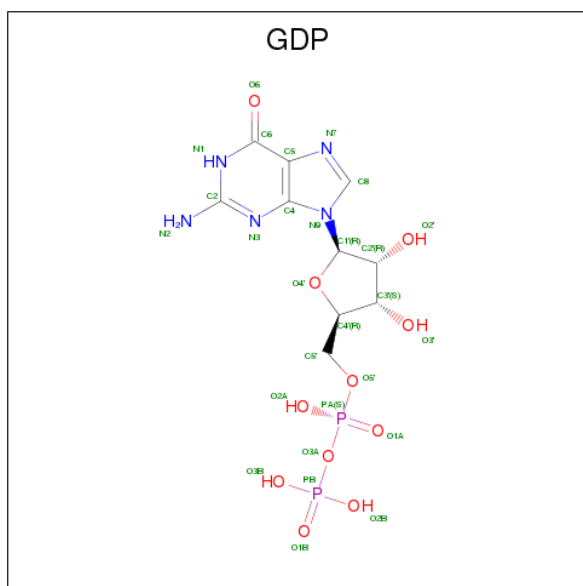
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



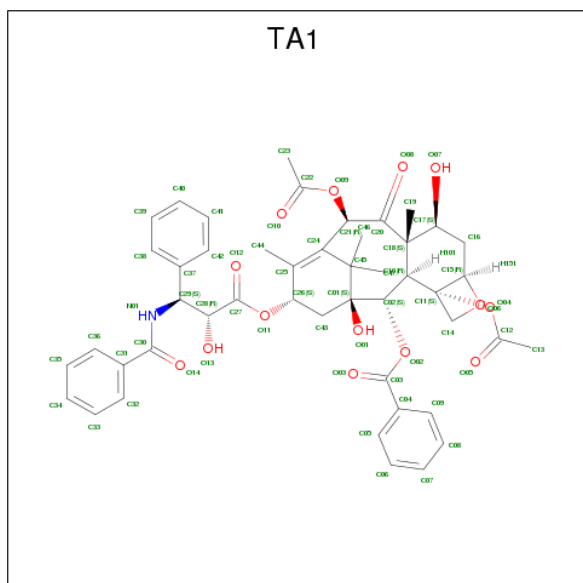
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
7	B	1	32	10	5	14	3	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).

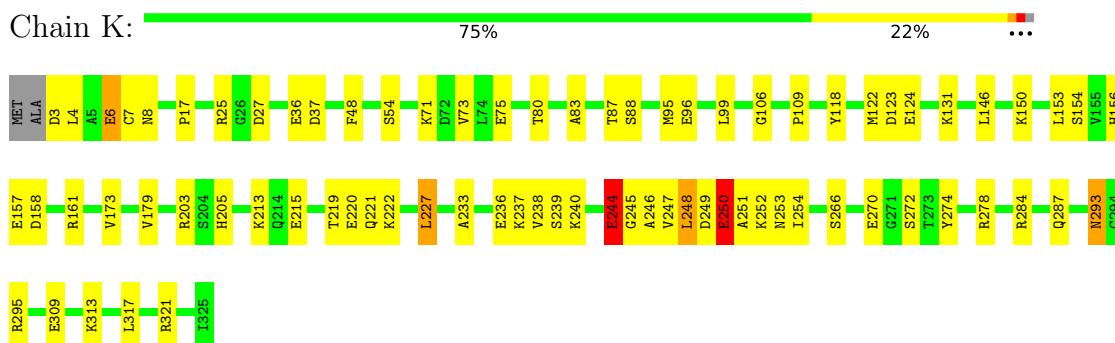


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	62	47	1	14	0

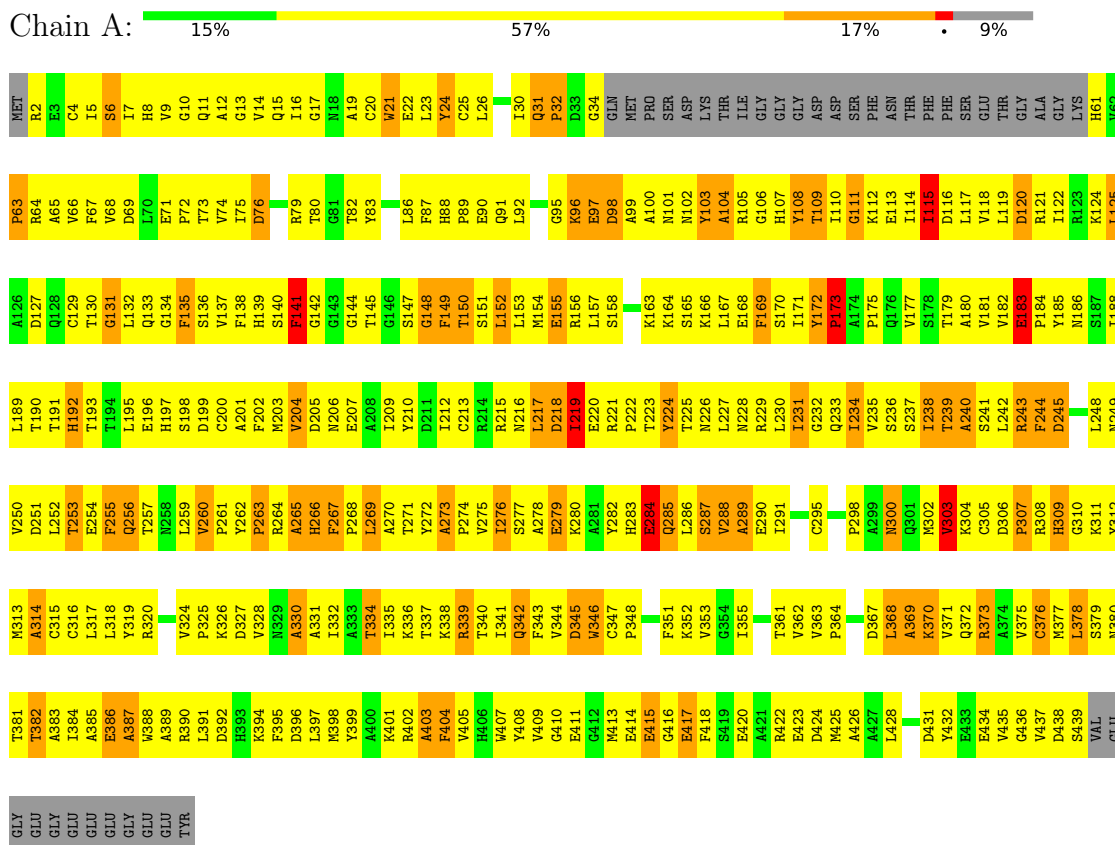
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

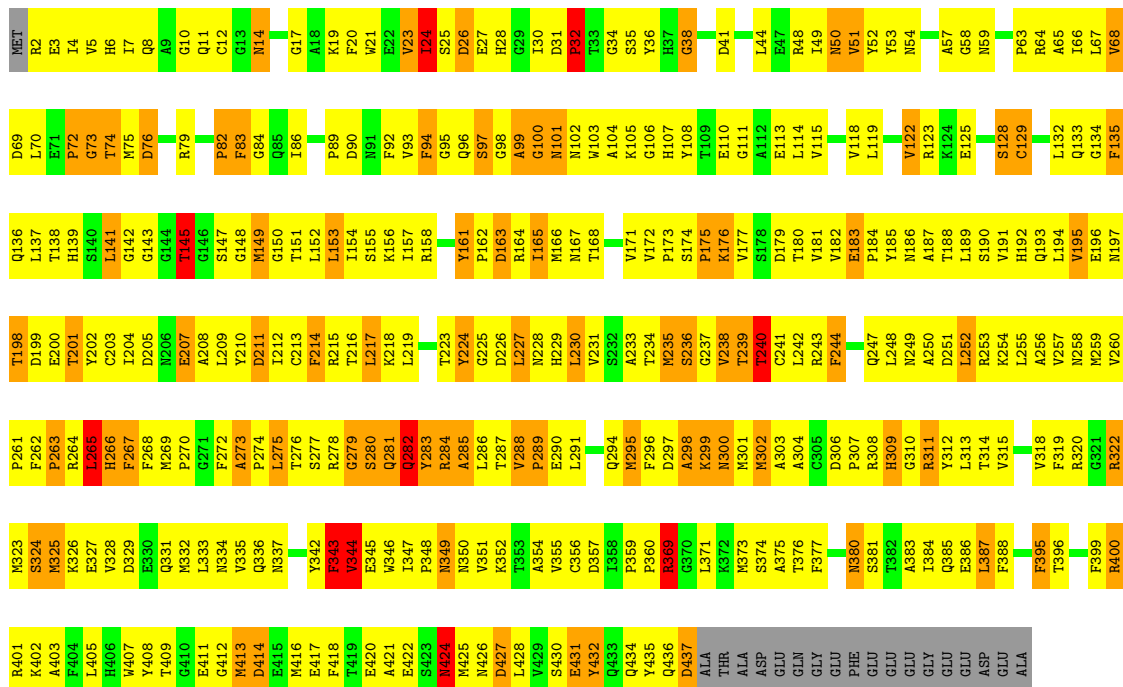
- Molecule 1: Kinesin heavy chain



- Molecule 2: Tubulin alpha chain



● Molecule 3: Tubulin beta chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	150000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction was integrated into the back projection process with a customized C program	Depositor
Microscope	JEOL 4000	Depositor
Voltage (kV)	400	Depositor
Electron dose ($e^-/\text{Å}^2$)	16	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	60000	Depositor
Image detector	KODAK SO-163 FILM	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: GDP, MG, TA1, ADP, ZN, 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 >2	RMSZ	# Z >2
1	K	0.36	0/2573	0.63	0/3467
2	A	0.50	0/3300	0.73	0/4482
3	B	0.51	0/3426	0.76	2/4642 (0.0%)
All	All	0.47	0/9299	0.71	2/12591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	235	MET	CG-SD-CE	6.09	109.94	100.20
3	B	217	LEU	N-CA-C	-5.37	96.50	111.00

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	K	2534	0	2498	214	0
2	A	3227	0	3138	659	0
3	B	3351	0	3229	598	0
4	A	1	0	0	0	0
4	K	1	0	0	0	0
5	K	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	B	32	0	12	5	0
8	B	28	0	12	1	0
9	B	62	0	51	6	0
All	All	9264	0	8952	1276	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 70.

The worst 5 of 1276 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:237:LYS:HE2	2:A:414:GLU:CG	1.28	1.57
1:K:247:VAL:CG2	2:A:156:ARG:NH1	1.67	1.55
1:K:247:VAL:CG2	2:A:156:ARG:CZ	1.84	1.52
1:K:237:LYS:CE	2:A:414:GLU:HG3	1.37	1.51
1:K:247:VAL:HG23	2:A:156:ARG:NH2	1.27	1.46

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	321/325 (99%)	292 (91%)	24 (8%)	5 (2%)	11	50
2	A	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	5
3	B	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	6
All	All	1153/1221 (94%)	832 (72%)	201 (17%)	120 (10%)	1	10

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	123	ASP
1	K	250	GLU
2	A	96	LYS
2	A	97	GLU
2	A	108	TYR

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	288/289 (100%)	278 (96%)	10 (4%)	39	66
2	A	347/377 (92%)	298 (86%)	49 (14%)	4	20
3	B	367/381 (96%)	307 (84%)	60 (16%)	2	15
All	All	1002/1047 (96%)	883 (88%)	119 (12%)	9	24

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	380	ASN
3	B	90	ASP
3	B	369	ARG
2	A	415	GLU
3	B	24	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	256	GLN
3	B	91	ASN
3	B	406	HIS
2	A	309	HIS
2	A	380	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
7	GTP	B	500	4	27,34,34	1.55	4 (14%)	29,54,54	2.14	5 (17%)
8	GDP	B	600	-	25,30,30	3.49	8 (32%)	27,47,47	3.61	9 (33%)
9	TA1	B	601	-	68,68,68	1.97	20 (29%)	105,105,105	1.34	9 (8%)
5	ADP	K	401	4	25,29,29	0.98	0	25,45,45	1.97	3 (12%)

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
7	GTP	B	500	4	-	0/18/38/38	0/3/3/3
8	GDP	B	600	-	-	0/12/32/32	0/3/3/3
9	TA1	B	601	-	-	0/41/127/127	0/7/7/7
5	ADP	K	401	4	-	0/12/32/32	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	TA1	C08-C07	-5.11	1.25	1.38
8	B	600	GDP	PB-O2B	-3.62	1.40	1.54
9	B	601	TA1	C04-C03	-2.33	1.44	1.49
7	B	500	GTP	C8-N7	-2.02	1.31	1.34
9	B	601	TA1	C41-C42	2.06	1.42	1.38

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	600	GDP	C6-C5-C4	-11.56	109.51	120.85
5	K	401	ADP	N3-C2-N1	-7.88	122.12	128.86
7	B	500	GTP	C5-C6-N1	-7.10	113.37	123.47
8	B	600	GDP	N2-C2-N1	-6.03	107.77	117.25
8	B	600	GDP	C4-C5-N7	-5.04	104.54	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	500	GTP	5	0
8	B	600	GDP	1	0
9	B	601	TA1	6	0

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.