



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Apr 28, 2018 – 01:16 PM EDT

PDB ID : 6B0L  
EMDB ID: : EMD-7028  
Title : KLP10A-AMPPNP in complex with a microtubule  
Authors : Benoit, M.P.M.H.; Asenjo, A.B.; Sosa, H.  
Deposited on : 2017-09-14  
Resolution : 3.98 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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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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-20031021

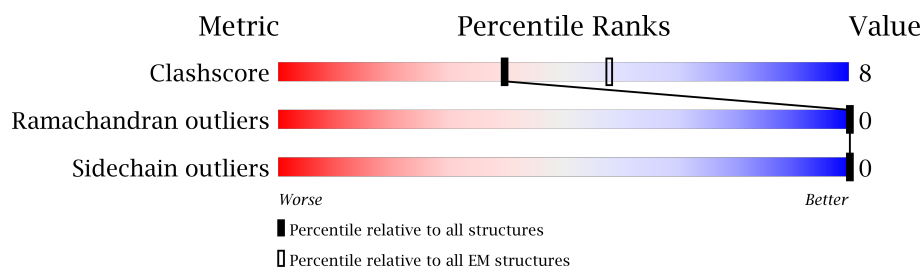
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.98 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  $\geq 3$ , 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	A	451	
2	B	445	
3	K	419	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9861 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3446	2180	585	659	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3376	2119	578	652	27		

- Molecule 3 is a protein called Kinesin-like protein Klp10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	368	Total	C	N	O	S	0	0
			2884	1809	516	541	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	197	GLY	-	expression tag	UNP Q960Z0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

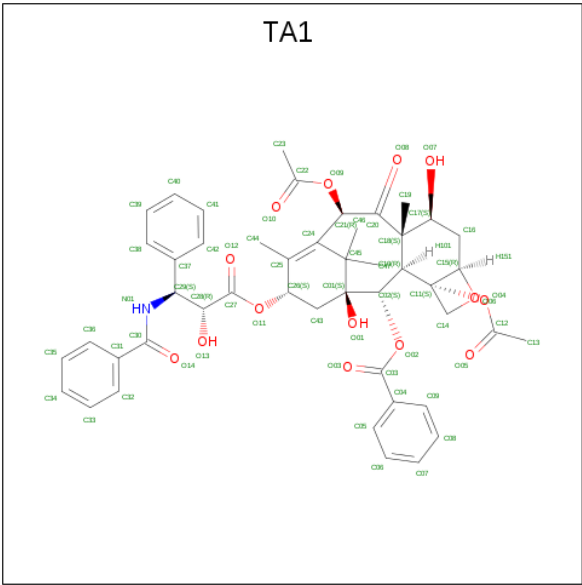
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Mg 1 1	0
5	K	1	Total Mg 1 1	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



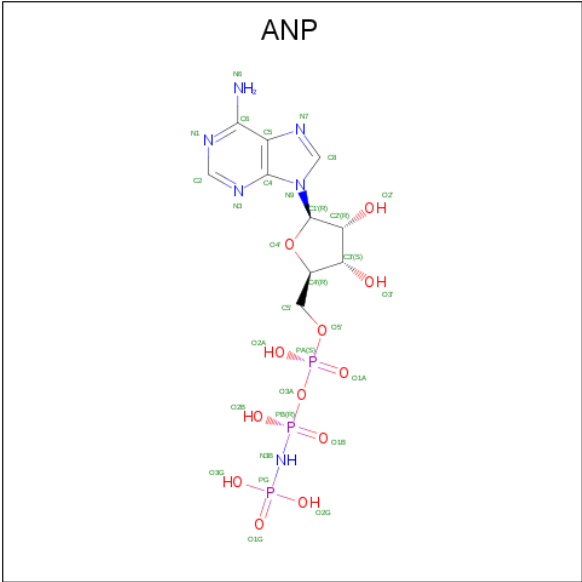
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: C<sub>47</sub>H<sub>51</sub>NO<sub>14</sub>).



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

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	K	1	31	10	6	12	3	0

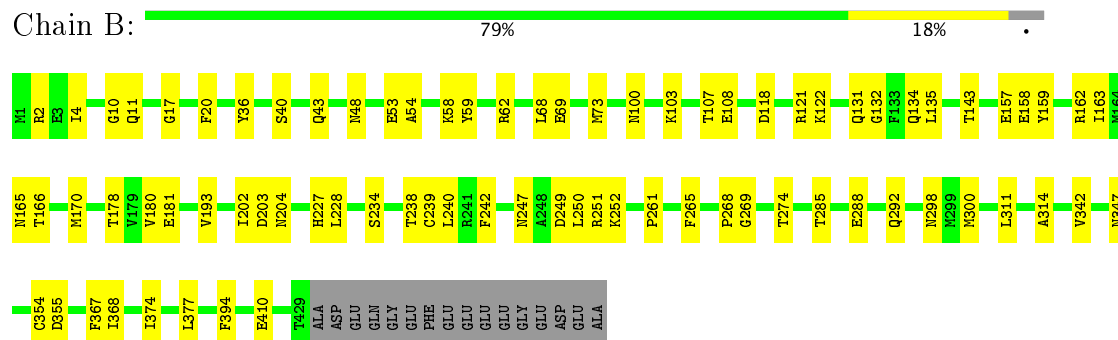
### 3 Residue-property plots [i](#)

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.

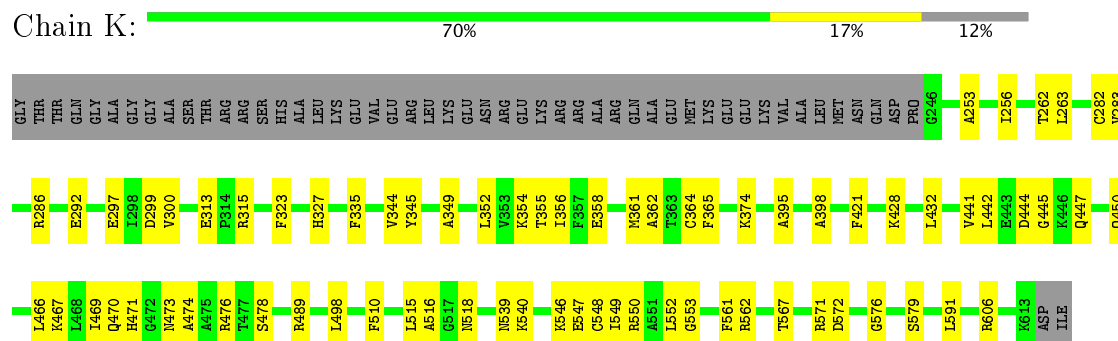
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain



- Molecule 3: Kinesin-like protein Klp10A



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=168.083°, rise=5.50 Å, axial sym=C1	Depositor
Number of segments used	6040	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	1.28	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	46598	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: GDP, GTP, MG, ANP, TA1

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	A	0.41	1/3524 (0.0%)	0.64	4/4784 (0.1%)
2	B	0.35	0/3451	0.54	0/4674
3	K	0.34	0/2930	0.61	0/3941
All	All	0.37	1/9905 (0.0%)	0.60	4/13399 (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	A	0	2
2	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	PRO	N-CD	-10.80	1.32	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	SER	CB-CA-C	-7.47	95.90	110.10
1	A	72	PRO	CA-N-CD	7.25	121.84	111.70
1	A	277	SER	N-CA-C	5.84	126.76	111.00
1	A	72	PRO	N-CA-CB	-5.47	96.59	102.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	PRO	Peptide
1	A	93	ILE	Peptide
2	B	69	GLU	Peptide

## 5.2 Too-close contacts

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	3446	0	3355	60	0
2	B	3376	0	3257	58	0
3	K	2884	0	2922	56	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
5	K	1	0	0	0	0
6	B	28	0	12	1	0
7	B	62	0	51	16	0
8	K	31	0	13	0	0
All	All	9861	0	9622	164	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 8.

All (164) 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:B:227:HIS:HB3	7:B:502:TA1:HC71	1.23	1.14
2:B:227:HIS:HB3	7:B:502:TA1:C07	2.08	0.81
1:A:406:HIS:HB2	3:K:540:LYS:HZ2	1.45	0.80
2:B:227:HIS:NE2	7:B:502:TA1:O14	2.18	0.76
7:B:502:TA1:H261	7:B:502:TA1:H463	1.69	0.73
1:A:406:HIS:O	3:K:540:LYS:NZ	2.21	0.73
3:K:567:THR:O	3:K:571:ARG:N	2.24	0.71
1:A:11:GLN:NE2	2:B:247:ASN:OD1	2.27	0.68
1:A:71:GLU:CD	1:A:72:PRO:HD2	2.17	0.66
3:K:470:GLN:O	3:K:474:ALA:N	2.31	0.64
2:B:311:LEU:HD23	2:B:342:VAL:HG21	1.80	0.64
3:K:395:ALA:HA	3:K:398:ALA:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:HIS:HB2	3:K:540:LYS:NZ	2.14	0.63
1:A:297:GLU:HG3	1:A:299:ALA:H	1.64	0.62
2:B:274:THR:HG22	7:B:502:TA1:H162	1.82	0.62
3:K:546:LYS:O	3:K:550:ARG:N	2.32	0.61
1:A:241:SER:HB2	1:A:250:VAL:H	1.64	0.61
2:B:17:GLY:HA2	2:B:20:PHE:HB3	1.81	0.61
3:K:374:LYS:HZ1	3:K:515:LEU:HD22	1.64	0.61
2:B:68:LEU:HD22	2:B:73:MET:HA	1.81	0.61
2:B:249:ASP:H	2:B:252:LYS:HD3	1.65	0.61
2:B:11:GLN:HB2	6:B:501:GDP:O2B	2.02	0.60
2:B:227:HIS:CB	7:B:502:TA1:HC71	2.14	0.60
3:K:282:CYS:SG	3:K:283:VAL:N	2.74	0.59
3:K:361:MET:SD	3:K:572:ASP:OD1	2.59	0.59
2:B:4:ILE:HG12	2:B:132:GLY:HA3	1.85	0.59
3:K:478:SER:O	3:K:489:ARG:N	2.34	0.59
3:K:442:LEU:O	3:K:450:GLN:N	2.35	0.59
1:A:79:ARG:HH21	1:A:91:GLN:HB2	1.68	0.58
7:B:502:TA1:C26	7:B:502:TA1:H463	2.33	0.58
3:K:364:CYS:SG	3:K:365:PHE:N	2.76	0.58
1:A:254:GLU:O	1:A:258:ASN:ND2	2.36	0.58
1:A:136:LEU:HA	1:A:167:LEU:O	2.04	0.57
1:A:400:ALA:O	3:K:550:ARG:NH2	2.38	0.57
1:A:402:ARG:NH2	3:K:606:ARG:HE	2.03	0.57
3:K:352:LEU:HD22	3:K:362:ALA:HB1	1.86	0.57
1:A:229:ARG:NH1	1:A:366:GLY:O	2.38	0.57
1:A:268:PRO:O	1:A:379:SER:N	2.38	0.57
1:A:276:ILE:HG21	1:A:369:ALA:H	1.70	0.55
1:A:87:PHE:HB2	1:A:91:GLN:HE21	1.72	0.55
1:A:406:HIS:HA	1:A:409:VAL:HG12	1.88	0.55
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.88	0.55
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.88	0.55
2:B:238:THR:HG23	2:B:239:CYS:N	2.22	0.55
1:A:178:SER:O	2:B:347:ASN:ND2	2.39	0.55
2:B:68:LEU:HD13	2:B:73:MET:HG3	1.89	0.54
1:A:16:ILE:HD11	1:A:171:ILE:HD11	1.90	0.54
1:A:409:VAL:HG22	3:K:539:ASN:HB3	1.90	0.54
2:B:2:ARG:NH1	2:B:131:GLN:OE1	2.41	0.54
2:B:234:SER:OG	7:B:502:TA1:H401	2.08	0.54
1:A:101:ASN:HD22	1:A:143:GLY:HA2	1.73	0.53
3:K:478:SER:OG	3:K:489:ARG:O	2.26	0.53
3:K:262:THR:HG23	3:K:263:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:OH	3:K:606:ARG:NH2	2.41	0.53
2:B:354:CYS:SG	2:B:355:ASP:N	2.82	0.53
1:A:27:GLU:OE1	1:A:243:ARG:NH1	2.42	0.53
2:B:135:LEU:HB3	2:B:166:THR:HG22	1.91	0.52
2:B:178:THR:HB	2:B:181:GLU:HB2	1.91	0.52
2:B:227:HIS:ND1	7:B:502:TA1:C07	2.72	0.52
1:A:402:ARG:HG2	3:K:547:GLU:OE2	2.10	0.52
3:K:561:PHE:CZ	3:K:571:ARG:CZ	2.93	0.52
2:B:410:GLU:HB2	3:K:442:LEU:HD23	1.92	0.52
3:K:473:ASN:O	3:K:476:ARG:N	2.42	0.51
1:A:135:PHE:HB2	1:A:166:LYS:HA	1.92	0.51
3:K:355:THR:HB	3:K:362:ALA:HB2	1.93	0.51
1:A:180:ALA:HB3	1:A:183:GLU:HB2	1.93	0.51
2:B:121:ARG:NH1	2:B:158:GLU:OE2	2.44	0.51
3:K:345:TYR:O	3:K:349:ALA:N	2.42	0.51
1:A:195:LEU:HD11	1:A:264:ARG:HB3	1.91	0.50
2:B:134:GLN:HG2	2:B:165:ASN:HD21	1.77	0.50
3:K:515:LEU:HD23	3:K:516:ALA:O	2.12	0.50
3:K:549:ILE:O	3:K:553:GLY:N	2.42	0.50
3:K:562:ARG:O	3:K:562:ARG:HG2	2.12	0.49
2:B:163:ILE:HD11	2:B:251:ARG:HB2	1.95	0.49
2:B:249:ASP:HB3	2:B:252:LYS:H	1.77	0.49
1:A:8:HIS:HB2	1:A:67:PHE:HB3	1.95	0.49
2:B:410:GLU:CB	3:K:442:LEU:HD23	2.43	0.48
2:B:159:TYR:HB3	2:B:162:ARG:HG3	1.94	0.48
1:A:185:TYR:OH	1:A:398:MET:O	2.31	0.48
1:A:277:SER:H	1:A:278:ALA:HA	1.77	0.48
2:B:157:GLU:OE1	3:K:428:LYS:NZ	2.36	0.48
2:B:240:LEU:HD11	2:B:250:LEU:H	1.79	0.48
1:A:259:LEU:HD21	1:A:316:CYS:HB2	1.95	0.48
3:K:548:CYS:O	3:K:552:LEU:N	2.44	0.48
1:A:286:LEU:O	1:A:373:ARG:NH1	2.42	0.48
1:A:316:CYS:HB3	1:A:378:LEU:HB2	1.96	0.47
3:K:354:LYS:O	3:K:358:GLU:N	2.47	0.47
3:K:515:LEU:HD21	3:K:518:ASN:OD1	2.14	0.47
1:A:8:HIS:HA	1:A:138:PHE:HB2	1.95	0.47
1:A:139:HIS:NE2	1:A:168:GLU:OE1	2.40	0.47
1:A:175:PRO:HB3	1:A:390:ARG:HB3	1.95	0.47
1:A:213:CYS:HA	1:A:217:LEU:HB2	1.95	0.47
7:B:502:TA1:H101	7:B:502:TA1:C25	2.45	0.47
3:K:467:LYS:O	3:K:471:HIS:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:N	2:B:202:ILE:O	2.44	0.47
2:B:227:HIS:ND1	7:B:502:TA1:C06	2.78	0.47
3:K:374:LYS:NZ	3:K:515:LEU:HD22	2.30	0.47
1:A:102:ASN:HD21	1:A:105:ARG:HD3	1.80	0.46
3:K:253:ALA:HA	3:K:256:ILE:HD12	1.97	0.46
3:K:361:MET:SD	3:K:572:ASP:CG	2.94	0.46
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.97	0.46
2:B:43:GLN:HA	2:B:242:PHE:HE1	1.81	0.46
2:B:193:VAL:HG22	2:B:265:PHE:HZ	1.79	0.46
3:K:466:LEU:HD23	3:K:469:ILE:HD12	1.98	0.46
1:A:402:ARG:HG3	1:A:405:VAL:HG11	1.98	0.45
3:K:313:GLU:OE1	3:K:327:HIS:NE2	2.44	0.45
3:K:561:PHE:O	3:K:567:THR:OG1	2.18	0.45
1:A:79:ARG:NH2	1:A:91:GLN:O	2.49	0.45
2:B:238:THR:CG2	2:B:239:CYS:N	2.80	0.45
3:K:444:ASP:OD1	3:K:445:GLY:N	2.49	0.45
3:K:297:GLU:OE2	3:K:591:LEU:N	2.47	0.45
2:B:314:ALA:HB3	2:B:368:ILE:HB	1.99	0.45
3:K:335:PHE:HE2	3:K:344:VAL:HG13	1.82	0.45
3:K:362:ALA:HB3	3:K:510:PHE:CE1	2.52	0.45
1:A:1:MET:HB3	1:A:50:ASN:HD22	1.82	0.44
1:A:219:ILE:HG22	1:A:221:ARG:H	1.83	0.44
3:K:447:GLN:OE1	3:K:571:ARG:NH2	2.49	0.44
2:B:107:THR:OG1	2:B:108:GLU:OE1	2.30	0.44
2:B:227:HIS:CB	7:B:502:TA1:C07	2.87	0.44
2:B:53:GLU:HG3	2:B:59:TYR:HE1	1.83	0.44
3:K:441:VAL:C	3:K:442:LEU:HD12	2.39	0.43
1:A:414:GLU:HG2	1:A:416:GLY:H	1.82	0.43
2:B:36:TYR:OH	2:B:43:GLN:NE2	2.51	0.43
2:B:227:HIS:CG	7:B:502:TA1:C07	3.00	0.43
3:K:576:GLY:O	3:K:579:SER:HB3	2.18	0.43
2:B:48:ASN:O	2:B:62:ARG:NH2	2.40	0.43
1:A:242:LEU:HD11	1:A:252:LEU:HG	1.99	0.43
2:B:285:THR:H	2:B:288:GLU:HB3	1.84	0.43
2:B:292:GLN:HG2	2:B:298:ASN:HD22	1.84	0.42
3:K:356:ILE:HG12	3:K:498:LEU:HD22	2.01	0.42
1:A:134:GLY:HA2	1:A:165:SER:HB2	2.01	0.42
1:A:105:ARG:N	1:A:106:GLY:HA3	2.35	0.42
1:A:341:ILE:HG13	1:A:341:ILE:O	2.19	0.42
2:B:292:GLN:HG2	2:B:298:ASN:ND2	2.34	0.42
2:B:40:SER:OG	2:B:43:GLN:OE1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:502:TA1:H101	7:B:502:TA1:C24	2.49	0.42
3:K:352:LEU:CD2	3:K:362:ALA:HB1	2.48	0.42
2:B:268:PRO:HG2	2:B:300:MET:HB2	2.01	0.42
1:A:213:CYS:O	1:A:219:ILE:N	2.46	0.42
2:B:269:GLY:N	2:B:367:PHE:O	2.53	0.42
2:B:100:ASN:HB3	2:B:103:LYS:HB2	2.01	0.42
2:B:10:GLY:HA2	2:B:143:THR:HB	2.02	0.42
2:B:228:LEU:HD23	7:B:502:TA1:H081	2.01	0.42
1:A:88:HIS:HA	1:A:89:PRO:HD3	1.85	0.41
1:A:269:LEU:HD12	1:A:384:ILE:HD13	2.02	0.41
1:A:333:ALA:O	1:A:337:THR:N	2.53	0.41
3:K:299:ASP:OD1	3:K:300:VAL:N	2.53	0.41
3:K:315:ARG:N	3:K:323:PHE:O	2.51	0.41
1:A:406:HIS:CG	2:B:261:PRO:HG3	2.55	0.41
7:B:502:TA1:C26	7:B:502:TA1:C46	2.98	0.41
3:K:286:ARG:NH2	3:K:292:GLU:OE2	2.52	0.41
2:B:118:ASP:OD2	2:B:122:LYS:NZ	2.52	0.41
1:A:212:ILE:HG23	1:A:216:ASN:HD22	1.86	0.41
2:B:374:ILE:HA	2:B:377:LEU:HD13	2.03	0.41
2:B:410:GLU:HG2	3:K:442:LEU:HG	2.02	0.41
3:K:335:PHE:CE2	3:K:344:VAL:HG13	2.56	0.41
3:K:421:PHE:HB3	3:K:432:LEU:HD12	2.03	0.40
1:A:119:LEU:HA	1:A:122:ILE:HD12	2.03	0.40
1:A:106:GLY:HA2	1:A:148:GLY:HA3	2.03	0.40
1:A:122:ILE:O	1:A:126:ALA:N	2.51	0.40
1:A:50:ASN:OD1	1:A:64:ARG:NH2	2.54	0.40
2:B:203:ASP:OD1	2:B:204:ASN:N	2.55	0.40
1:A:356:ASN:OD1	1:A:357:TYR:N	2.55	0.40
2:B:180:VAL:HG12	2:B:394:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	439/451 (97%)	409 (93%)	30 (7%)	0	100	100
2	B	427/445 (96%)	397 (93%)	30 (7%)	0	100	100
3	K	366/419 (87%)	323 (88%)	43 (12%)	0	100	100
All	All	1232/1315 (94%)	1129 (92%)	103 (8%)	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	A	372/379 (98%)	372 (100%)	0	100	100
2	B	371/383 (97%)	371 (100%)	0	100	100
3	K	319/360 (89%)	319 (100%)	0	100	100
All	All	1062/1122 (95%)	1062 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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$
4	GTP	A	501	5	27,34,34	1.32	4 (14%)	29,54,54	1.93	6 (20%)
6	GDP	B	501	-	25,30,30	1.21	3 (12%)	27,47,47	2.09	6 (22%)
7	TA1	B	502	-	68,68,68	0.53	0	105,105,105	0.73	2 (1%)
8	ANP	K	702	5	29,33,33	1.47	4 (13%)	29,52,52	2.01	6 (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
4	GTP	A	501	5	-	0/18/38/38	0/3/3/3
6	GDP	B	501	-	-	0/12/32/32	0/3/3/3
7	TA1	B	502	-	-	0/41/127/127	0/7/7/7
8	ANP	K	702	5	-	1/13/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GTP	C8-N9	-2.98	1.33	1.36
4	A	501	GTP	PG-O3G	-2.46	1.44	1.54
6	B	501	GDP	C5-C4	2.07	1.45	1.40
4	A	501	GTP	C5-C4	2.18	1.45	1.40
8	K	702	ANP	C5-C4	2.19	1.45	1.40
8	K	702	ANP	C2-N3	2.43	1.36	1.32
6	B	501	GDP	C6-C5	3.11	1.46	1.41
4	A	501	GTP	C6-C5	3.30	1.47	1.41
8	K	702	ANP	PB-O1B	3.72	1.50	1.46
6	B	501	GDP	O4'-C1'	3.73	1.46	1.41
8	K	702	ANP	PG-O1G	4.33	1.51	1.46



All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	702	ANP	N3-C2-N1	-7.09	122.80	128.86
6	B	501	GDP	C6-C5-C4	-5.09	115.86	120.85
8	K	702	ANP	O1G-PG-N3B	-4.48	105.10	111.79
4	A	501	GTP	C6-C5-C4	-4.02	116.90	120.85
4	A	501	GTP	C5-C6-N1	-3.93	117.88	123.47
6	B	501	GDP	C5-C6-N1	-3.54	118.44	123.47
6	B	501	GDP	N3-C2-N1	-3.44	122.37	127.41
6	B	501	GDP	C1'-N9-C4	-3.32	120.89	126.64
4	A	501	GTP	N3-C2-N1	-2.93	123.11	127.41
7	B	502	TA1	O04-C11-C14	-2.66	102.10	108.12
4	A	501	GTP	C4-C5-N7	-2.65	106.85	109.41
8	K	702	ANP	C4-C5-N7	-2.50	106.99	109.41
8	K	702	ANP	O2A-PA-O1A	2.11	122.84	112.14
7	B	502	TA1	O09-C21-C24	2.32	112.94	109.73
8	K	702	ANP	C2-N1-C6	2.69	123.32	118.75
8	K	702	ANP	O2B-PB-O1B	3.13	116.36	109.88
6	B	501	GDP	C2-N3-C4	3.44	119.17	115.16
4	A	501	GTP	C6-N1-C2	4.27	122.21	116.06
4	A	501	GTP	C2-N3-C4	4.53	120.45	115.16
6	B	501	GDP	C6-N1-C2	4.93	123.15	116.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	K	702	ANP	O1B-PB-N3B-PG

There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GDP	1	0
7	B	502	TA1	16	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.