



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 9, 2017 – 08:40 AM EST

PDB ID : 5OCU
EMDB ID: : EMD-3780
Title : Molecular basis of human kinesin-8 function and inhibition
Authors : Locke, J.; Joseph, A.P.; Topf, M.; Moores, C.A.
Deposited on : unknown
Resolution : 5.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

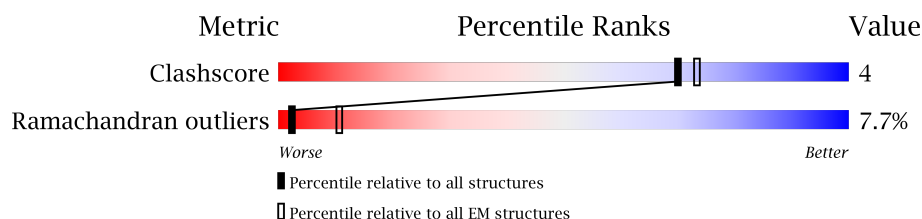
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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	125131	1336
Ramachandran outliers	121729	1120

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	377	 80% 7% • 12%
2	A	451	 79% 11% • 9%
3	B	445	 84% 11% •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4840 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-like protein KIF18A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	333	Total	C	N	O	0	0
			1332	666	333	333		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP Q8NI77
K	-1	SER	-	expression tag	UNP Q8NI77
K	0	HIS	-	expression tag	UNP Q8NI77

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	412	Total	C	N	O	0	0
			1648	824	412	412		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

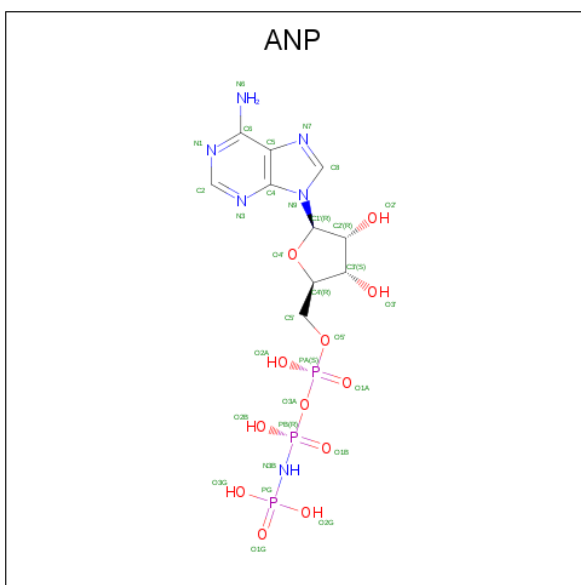
- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	426	Total	C	N	O	0	0
			1704	852	426	426		

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

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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).

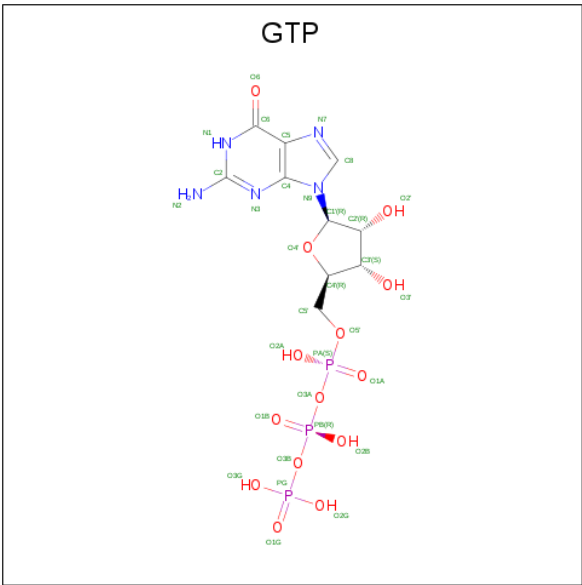


Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	P	0
			31	10	6	12	3	

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

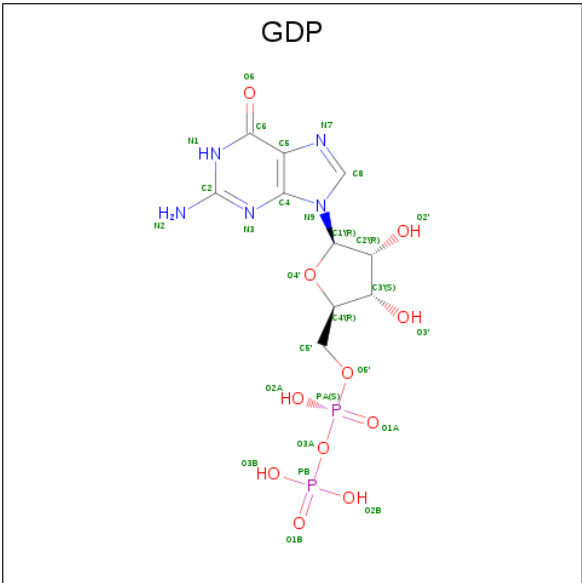
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Zn 1 1	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



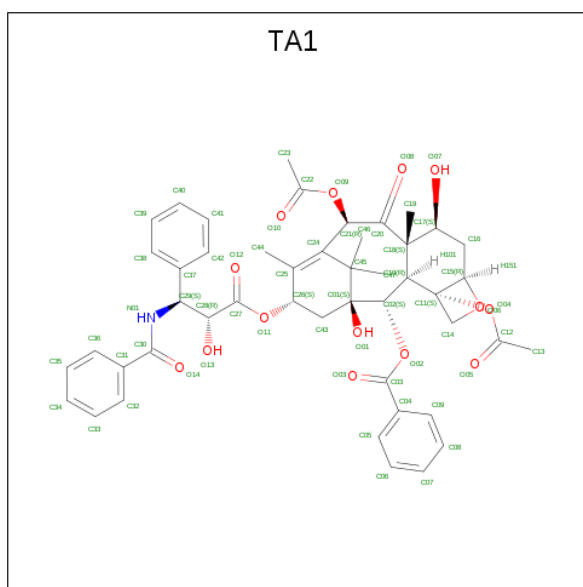
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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
8	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

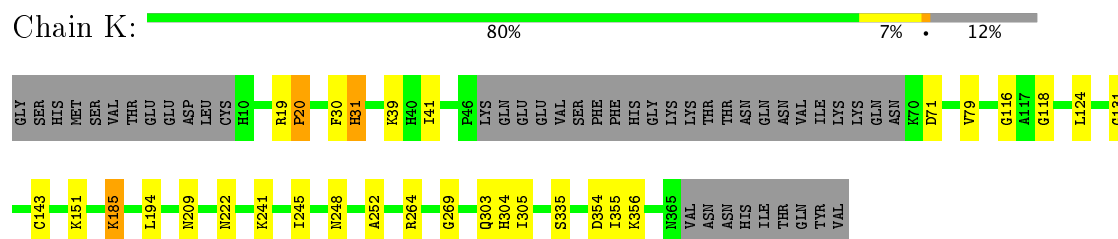


Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			62	47	1	14	

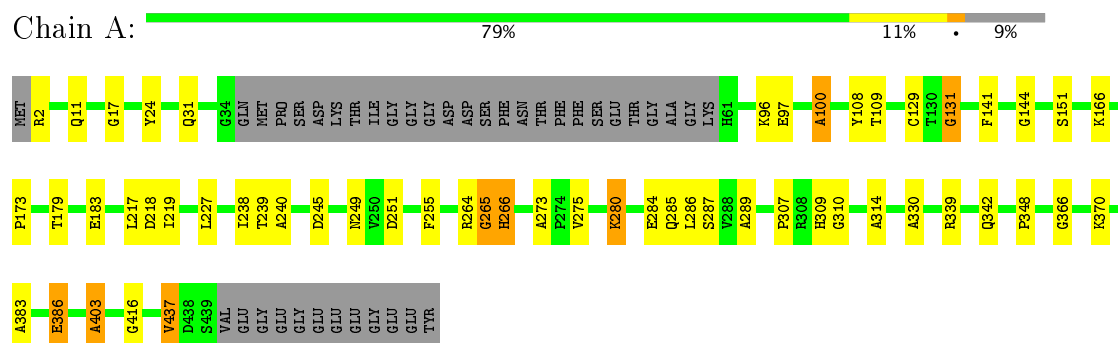
3 Residue-property plots

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.

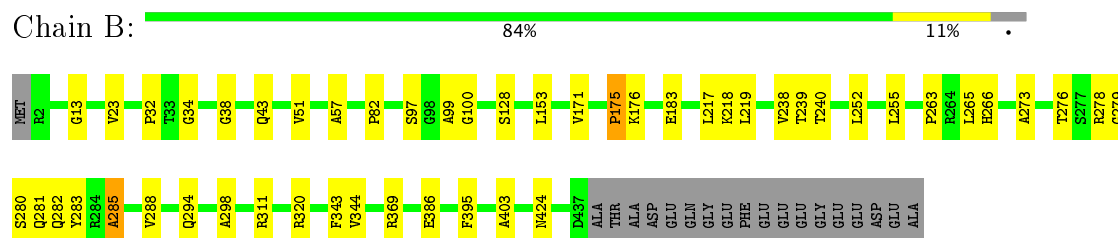
- Molecule 1: Kinesin-like protein KIF18A



- Molecule 2: Tubulin alpha chain



- Molecule 3: Tubulin beta chain



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=81 Å, axial sym=C1	Depositor
Number of segments used	70473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	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, MG, TA1, ZN, GTP, ANP

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	0.44	0/1330	0.86	0/1659
2	A	0.45	0/1646	0.90	1/2054 (0.0%)
3	B	0.47	0/1703	0.92	0/2127
All	All	0.45	0/4679	0.90	1/5840 (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	16
2	A	0	11
3	B	0	7
All	All	0	34

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	265	GLY	C-N-CA	5.63	135.77	121.70

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	151	SER	Mainchain
2	A	166	LYS	Mainchain
2	A	17	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	A	179	THR	Mainchain
2	A	227	LEU	Mainchain
2	A	280	LYS	Mainchain
2	A	286	LEU	Mainchain
2	A	386	GLU	Mainchain
2	A	403	ALA	Mainchain
2	A	416	GLY	Mainchain
2	A	437	VAL	Mainchain
3	B	13	GLY	Mainchain
3	B	153	LEU	Mainchain
3	B	171	VAL	Mainchain
3	B	175	PRO	Mainchain
3	B	255	LEU	Mainchain
3	B	285	ALA	Mainchain
3	B	320	ARG	Mainchain
1	K	143	CYS	Mainchain
1	K	151	LYS	Mainchain
1	K	185	LYS	Mainchain
1	K	194	LEU	Mainchain
1	K	209	ASN	Mainchain
1	K	222	ASN	Mainchain
1	K	241	LYS	Mainchain
1	K	248	ASN	Mainchain
1	K	252	ALA	Peptide
1	K	264	ARG	Mainchain
1	K	303	GLN	Peptide
1	K	335	SER	Mainchain
1	K	354	ASP	Mainchain
1	K	355	ILE	Mainchain
1	K	356	LYS	Mainchain
1	K	41	ILE	Mainchain

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	K	1332	0	358	13	0
2	A	1648	0	451	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1704	0	471	3	0
4	A	1	0	0	0	0
4	K	1	0	0	0	0
5	K	31	0	13	4	0
6	A	1	0	0	0	0
7	A	32	0	12	3	0
8	B	28	0	12	0	0
9	B	62	0	51	3	0
All	All	4840	0	1368	26	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 4.

All (26) 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:116:GLY:HA2	5:K:501:ANP:H5'1	1.75	0.69
1:K:30:PHE:O	1:K:31:HIS:C	2.27	0.69
1:K:30:PHE:O	1:K:31:HIS:O	2.12	0.67
9:B:601:TA1:H261	9:B:601:TA1:H463	1.80	0.62
1:K:19:ARG:O	1:K:20:PRO:C	2.44	0.55
1:K:118:GLY:HA2	5:K:501:ANP:C8	2.40	0.51
2:A:310:GLY:HA3	2:A:383:ALA:N	2.28	0.49
1:K:19:ARG:O	1:K:20:PRO:O	2.31	0.49
1:K:304:HIS:O	1:K:305:ILE:C	2.50	0.48
2:A:144:GLY:H	7:A:503:GTP:PG	2.37	0.48
2:A:144:GLY:N	7:A:503:GTP:O3G	2.43	0.47
2:A:11:GLN:N	7:A:503:GTP:O2B	2.50	0.45
1:K:118:GLY:HA2	5:K:501:ANP:H8	1.97	0.45
2:A:264:ARG:C	2:A:266:HIS:H	2.20	0.44
2:A:100:ALA:O	2:A:144:GLY:HA3	2.17	0.44
1:K:39:LYS:O	1:K:79:VAL:O	2.36	0.43
9:B:601:TA1:H463	9:B:601:TA1:C26	2.46	0.43
3:B:281:GLN:O	3:B:283:TYR:N	2.51	0.43
1:K:30:PHE:C	1:K:31:HIS:O	2.57	0.42
1:K:124:LEU:C	1:K:131:GLY:HA3	2.40	0.42
1:K:124:LEU:O	1:K:131:GLY:HA3	2.20	0.42
3:B:276:THR:O	9:B:601:TA1:H192	2.19	0.41
2:A:310:GLY:HA3	2:A:383:ALA:CA	2.50	0.41
2:A:2:ARG:N	2:A:131:GLY:O	2.53	0.41
1:K:116:GLY:CA	5:K:501:ANP:H5'1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:217:LEU:C	3:B:219:LEU:H	2.25	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	329/377 (87%)	298 (91%)	25 (8%)	6 (2%)	10	49
2	A	408/451 (90%)	296 (72%)	69 (17%)	43 (10%)	0	10
3	B	424/445 (95%)	305 (72%)	79 (19%)	40 (9%)	1	14
All	All	1161/1273 (91%)	899 (77%)	173 (15%)	89 (8%)	2	18

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	71	ASP
2	A	97	GLU
2	A	108	TYR
2	A	109	THR
2	A	141	PHE
2	A	183	GLU
2	A	245	ASP
2	A	266	HIS
2	A	280	LYS
2	A	284	GLU
2	A	285	GLN
2	A	287	SER
2	A	437	VAL
3	B	82	PRO
3	B	97	SER
3	B	175	PRO

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Mol	Chain	Res	Type
3	B	176	LYS
3	B	183	GLU
3	B	239	THR
3	B	252	LEU
3	B	278	ARG
3	B	282	GLN
3	B	288	VAL
3	B	344	VAL
3	B	369	ARG
3	B	403	ALA
1	K	20	PRO
1	K	31	HIS
2	A	96	LYS
2	A	217	LEU
2	A	240	ALA
2	A	249	ASN
2	A	251	ASP
2	A	255	PHE
2	A	309	HIS
2	A	342	GLN
2	A	370	LYS
2	A	403	ALA
3	B	32	PRO
3	B	38	GLY
3	B	128	SER
3	B	238	VAL
3	B	240	THR
3	B	265	LEU
3	B	266	HIS
3	B	273	ALA
3	B	279	GLY
3	B	294	GLN
3	B	298	ALA
3	B	311	ARG
3	B	343	PHE
1	K	185	LYS
2	A	100	ALA
2	A	173	PRO
2	A	218	ASP
2	A	238	ILE
2	A	289	ALA
2	A	314	ALA

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Mol	Chain	Res	Type
2	A	330	ALA
2	A	339	ARG
2	A	386	GLU
3	B	280	SER
3	B	386	GLU
2	A	129	CYS
3	B	263	PRO
2	A	24	TYR
2	A	219	ILE
2	A	239	THR
2	A	265	GLY
2	A	366	GLY
3	B	23	VAL
3	B	43	GLN
3	B	57	ALA
3	B	99	ALA
3	B	218	LYS
3	B	285	ALA
3	B	395	PHE
3	B	424	ASN
2	A	273	ALA
2	A	307	PRO
2	A	348	PRO
3	B	51	VAL
2	A	131	GLY
2	A	31	GLN
2	A	275	VAL
3	B	100	GLY
1	K	245	ILE
1	K	269	GLY
3	B	34	GLY

5.3.2 Protein sidechains ⓘ

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

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 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	A	503	4	27,34,34	1.53	4 (14%)	27,54,54	2.16	5 (18%)
8	GDP	B	600	-	25,30,30	2.63	8 (32%)	26,47,47	3.64	9 (34%)
9	TA1	B	601	-	68,68,68	1.97	20 (29%)	105,105,105	1.33	8 (7%)
5	ANP	K	501	4	29,33,33	1.66	5 (17%)	28,52,52	2.68	6 (21%)

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	A	503	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	0/5/7/7
5	ANP	K	501	4	-	1/13/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	TA1	C08-C07	-5.09	1.25	1.38
5	K	501	ANP	PG-O3G	-4.75	1.43	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	501	ANP	PG-O2G	-3.59	1.46	1.56
8	B	600	GDP	PB-O2B	-3.54	1.40	1.54
5	K	501	ANP	PB-O2B	-3.33	1.47	1.56
9	B	601	TA1	C04-C03	-2.32	1.44	1.49
7	A	503	GTP	C8-N7	-2.00	1.30	1.34
7	A	503	GTP	O4'-C1'	2.01	1.44	1.41
9	B	601	TA1	C10-C02	2.02	1.62	1.57
9	B	601	TA1	C41-C42	2.09	1.42	1.38
5	K	501	ANP	PB-N3B	2.10	1.68	1.63
8	B	600	GDP	O3'-C3'	2.11	1.47	1.43
9	B	601	TA1	C18-C20	2.18	1.62	1.56
9	B	601	TA1	C37-C29	2.20	1.54	1.51
9	B	601	TA1	C16-C15	2.22	1.56	1.52
9	B	601	TA1	C01-C45	2.22	1.66	1.56
8	B	600	GDP	PB-O3B	2.22	1.63	1.54
9	B	601	TA1	C11-C10	2.26	1.61	1.55
8	B	600	GDP	C5-C4	2.45	1.46	1.40
9	B	601	TA1	C26-C25	2.47	1.56	1.51
9	B	601	TA1	C43-C26	2.51	1.58	1.52
5	K	501	ANP	O4'-C1'	2.61	1.44	1.41
9	B	601	TA1	C43-C01	2.93	1.60	1.54
9	B	601	TA1	C25-C24	2.99	1.39	1.34
9	B	601	TA1	C46-C45	3.08	1.60	1.53
8	B	600	GDP	C8-N7	3.40	1.41	1.34
9	B	601	TA1	C45-C24	3.44	1.61	1.54
9	B	601	TA1	O02-C03	3.45	1.41	1.34
9	B	601	TA1	C36-C31	3.50	1.45	1.39
7	A	503	GTP	PG-O3B	3.80	1.66	1.60
8	B	600	GDP	O6-C6	4.08	1.34	1.24
9	B	601	TA1	C18-C10	4.31	1.69	1.57
9	B	601	TA1	C05-C04	4.52	1.46	1.39
7	A	503	GTP	C6-N1	4.81	1.41	1.33
9	B	601	TA1	C06-C05	5.82	1.50	1.38
8	B	600	GDP	O4'-C1'	6.20	1.49	1.41
8	B	600	GDP	C2-N1	7.66	1.49	1.35

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	600	GDP	C6-C5-C4	-11.35	109.55	120.84
7	A	503	GTP	C5-C6-N1	-7.11	113.36	123.48
8	B	600	GDP	N2-C2-N1	-5.93	107.76	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	600	GDP	C4-C5-N7	-5.05	104.53	109.41
8	B	600	GDP	N3-C2-N1	-4.94	120.25	127.46
9	B	601	TA1	C06-C05-C04	-4.87	114.62	120.35
5	K	501	ANP	O3A-PB-N3B	-4.40	94.38	106.59
5	K	501	ANP	O2G-PG-O1G	-4.26	102.60	113.41
5	K	501	ANP	O3G-PG-O2G	-4.05	96.34	107.69
9	B	601	TA1	C05-C04-C03	-3.98	111.44	120.39
7	A	503	GTP	N3-C2-N1	-3.15	122.85	127.46
9	B	601	TA1	O04-C11-C14	-2.76	101.74	108.14
7	A	503	GTP	C6-C5-C4	-2.44	118.42	120.84
5	K	501	ANP	PA-O3A-PB	-2.33	124.14	132.38
7	A	503	GTP	O5'-C5'-C4'	2.02	116.16	109.00
8	B	600	GDP	O2'-C2'-C3'	2.29	119.15	111.83
9	B	601	TA1	O01-C01-C43	2.48	113.41	106.86
9	B	601	TA1	C45-C01-C02	2.67	115.20	111.85
9	B	601	TA1	C17-C18-C20	2.84	109.81	102.33
8	B	600	GDP	C2'-C3'-C4'	3.39	109.22	102.62
9	B	601	TA1	C09-C04-C03	3.55	128.39	120.39
8	B	600	GDP	C2-N3-C4	3.66	119.43	115.16
8	B	600	GDP	C4'-O4'-C1'	4.00	114.02	109.77
9	B	601	TA1	C07-C08-C09	5.18	127.33	120.21
5	K	501	ANP	O1G-PG-N3B	5.52	120.05	111.79
7	A	503	GTP	C6-N1-C2	5.98	124.66	116.06
8	B	600	GDP	N2-C2-N3	7.71	131.98	117.75
5	K	501	ANP	O1B-PB-N3B	9.02	125.29	111.79

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	501	ANP	O1B-PB-N3B-PG

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	503	GTP	3	0
9	B	601	TA1	3	0
5	K	501	ANP	4	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.