



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

May 25, 2019 – 12:35 PM EDT

PDB ID : 6O2Q  
EMDB ID: : EMD-0612  
Title : Acetylated Microtubules  
Authors : Eshun-Wilson, L.; Zhang, R.; Portran, D.; Nachury, M.V.; Toso, D.; Lohr, T.;  
Vendruscolo, M.; Bonomi, M.; Fraser, J.S.; Nogales, E.  
Deposited on : 2019-02-24  
Resolution : 3.70 Å(reported)  
Based on PDB ID : 3JAR

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](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 : 1.8.0 (224370), CSD as540be (2019)  
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-20031633

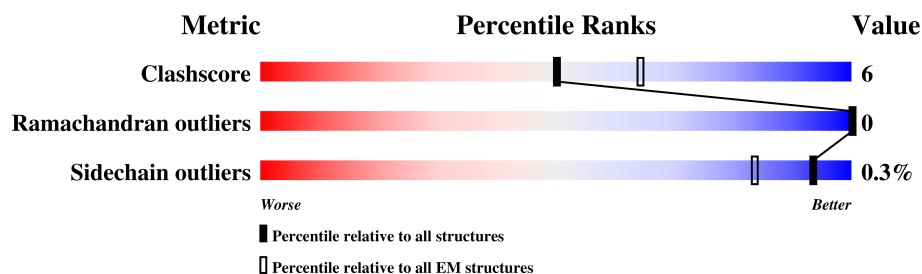
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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	78%	18% .
1	C	451	78%	18% .
1	E	451	77%	19% .
1	J	451	77%	19% .
1	K	451	78%	17% .
1	L	451	78%	18% .
2	B	445	78%	18% .
2	D	445	78%	18% .
2	F	445	80%	17% .

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Mol	Chain	Length	Quality of chain
2	G	445	<div><div></div><div>81%</div><div>16%</div><div></div></div>
2	H	445	<div><div></div><div>80%</div><div>16%</div><div></div></div>
2	I	445	<div><div></div><div>78%</div><div>18%</div><div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 40866 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.

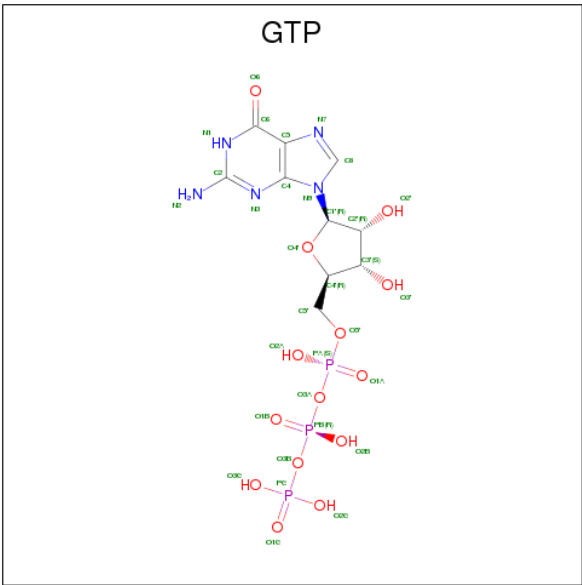
- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		
1	C	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		
1	E	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		
1	J	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		
1	K	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		
1	L	432	Total	C	N	O	S	0	0
			3382	2144	575	642	21		

- 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
			3368	2115	578	650	25		
2	D	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	F	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	G	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	H	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		
2	I	429	Total	C	N	O	S	0	0
			3368	2115	578	650	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

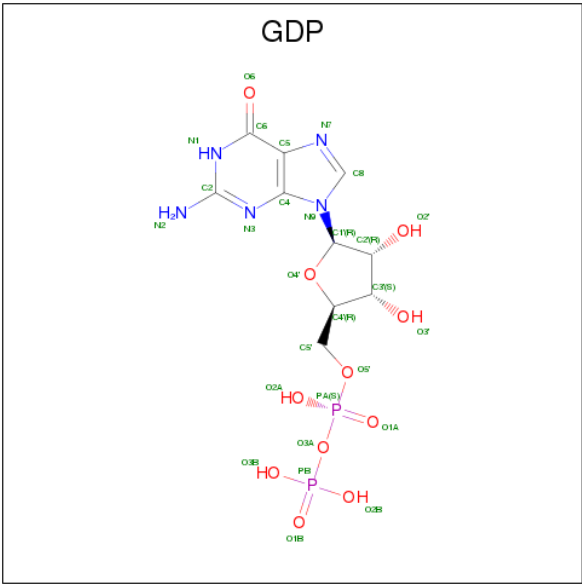


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	L	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

Mol	Chain	Residues	Atoms		AltConf
4	J	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	L	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

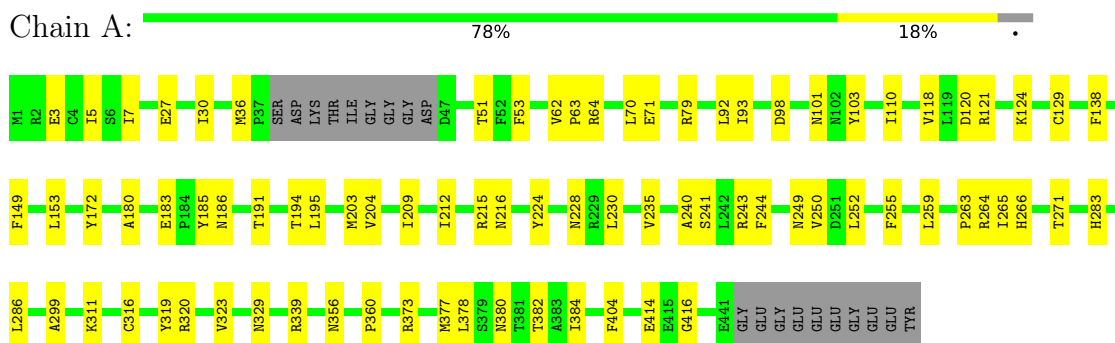


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	D	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	G	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	H	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	I	1	Total	C	N	O	P	0
			28	10	5	11	2	

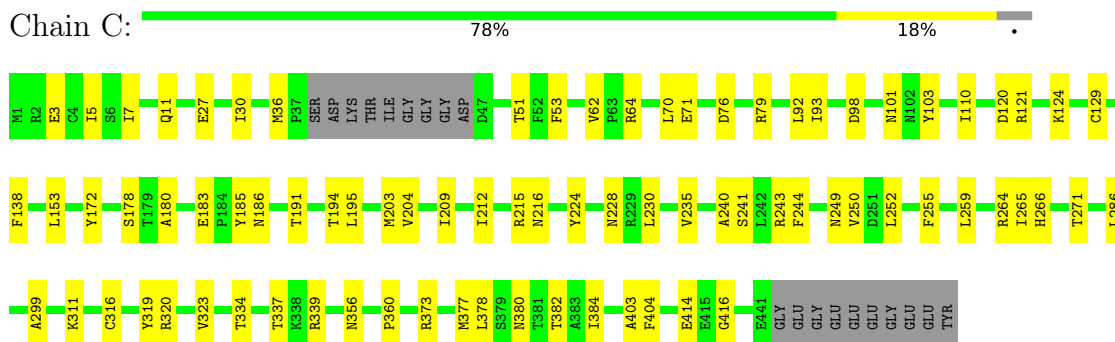
### 3 Residue-property plots

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.

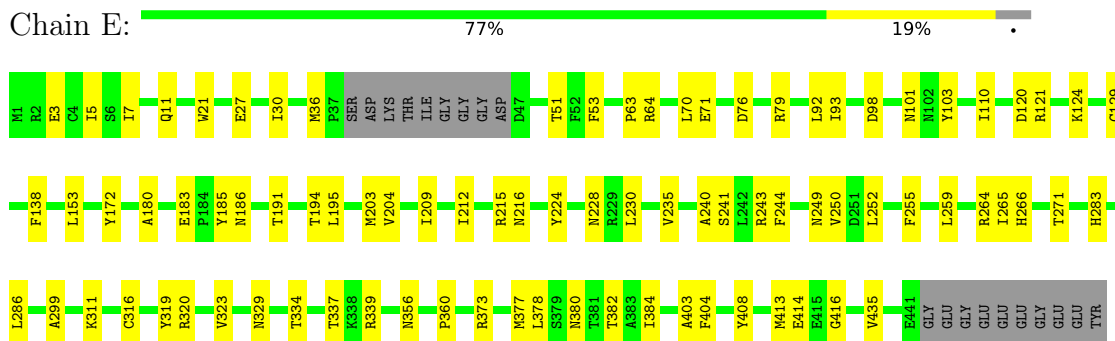
- Molecule 1: Tubulin alpha-1B chain




- Molecule 1: Tubulin alpha-1B chain

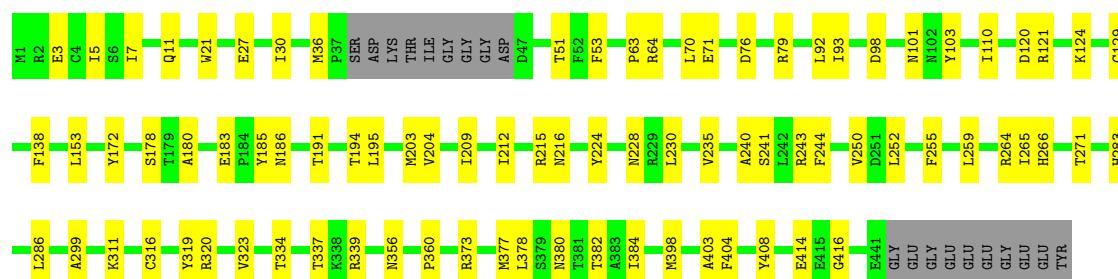


- Molecule 1: Tubulin alpha-1B chain




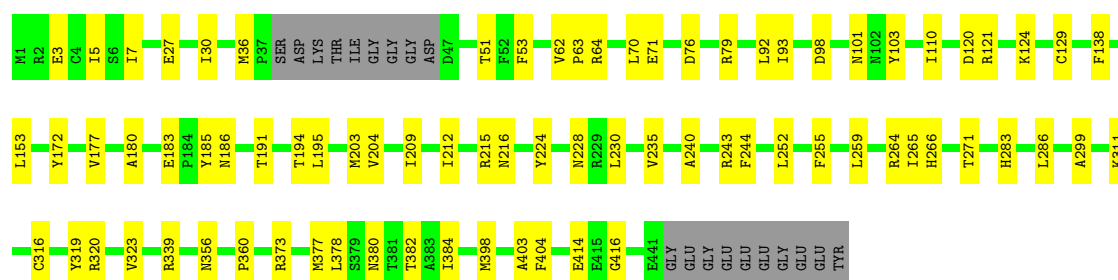
- Molecule 1: Tubulin alpha-1B chain

Chain J:  77% 19% .




- Molecule 1: Tubulin alpha-1B chain

Chain K:  78% 17% .




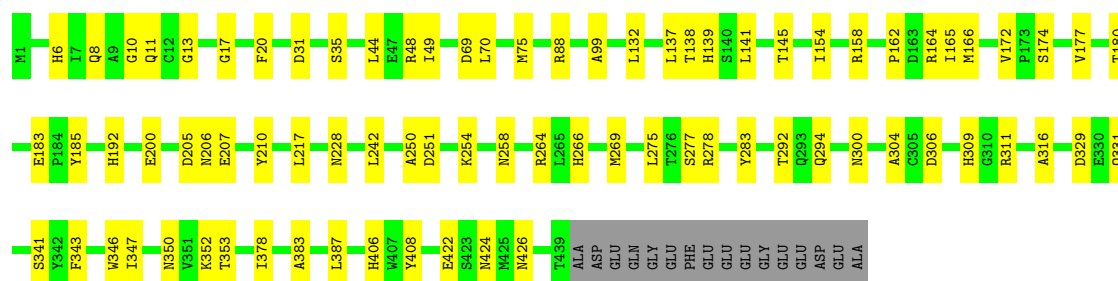
- Molecule 1: Tubulin alpha-1B chain

Chain L:  78% 18% .



- Molecule 2: Tubulin beta chain

Chain B:  78% 18% .



- Molecule 2: Tubulin beta chain

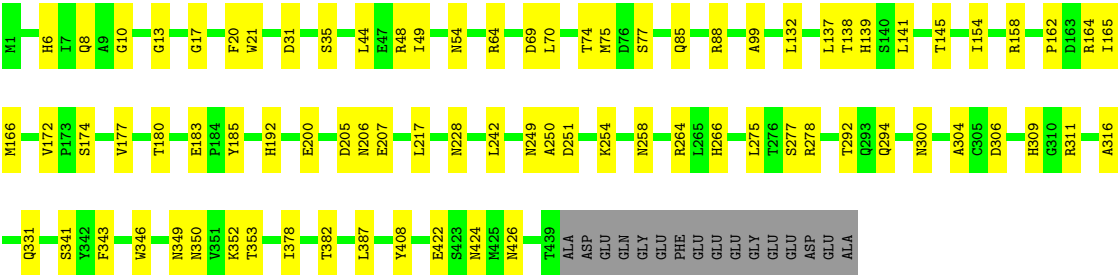




Chain I: 

78%

18%



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-27.7°, rise=9.3 Å, axial sym=C1	Depositor
Number of segments used	18432	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	1422.3	Depositor
Maximum defocus (nm)	2706.1	Depositor
Magnification	23364	Depositor
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: GDP, GTP, MG

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	0.36	0/3459	0.51	0/4697
1	C	0.36	0/3459	0.51	0/4697
1	E	0.36	0/3459	0.51	0/4697
1	J	0.36	0/3459	0.51	0/4697
1	K	0.36	0/3459	0.50	0/4697
1	L	0.36	0/3459	0.51	0/4697
2	B	0.36	0/3443	0.51	0/4666
2	D	0.36	0/3443	0.51	0/4666
2	F	0.36	0/3443	0.51	0/4666
2	G	0.36	0/3443	0.51	0/4666
2	H	0.36	0/3443	0.51	0/4666
2	I	0.36	0/3443	0.51	0/4666
All	All	0.36	0/41412	0.51	0/56178

There are no bond length outliers.

There are no bond angle outliers.

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	3382	0	3292	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3382	0	3292	46	0
1	E	3382	0	3292	50	0
1	J	3382	0	3292	48	0
1	K	3382	0	3292	45	0
1	L	3382	0	3292	46	0
2	B	3368	0	3246	49	0
2	D	3368	0	3246	52	0
2	F	3368	0	3246	47	0
2	G	3368	0	3246	40	0
2	H	3368	0	3246	43	0
2	I	3368	0	3246	49	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	E	32	0	12	0	0
3	J	32	0	12	0	0
3	K	32	0	12	0	0
3	L	32	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	2	0
5	F	28	0	12	2	0
5	G	28	0	12	2	0
5	H	28	0	12	2	0
5	I	28	0	12	2	0
All	All	40866	0	39372	518	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 6.

The worst 5 of 518 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:H:283:TYR:HB3	2:I:88:ARG:HG2	1.68	0.73
2:B:258:ASN:HD21	1:K:101:ASN:HD22	1.43	0.67
1:A:249:ASN:H	2:B:11:GLN:HE22	1.40	0.66
2:B:283:TYR:HB3	2:D:88:ARG:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:ASN:HD21	1:J:101:ASN:HD22	1.42	0.65

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	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
1	C	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
1	E	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
1	J	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
1	K	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
1	L	428/451 (95%)	417 (97%)	11 (3%)	0	100	100
2	B	427/445 (96%)	410 (96%)	17 (4%)	0	100	100
2	D	427/445 (96%)	410 (96%)	17 (4%)	0	100	100
2	F	427/445 (96%)	411 (96%)	16 (4%)	0	100	100
2	G	427/445 (96%)	410 (96%)	17 (4%)	0	100	100
2	H	427/445 (96%)	410 (96%)	17 (4%)	0	100	100
2	I	427/445 (96%)	410 (96%)	17 (4%)	0	100	100
All	All	5130/5376 (95%)	4963 (97%)	167 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	364/379 (96%)	363 (100%)	1 (0%)	93	97
1	C	364/379 (96%)	363 (100%)	1 (0%)	93	97
1	E	364/379 (96%)	363 (100%)	1 (0%)	93	97
1	J	364/379 (96%)	363 (100%)	1 (0%)	93	97
1	K	364/379 (96%)	363 (100%)	1 (0%)	93	97
1	L	364/379 (96%)	363 (100%)	1 (0%)	93	97
2	B	368/381 (97%)	367 (100%)	1 (0%)	93	97
2	D	368/381 (97%)	367 (100%)	1 (0%)	93	97
2	F	368/381 (97%)	367 (100%)	1 (0%)	93	97
2	G	368/381 (97%)	367 (100%)	1 (0%)	93	97
2	H	368/381 (97%)	367 (100%)	1 (0%)	93	97
2	I	368/381 (97%)	367 (100%)	1 (0%)	93	97
All	All	4392/4560 (96%)	4380 (100%)	12 (0%)	93	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	300	ASN
2	G	300	ASN
1	J	339	ARG
1	E	339	ARG
2	I	300	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	133	GLN
2	G	133	GLN
1	K	186	ASN
2	F	192	HIS
2	F	294	GLN

### 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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
3	GTP	A	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
5	GDP	B	501	-	24,30,30	1.07	2 (8%)	27,47,47	2.13	7 (25%)
3	GTP	C	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
5	GDP	D	501	-	24,30,30	1.07	2 (8%)	27,47,47	2.13	7 (25%)
3	GTP	E	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
5	GDP	F	501	-	24,30,30	1.07	2 (8%)	27,47,47	2.12	7 (25%)
5	GDP	G	501	-	24,30,30	1.06	2 (8%)	27,47,47	2.13	7 (25%)
5	GDP	H	501	-	24,30,30	1.06	2 (8%)	27,47,47	2.13	7 (25%)
5	GDP	I	501	-	24,30,30	1.08	2 (8%)	27,47,47	2.12	7 (25%)
3	GTP	J	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	K	501	4	26,34,34	0.96	1 (3%)	29,54,54	1.91	6 (20%)
3	GTP	L	501	4	26,34,34	0.95	1 (3%)	29,54,54	1.91	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
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
3	GTP	C	501	4	-	0/18/38/38	0/3/3/3
5	GDP	D	501	-	-	0/12/32/32	0/3/3/3
3	GTP	E	501	4	-	0/18/38/38	0/3/3/3
5	GDP	F	501	-	-	0/12/32/32	0/3/3/3
5	GDP	G	501	-	-	0/12/32/32	0/3/3/3
5	GDP	H	501	-	-	0/12/32/32	0/3/3/3
5	GDP	I	501	-	-	0/12/32/32	0/3/3/3
3	GTP	J	501	4	-	0/18/38/38	0/3/3/3
3	GTP	K	501	4	-	0/18/38/38	0/3/3/3
3	GTP	L	501	4	-	0/18/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	501	GDP	C5-C4	2.55	1.46	1.40
3	E	501	GTP	C6-N1	2.55	1.37	1.33
5	B	501	GDP	C5-C4	2.57	1.46	1.40
3	J	501	GTP	C6-N1	2.58	1.37	1.33
3	C	501	GTP	C6-N1	2.58	1.37	1.33

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	GTP	N3-C2-N1	-5.03	120.45	127.25
3	K	501	GTP	N3-C2-N1	-5.02	120.46	127.25
3	A	501	GTP	N3-C2-N1	-5.02	120.46	127.25
3	C	501	GTP	N3-C2-N1	-5.02	120.46	127.25
3	J	501	GTP	N3-C2-N1	-5.01	120.47	127.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GDP	2	0
5	D	501	GDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	501	GDP	2	0
5	G	501	GDP	2	0
5	H	501	GDP	2	0
5	I	501	GDP	2	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.