



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:42 am GMT

PDB ID : 3J6F
EMDB ID: : EMD-5896
Title : Minimized average structure of GDP-bound dynamic microtubules
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-19
Resolution : 4.90 Å(reported)
Based on PDB ID : 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
<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) : recalc29047

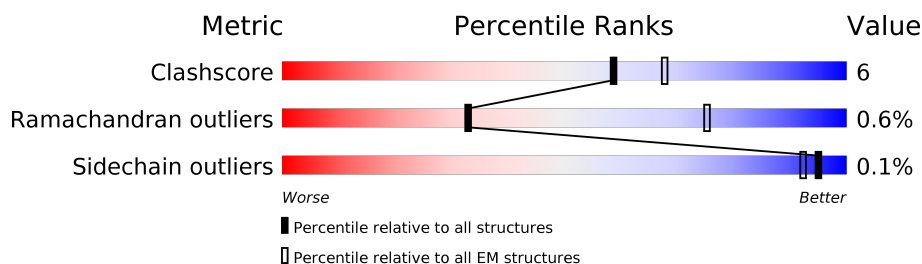
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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
Sidechain outliers	121581	1026

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	A	439	79% 17% . .
1	C	439	78% 18% . .
1	E	439	79% 17% . .
1	G	439	78% 17% . .
1	I	439	79% 17% . .
1	K	439	79% 17% . .
1	M	439	79% 16% . .
1	O	439	79% 16% . .
1	Q	439	79% 17% . .

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Mol	Chain	Length	Quality of chain
2	B	427	<div><div></div><div>85%13%</div><div></div></div>
2	D	427	<div><div></div><div>84%13%</div><div></div></div>
2	F	427	<div><div></div><div>85%13%</div><div></div></div>
2	H	427	<div><div></div><div>85%13%</div><div></div></div>
2	J	427	<div><div></div><div>85%13%</div><div></div></div>
2	L	427	<div><div></div><div>85%13%</div><div></div></div>
2	N	427	<div><div></div><div>84%13%</div><div></div></div>
2	P	427	<div><div></div><div>83%14%</div><div></div></div>
2	R	427	<div><div></div><div>83%15%</div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60903 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-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	C	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	E	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	G	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	I	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	K	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	M	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	O	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	Q	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		

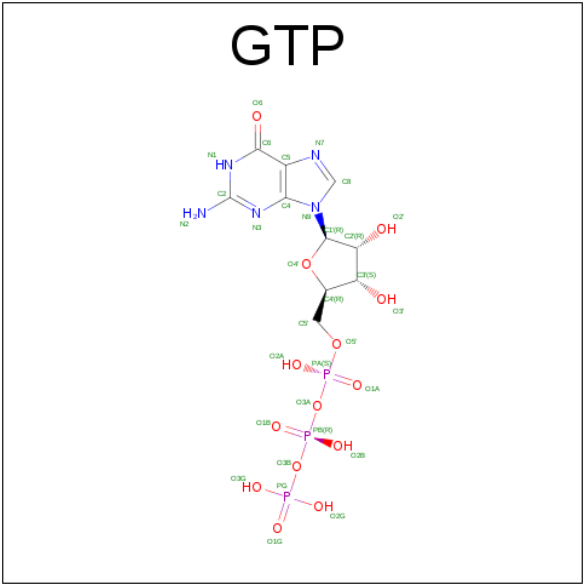
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	CONFLICT	UNP P02550
C	265	GLY	ALA	CONFLICT	UNP P02550
E	265	GLY	ALA	CONFLICT	UNP P02550
G	265	GLY	ALA	CONFLICT	UNP P02550
I	265	GLY	ALA	CONFLICT	UNP P02550
K	265	GLY	ALA	CONFLICT	UNP P02550
M	265	GLY	ALA	CONFLICT	UNP P02550
O	265	GLY	ALA	CONFLICT	UNP P02550
Q	265	GLY	ALA	CONFLICT	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	D	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	F	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	H	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	J	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	L	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	N	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	P	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	R	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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	

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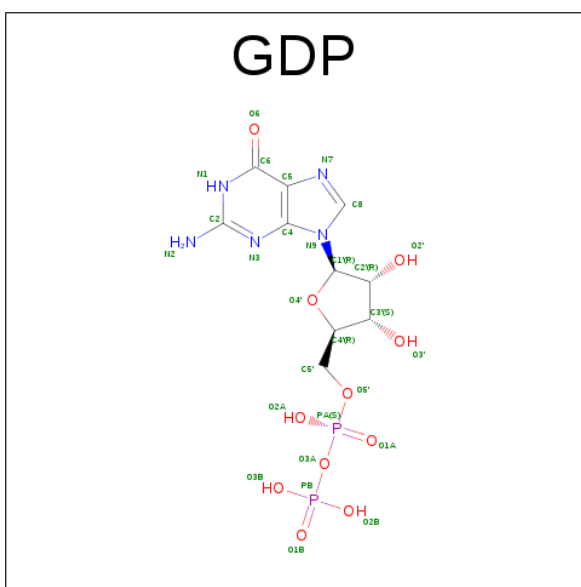
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Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	Q	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	G	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	4	Total O 4 4	0
6	C	4	Total O 4 4	0
6	E	4	Total O 4 4	0

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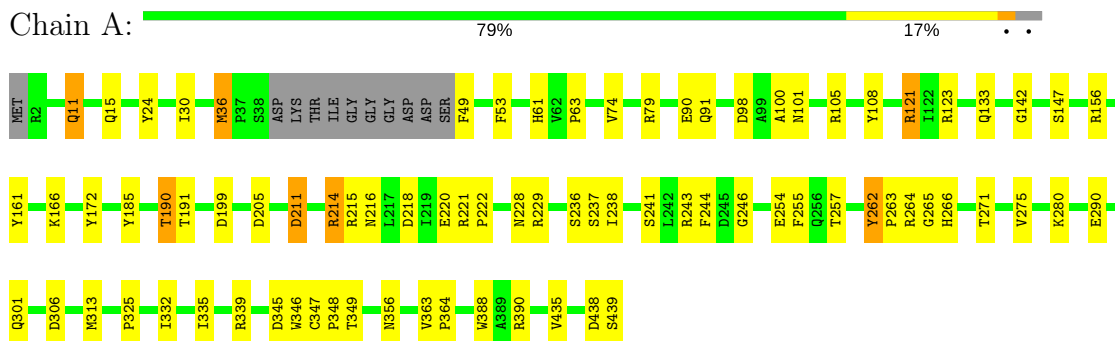
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Mol	Chain	Residues	Atoms		AltConf
6	G	4	Total 4	O 4	0
6	I	4	Total 4	O 4	0
6	K	4	Total 4	O 4	0
6	M	4	Total 4	O 4	0
6	O	4	Total 4	O 4	0
6	Q	4	Total 4	O 4	0

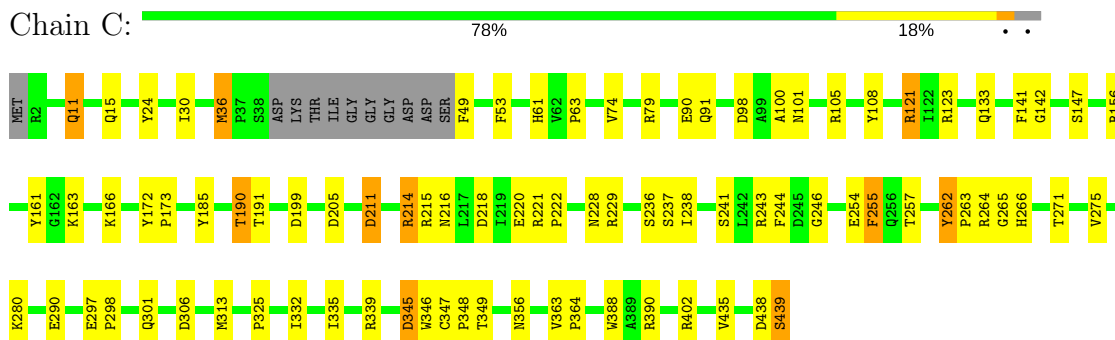
3 Residue-property plots

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.

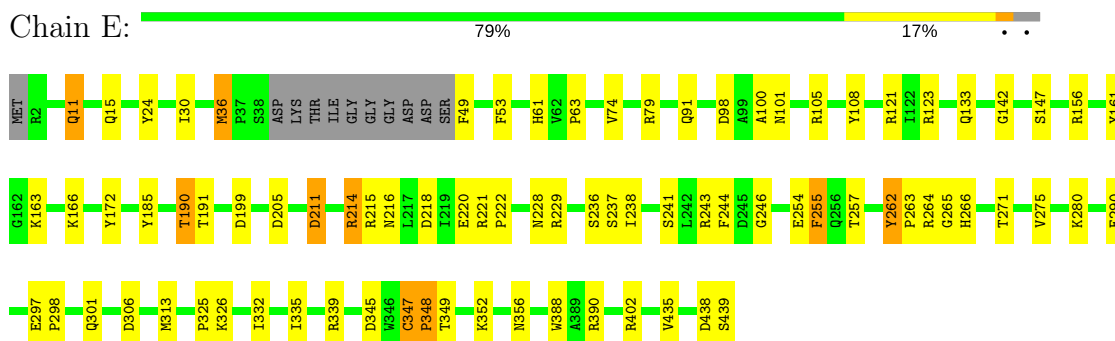
- Molecule 1: Tubulin alpha-1A chain



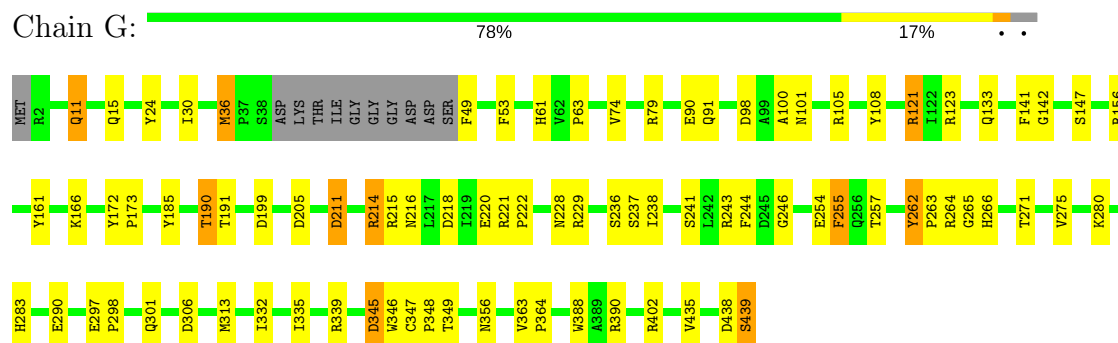
- Molecule 1: Tubulin alpha-1A chain



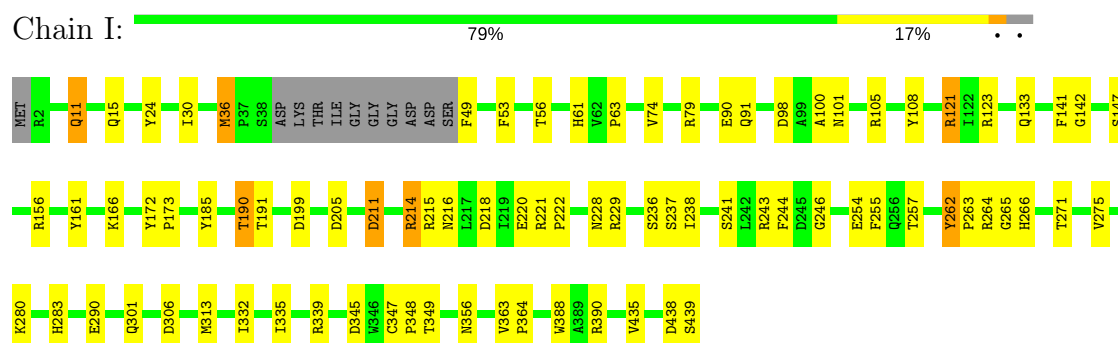
- Molecule 1: Tubulin alpha-1A chain



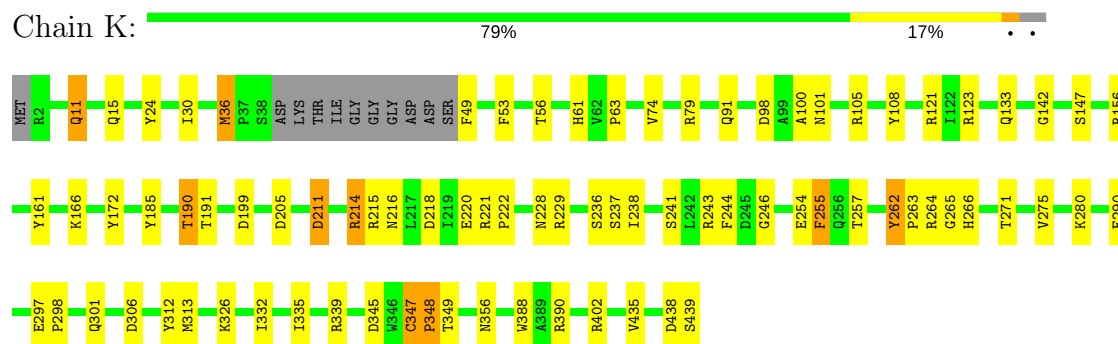
- Molecule 1: Tubulin alpha-1A chain



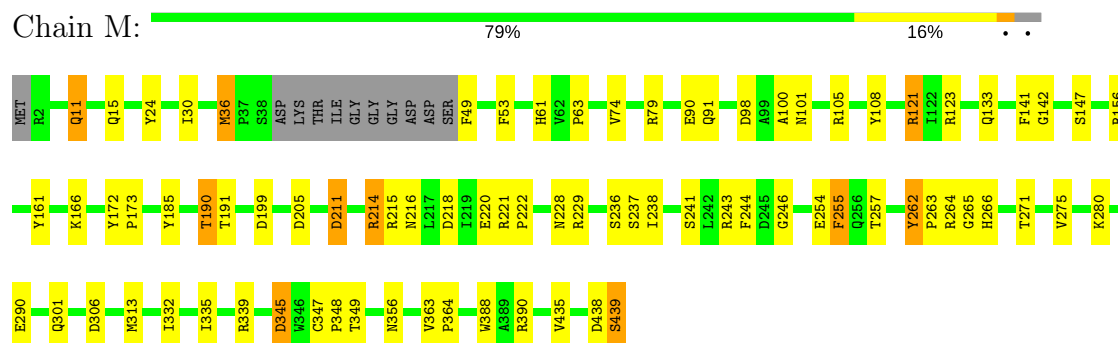
- Molecule 1: Tubulin alpha-1A chain



- Molecule 1: Tubulin alpha-1A chain



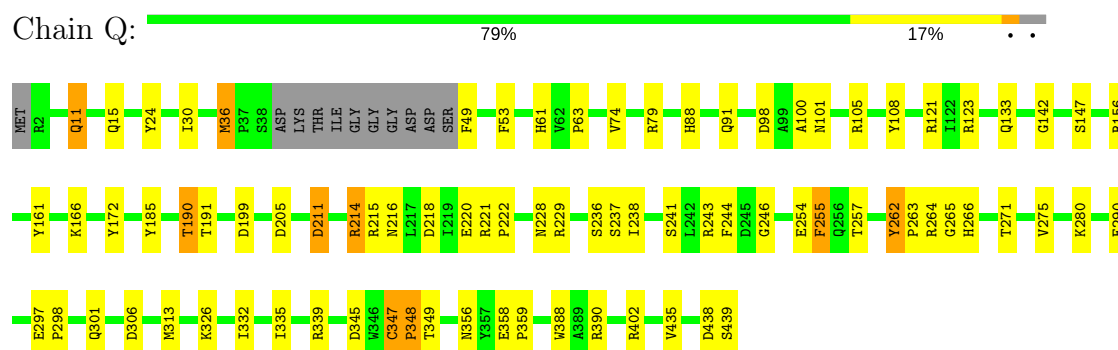
- Molecule 1: Tubulin alpha-1A chain



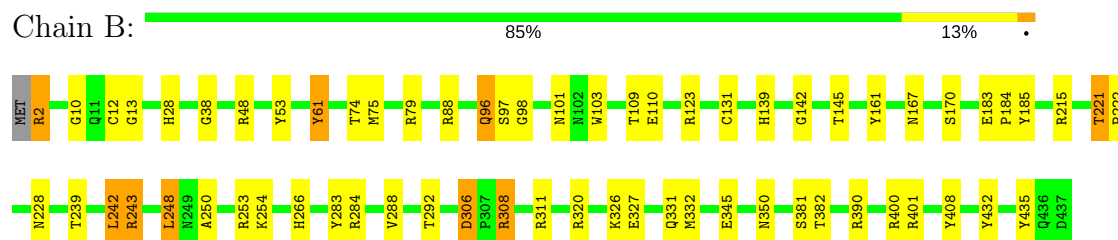
- Molecule 1: Tubulin alpha-1A chain



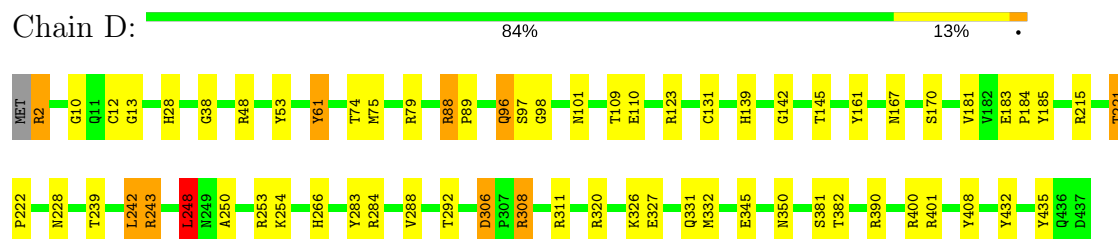
- Molecule 1: Tubulin alpha-1A chain



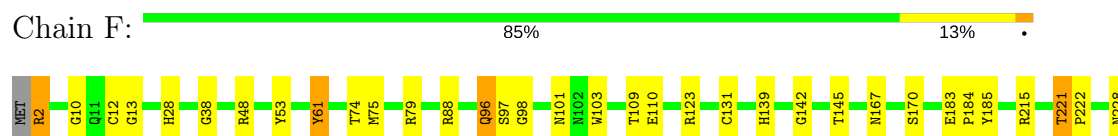
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain

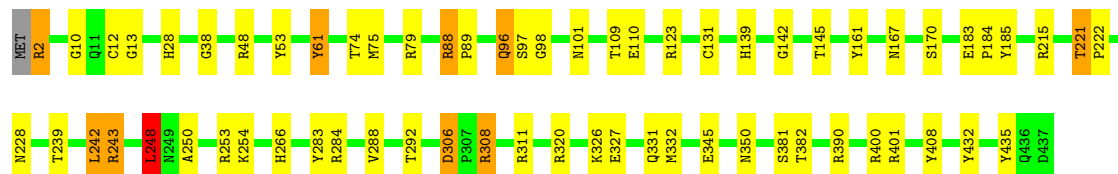
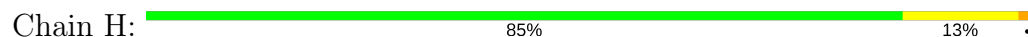


- Molecule 2: Tubulin beta chain

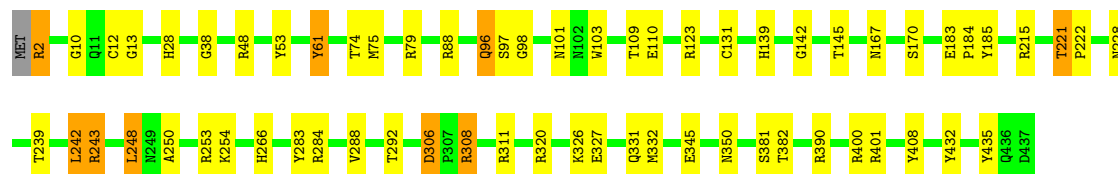
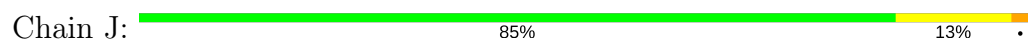




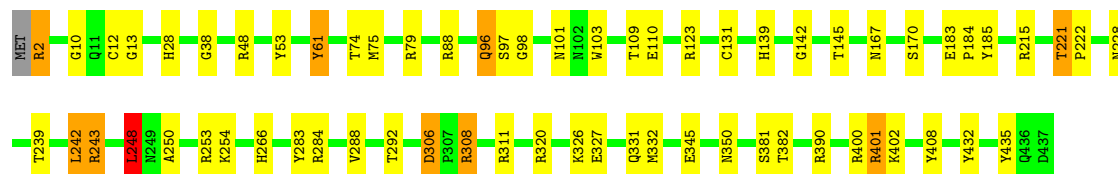
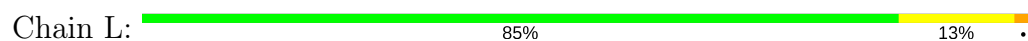
• Molecule 2: Tubulin beta chain



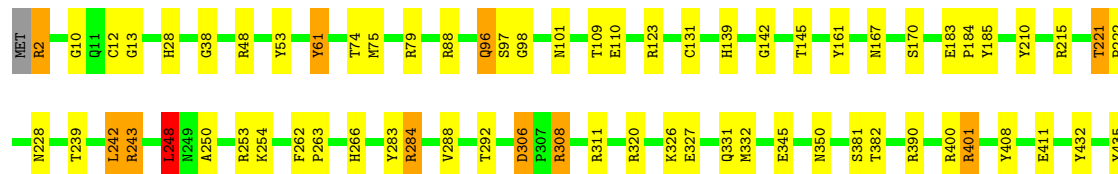
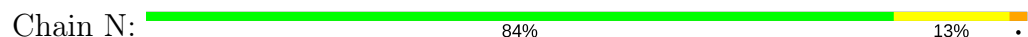
• Molecule 2: Tubulin beta chain



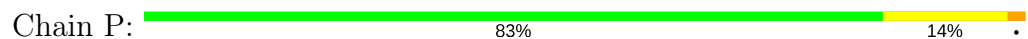
• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

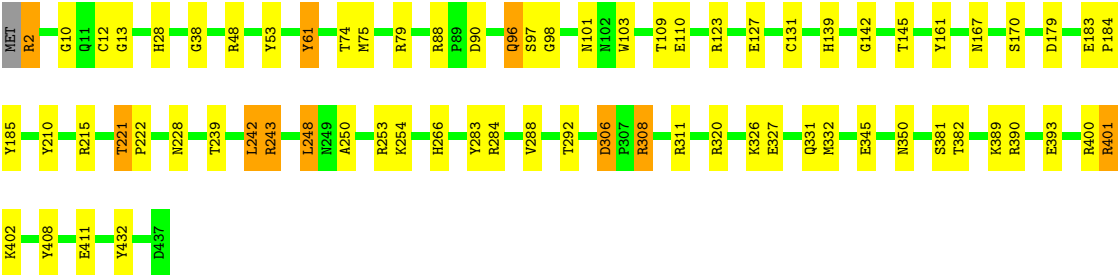
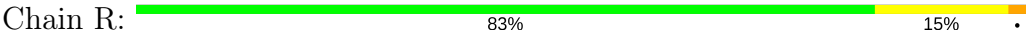


• Molecule 2: Tubulin beta chain





• Molecule 2: Tubulin beta chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	54445	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	ctftilt	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.0	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	72000	Depositor
Image detector	KODAK SO-163 film	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

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	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	C	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	E	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	G	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	I	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	K	1.14	10/3427 (0.3%)	1.44	45/4651 (1.0%)
1	M	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	O	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	Q	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
2	B	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	D	1.05	5/3427 (0.1%)	1.56	49/4642 (1.1%)
2	F	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	H	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	J	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	L	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	N	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	P	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	R	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
All	All	1.09	135/61686 (0.2%)	1.50	826/83637 (1.0%)

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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
All	All	0	9

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	265	GLY	CA-C	-15.06	1.27	1.51
1	M	265	GLY	CA-C	-15.03	1.27	1.51
1	E	265	GLY	CA-C	-15.01	1.27	1.51
1	I	265	GLY	CA-C	-15.01	1.27	1.51
1	G	265	GLY	CA-C	-15.00	1.27	1.51

The worst 5 of 826 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	48	ARG	NE-CZ-NH1	20.40	130.50	120.30
2	P	48	ARG	NE-CZ-NH1	20.32	130.46	120.30
2	J	48	ARG	NE-CZ-NH1	20.31	130.45	120.30
2	H	48	ARG	NE-CZ-NH1	20.30	130.45	120.30
2	B	48	ARG	NE-CZ-NH1	20.29	130.44	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	LEU	Peptide
2	D	248	LEU	Peptide
2	F	248	LEU	Peptide
2	H	248	LEU	Peptide
2	J	248	LEU	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	3350	0	3254	39	0
1	C	3350	0	3254	46	0
1	E	3350	0	3254	43	0
1	G	3350	0	3254	45	0
1	I	3350	0	3254	40	0
1	K	3350	0	3254	40	0
1	M	3350	0	3254	41	0
1	O	3350	0	3254	38	0
1	Q	3350	0	3254	42	0
2	B	3352	0	3227	34	0
2	D	3352	0	3227	36	0
2	F	3352	0	3227	35	0
2	H	3352	0	3227	35	0
2	J	3352	0	3227	34	0
2	L	3352	0	3227	36	0
2	N	3352	0	3227	40	0
2	P	3352	0	3227	44	0
2	R	3352	0	3227	42	0
3	A	32	0	12	2	0
3	C	32	0	12	2	0
3	E	32	0	12	2	0
3	G	32	0	12	2	0
3	I	32	0	12	2	0
3	K	32	0	12	2	0
3	M	32	0	12	2	0
3	O	32	0	12	2	0
3	Q	32	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	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	H	28	0	12	2	0
5	J	28	0	12	2	0
5	L	28	0	12	2	0
5	N	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	28	0	12	2	0
5	R	28	0	12	2	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
6	E	4	0	0	0	0
6	G	4	0	0	0	0
6	I	4	0	0	0	0
6	K	4	0	0	0	0
6	M	4	0	0	0	0
6	O	4	0	0	0	0
6	Q	4	0	0	0	0
All	All	60903	0	58545	666	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 666 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:J:228:ASN:HD21	5:J:901:GDP:HN1	1.17	0.91
2:L:228:ASN:HD21	5:L:901:GDP:HN1	1.17	0.90
2:B:228:ASN:HD21	5:B:901:GDP:HN1	1.17	0.90
2:F:228:ASN:HD21	5:F:901:GDP:HN1	1.17	0.90
2:R:228:ASN:HD21	5:R:901:GDP:HN1	1.17	0.90

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	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	E	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	G	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	I	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	K	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	M	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	O	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	Q	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	B	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	D	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	F	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	H	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	J	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	L	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	N	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	P	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	R	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
All	All	7632/7794 (98%)	7353 (96%)	234 (3%)	45 (1%)	33	71

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	GLY
2	D	98	GLY
2	F	98	GLY
2	H	98	GLY
2	J	98	GLY

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	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	C	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	E	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	G	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	I	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	K	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	M	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	O	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	Q	360/368 (98%)	359 (100%)	1 (0%)	94	96
2	B	367/368 (100%)	367 (100%)	0	100	100
2	D	367/368 (100%)	367 (100%)	0	100	100
2	F	367/368 (100%)	367 (100%)	0	100	100
2	H	367/368 (100%)	367 (100%)	0	100	100
2	J	367/368 (100%)	367 (100%)	0	100	100
2	L	367/368 (100%)	367 (100%)	0	100	100
2	N	367/368 (100%)	367 (100%)	0	100	100
2	P	367/368 (100%)	367 (100%)	0	100	100
2	R	367/368 (100%)	367 (100%)	0	100	100
All	All	6543/6624 (99%)	6534 (100%)	9 (0%)	95	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	255	PHE
1	Q	255	PHE
1	M	255	PHE
1	E	255	PHE
1	K	255	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	11	GLN
2	L	8	GLN
1	Q	301	GLN
2	J	96	GLN

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Mol	Chain	Res	Type
2	J	249	ASN

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 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 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	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	B	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	C	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	D	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	E	501	4	27,34,34	1.52	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	F	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	11 (42%)
3	GTP	G	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	H	901	-	25,30,30	2.71	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	I	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	J	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	K	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	4 (14%)
5	GDP	L	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	11 (42%)
3	GTP	M	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.16	5 (18%)
5	GDP	N	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	O	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.15	5 (18%)
5	GDP	P	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	Q	501	4	27,34,34	1.52	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	R	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.64	10 (38%)

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	901	-	-	0/12/32/32	0/3/3/3
3	GTP	C	501	4	-	0/18/38/38	0/3/3/3
5	GDP	D	901	-	-	0/12/32/32	0/3/3/3
3	GTP	E	501	4	-	0/18/38/38	0/3/3/3
5	GDP	F	901	-	-	0/12/32/32	0/3/3/3
3	GTP	G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	H	901	-	-	0/12/32/32	0/3/3/3
3	GTP	I	501	4	-	0/18/38/38	0/3/3/3
5	GDP	J	901	-	-	0/12/32/32	0/3/3/3
3	GTP	K	501	4	-	0/18/38/38	0/3/3/3
5	GDP	L	901	-	-	0/12/32/32	0/3/3/3
3	GTP	M	501	4	-	0/18/38/38	0/3/3/3
5	GDP	N	901	-	-	0/12/32/32	0/3/3/3
3	GTP	O	501	4	-	0/18/38/38	0/3/3/3
5	GDP	P	901	-	-	0/12/32/32	0/3/3/3
3	GTP	Q	501	4	-	0/18/38/38	0/3/3/3
5	GDP	R	901	-	-	0/12/32/32	0/3/3/3

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	901	GDP	PB-O2B	-3.55	1.40	1.54
5	D	901	GDP	PB-O2B	-3.55	1.40	1.54
5	R	901	GDP	PB-O2B	-3.54	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	GDP	PB-O2B	-3.54	1.40	1.54
5	P	901	GDP	PB-O2B	-3.54	1.40	1.54

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	GDP	C6-C5-C4	-11.54	109.37	120.84
5	P	901	GDP	C6-C5-C4	-11.49	109.42	120.84
5	N	901	GDP	C6-C5-C4	-11.49	109.42	120.84
5	B	901	GDP	C6-C5-C4	-11.48	109.42	120.84
5	L	901	GDP	C6-C5-C4	-11.48	109.43	120.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	2	0
5	B	901	GDP	2	0
3	C	501	GTP	2	0
5	D	901	GDP	2	0
3	E	501	GTP	2	0
5	F	901	GDP	2	0
3	G	501	GTP	2	0
5	H	901	GDP	2	0
3	I	501	GTP	2	0
5	J	901	GDP	2	0
3	K	501	GTP	2	0
5	L	901	GDP	2	0
3	M	501	GTP	2	0
5	N	901	GDP	2	0
3	O	501	GTP	2	0
5	P	901	GDP	2	0
3	Q	501	GTP	2	0
5	R	901	GDP	2	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.