



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:24 PM BST

PDB ID : 3J6G
EMDB ID: : EMD-5897
Title : Minimized average structure of microtubules stabilized by taxol
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-19
Resolution : 5.50 Å(reported)
Based on PDB ID : 1JFF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

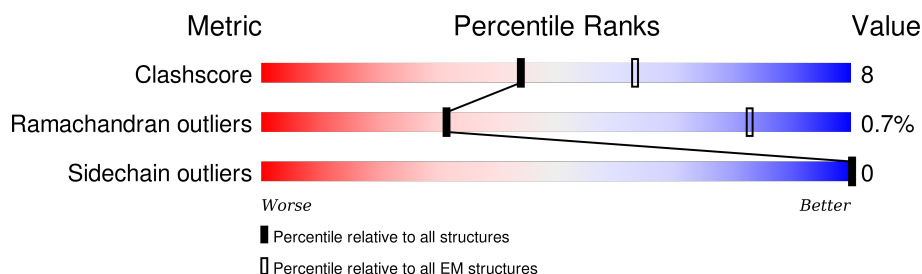
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	72% 19% 6% .
1	C	439	71% 20% 6% .
1	E	439	72% 19% 6% .
1	G	439	72% 19% 6% .
1	I	439	73% 18% 6% .
1	K	439	73% 18% 6% .
1	M	439	72% 20% 6% .
1	O	439	73% 19% 6% .
1	Q	439	73% 18% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	427	 75% 23% •
2	D	427	 77% 22% •
2	F	427	 77% 21% •
2	H	427	 76% 22% •
2	J	427	 76% 22% •
2	L	427	 77% 21% •
2	N	427	 76% 22% •
2	P	427	 75% 23% •
2	R	427	 76% 22% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 61461 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		

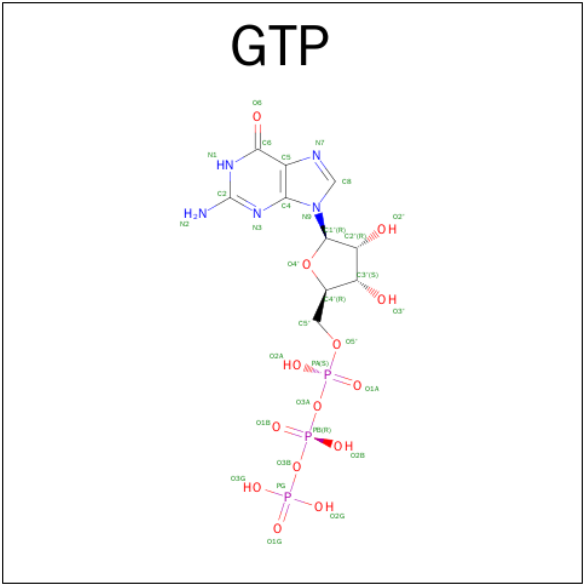
There are 9 discrepancies between the modelled and reference sequences:

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	

Continued on next page...

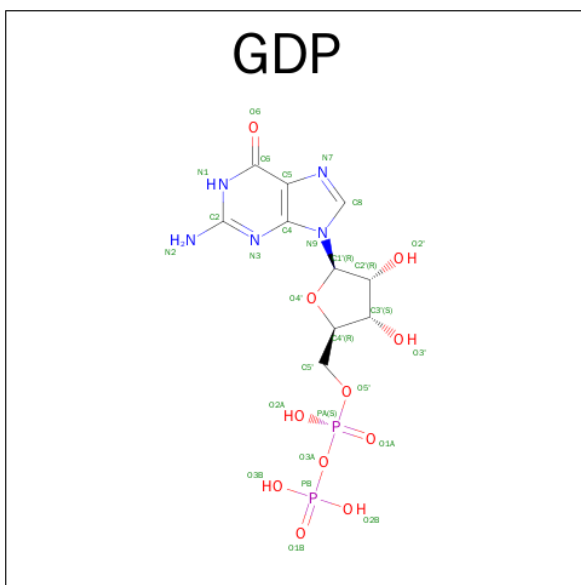
Continued from previous page...

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



- Molecule 7 is water.

Continued on next page...

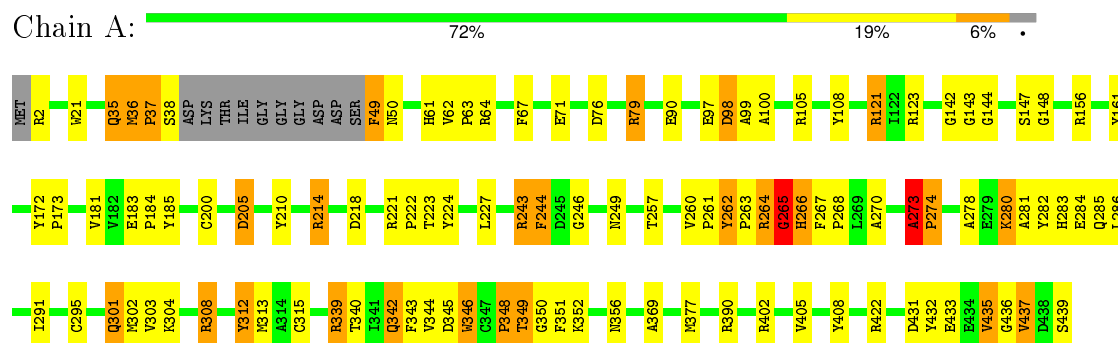
Continued from previous page...

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

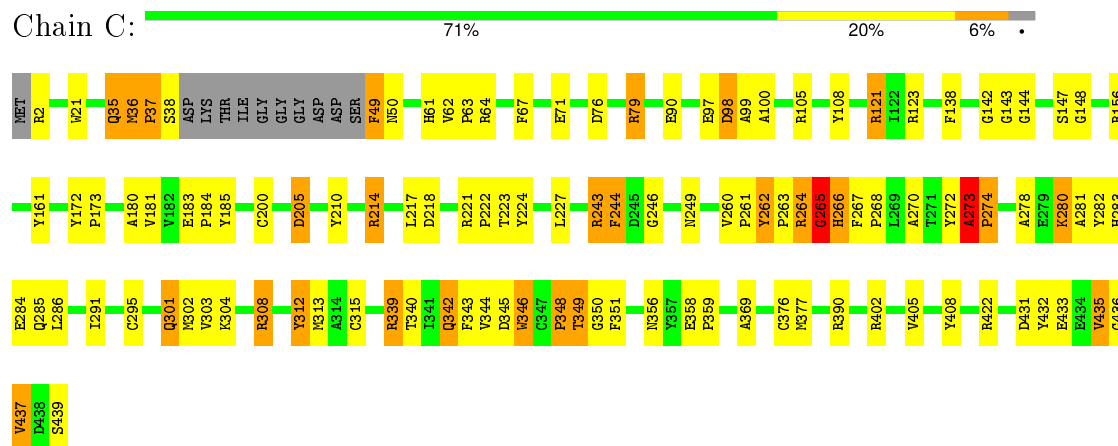
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

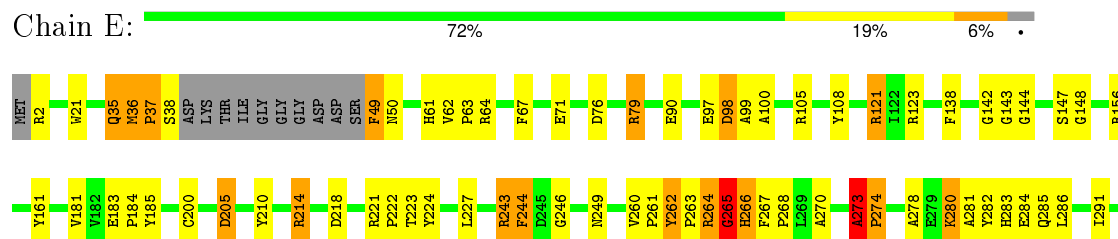
- Molecule 1: Tubulin alpha-1A chain



- Molecule 1: Tubulin alpha-1A chain



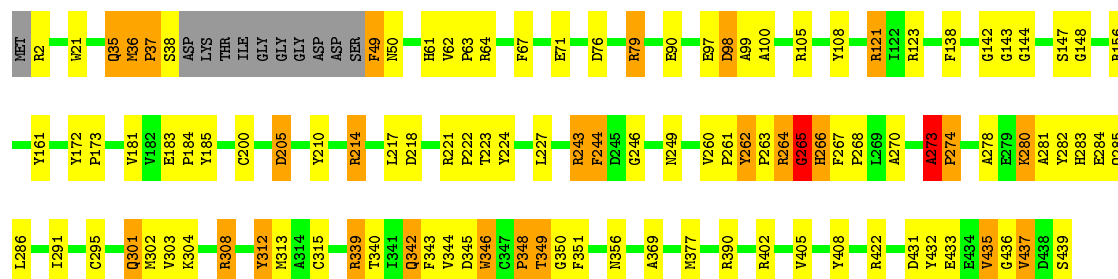
- Molecule 1: Tubulin alpha-1A chain





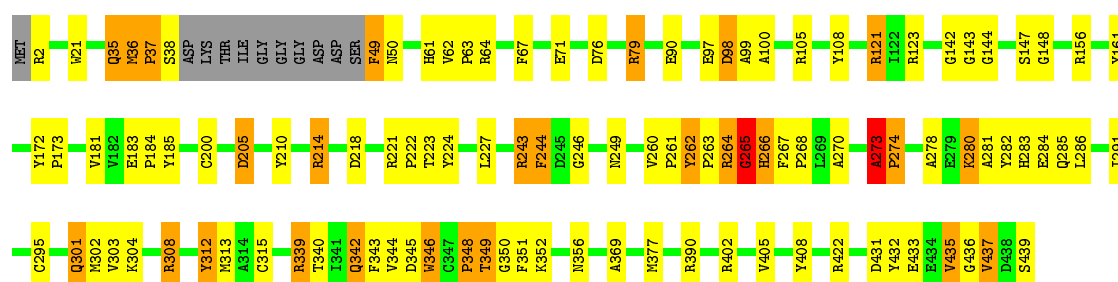
• Molecule 1: Tubulin alpha-1A chain

Chain G: 72% 19% 6%



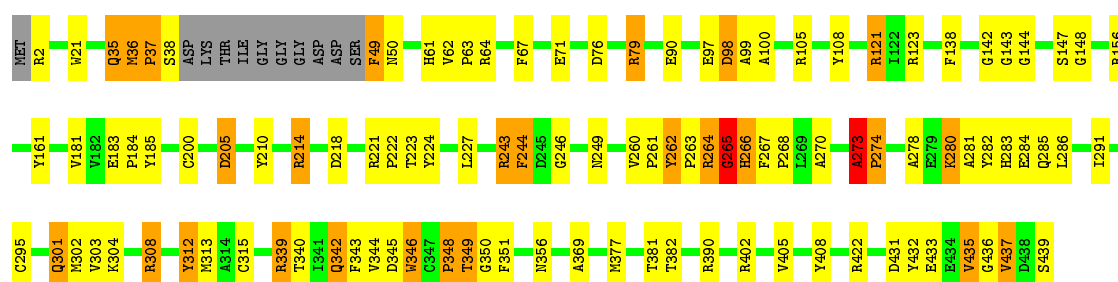
• Molecule 1: Tubulin alpha-1A chain

Chain I: 73% 18% 6%



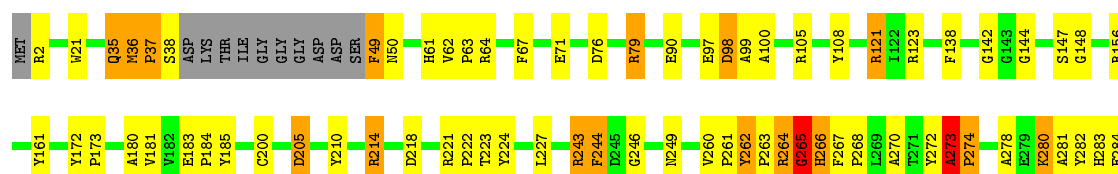
• Molecule 1: Tubulin alpha-1A chain

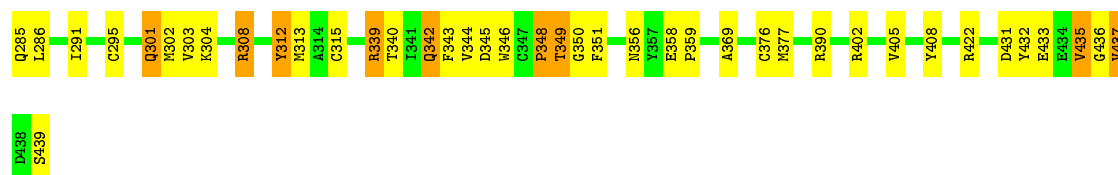
Chain K: 73% 18% 6%



• Molecule 1: Tubulin alpha-1A chain

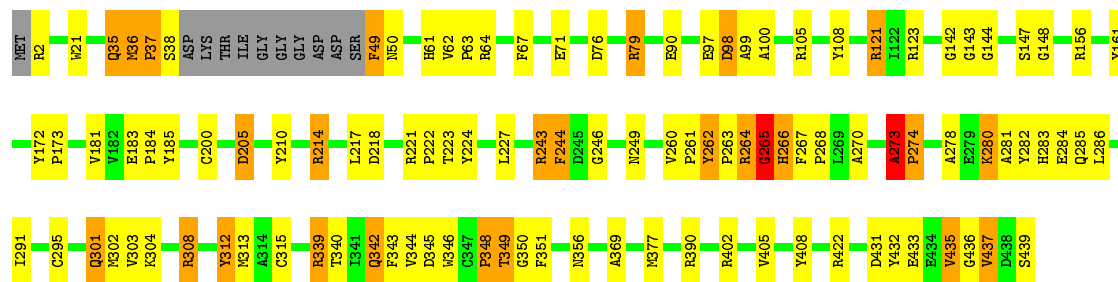
Chain M: 72% 20% 6%





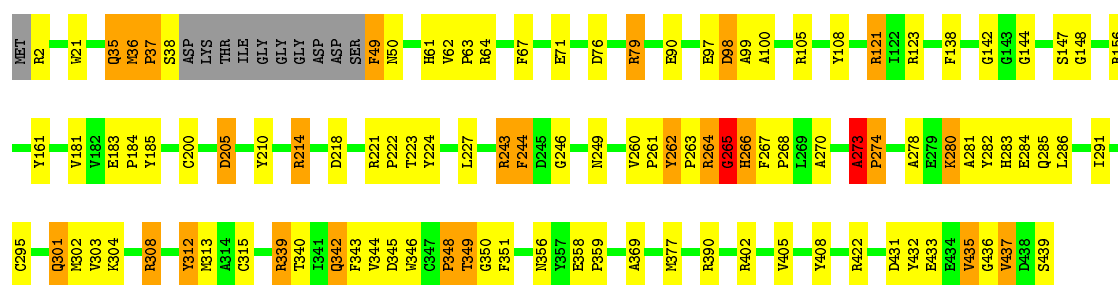
- Molecule 1: Tubulin alpha-1A chain

Chain O: 73% 19% 6% •



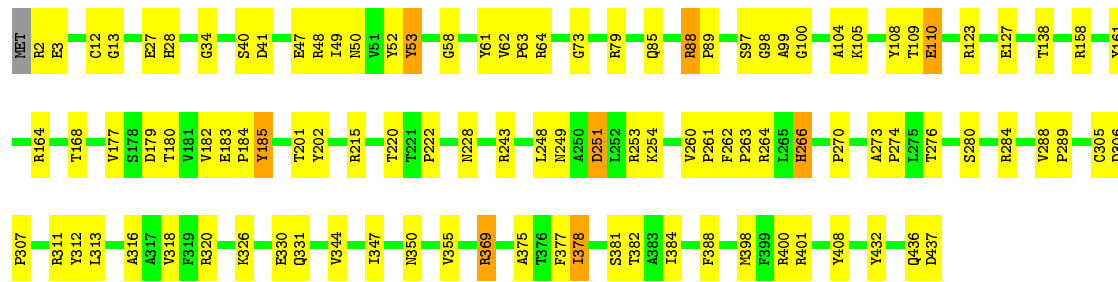
- Molecule 1: Tubulin alpha-1A chain

Chain Q: 73% 18% 6% •



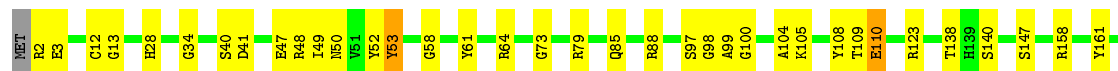
- Molecule 2: Tubulin beta chain

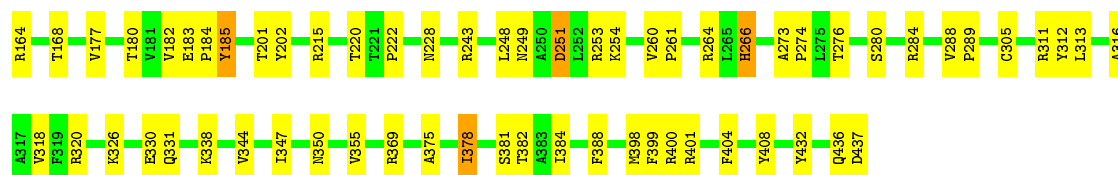
Chain B: 75% 23% •



- Molecule 2: Tubulin beta chain

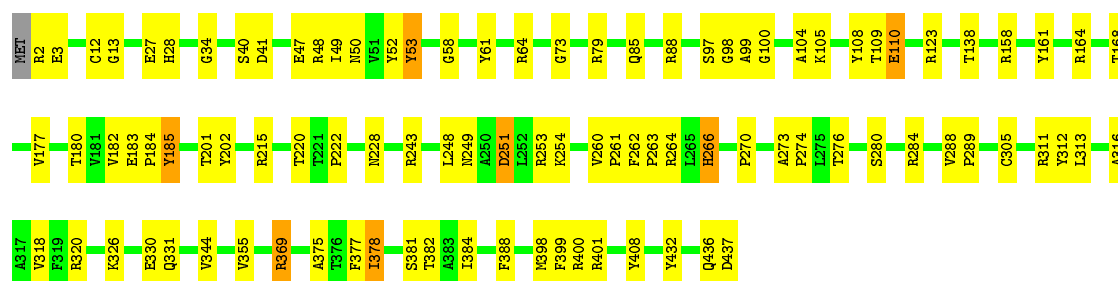
Chain D: 77% 22% •





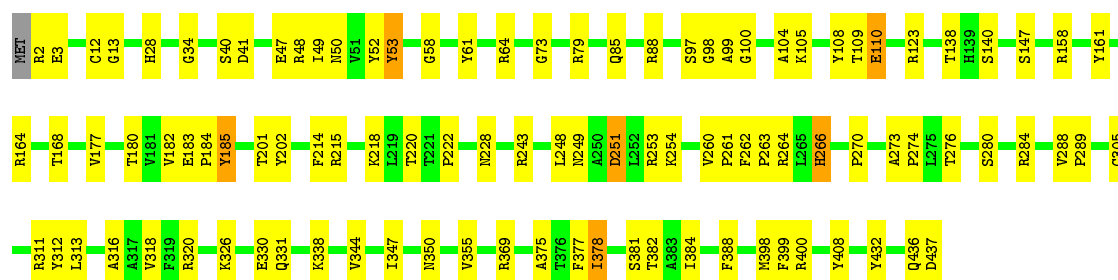
- Molecule 2: Tubulin beta chain

Chain F: 77% 21%



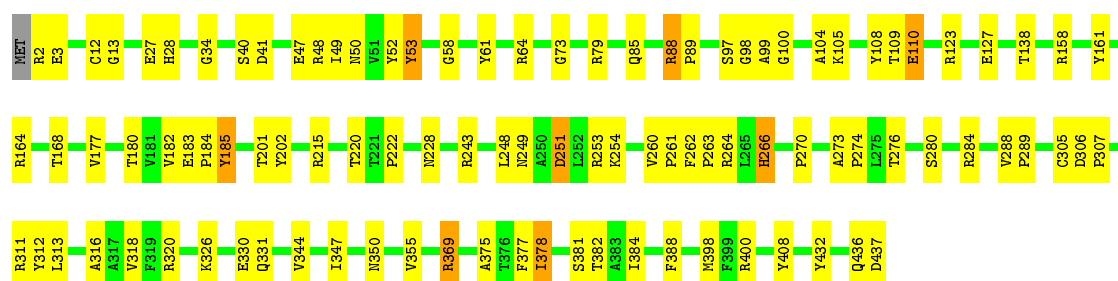
- Molecule 2: Tubulin beta chain

Chain H: 76% 22%



- Molecule 2: Tubulin beta chain

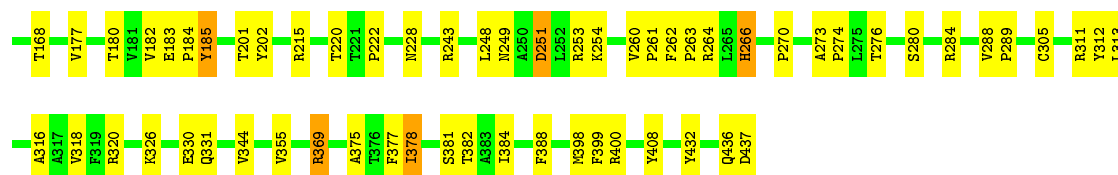
Chain J: 76% 22%



- Molecule 2: Tubulin beta chain

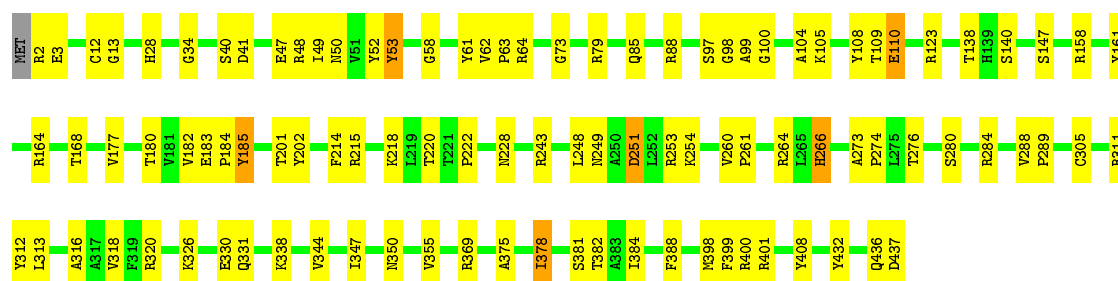
Chain L: 77% 21%





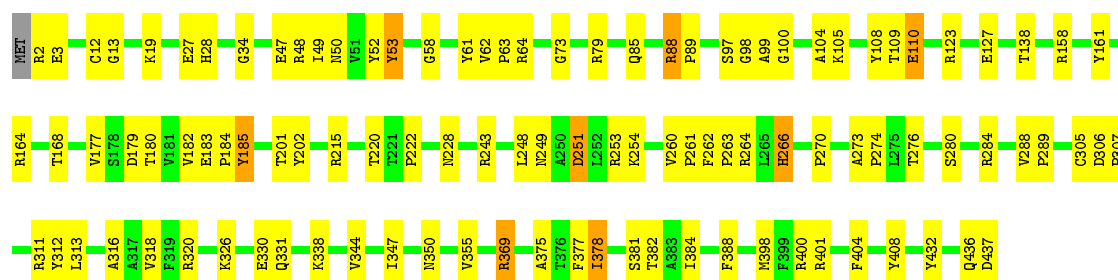
- Molecule 2: Tubulin beta chain

Chain N: 76% 22%



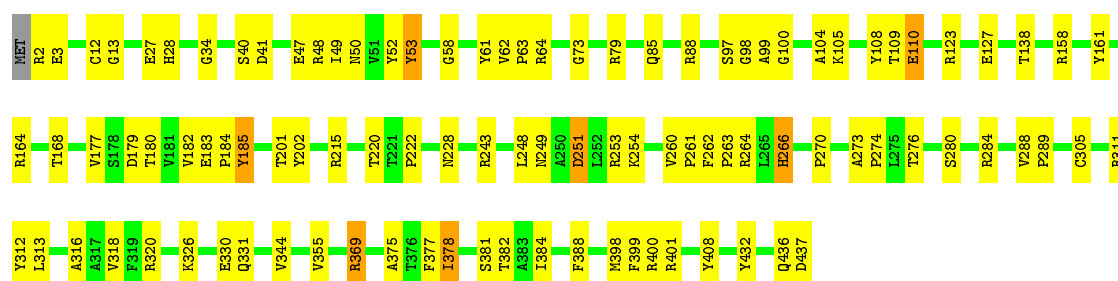
- Molecule 2: Tubulin beta chain

Chain P: 75% 23%



- Molecule 2: Tubulin beta chain

Chain R: 76% 22%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	24357	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, 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	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	C	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	E	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	G	1.34	32/3427 (0.9%)	1.68	86/4651 (1.8%)
1	I	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	K	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	M	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	O	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
1	Q	1.34	31/3427 (0.9%)	1.68	86/4651 (1.8%)
2	B	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	D	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	F	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	H	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	J	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	L	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	N	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	P	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
2	R	1.19	12/3427 (0.4%)	1.55	46/4642 (1.0%)
All	All	1.27	388/61686 (0.6%)	1.62	1188/83637 (1.4%)

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	6
1	C	0	6
1	E	0	6
1	G	0	6
1	I	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	6
1	M	0	6
1	O	0	6
1	Q	0	6
All	All	0	54

The worst 5 of 388 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	GLU	N-CA	-12.57	1.21	1.46
2	N	3	GLU	N-CA	-12.56	1.21	1.46
2	R	3	GLU	N-CA	-12.56	1.21	1.46
2	H	3	GLU	N-CA	-12.55	1.21	1.46
2	B	3	GLU	N-CA	-12.54	1.21	1.46

The worst 5 of 1188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	262	TYR	CB-CG-CD1	-17.46	110.53	121.00
1	G	262	TYR	CB-CG-CD1	-17.44	110.53	121.00
1	A	262	TYR	CB-CG-CD1	-17.43	110.54	121.00
1	E	262	TYR	CB-CG-CD1	-17.42	110.55	121.00
1	I	262	TYR	CB-CG-CD1	-17.41	110.55	121.00

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	PHE	Sidechain
1	A	264	ARG	Peptide
1	A	265	GLY	Peptide
1	A	273	ALA	Mainchain
1	A	37	PRO	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	3253	74	0
1	C	3350	0	3253	76	0
1	E	3350	0	3253	72	0
1	G	3350	0	3253	74	0
1	I	3350	0	3253	70	0
1	K	3350	0	3253	73	0
1	M	3350	0	3253	61	0
1	O	3350	0	3253	59	0
1	Q	3350	0	3253	59	0
2	B	3352	0	3229	59	0
2	D	3352	0	3229	56	0
2	F	3352	0	3229	58	0
2	H	3352	0	3229	47	0
2	J	3352	0	3229	46	0
2	L	3352	0	3229	45	0
2	N	3352	0	3229	58	0
2	P	3352	0	3229	64	0
2	R	3352	0	3229	59	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	E	32	0	12	0	0
3	G	32	0	12	0	0
3	I	32	0	12	0	0
3	K	32	0	12	0	0
3	M	32	0	12	0	0
3	O	32	0	12	0	0
3	Q	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	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

Continued on next page...

Continued from previous page...

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	B	62	0	51	4	0
6	D	62	0	51	4	0
6	F	62	0	51	4	0
6	H	62	0	51	4	0
6	J	62	0	51	4	0
6	L	62	0	51	4	0
6	N	62	0	51	4	0
6	P	62	0	51	4	0
6	R	62	0	51	4	0
7	A	4	0	0	1	0
7	C	4	0	0	1	0
7	E	4	0	0	1	0
7	G	4	0	0	1	0
7	I	4	0	0	1	0
7	K	4	0	0	1	0
7	M	4	0	0	1	0
7	O	4	0	0	1	0
7	Q	4	0	0	1	0
All	All	61461	0	59013	1008	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.

The worst 5 of 1008 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:C:346:TRP:CD1	2:N:401:ARG:HG3	1.38	1.57
2:F:401:ARG:HG3	1:K:346:TRP:CD1	1.38	1.55
2:D:401:ARG:HG3	1:G:346:TRP:CD1	1.36	1.54
1:E:346:TRP:CD1	2:R:401:ARG:HG3	1.43	1.53
1:A:346:TRP:CD1	2:P:401:ARG:HG3	1.49	1.48

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%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	C	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	E	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	G	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	I	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	K	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	M	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	O	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
1	Q	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	21	66
2	B	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	D	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	F	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	H	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	J	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	L	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	N	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	P	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
2	R	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	34	77
All	All	7632/7794 (98%)	7290 (96%)	288 (4%)	54 (1%)	31	71

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
1	A	274	PRO
1	A	342	GLN
2	B	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	98	ASP

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%)	360 (100%)	0	100	100
1	C	360/368 (98%)	360 (100%)	0	100	100
1	E	360/368 (98%)	360 (100%)	0	100	100
1	G	360/368 (98%)	360 (100%)	0	100	100
1	I	360/368 (98%)	360 (100%)	0	100	100
1	K	360/368 (98%)	360 (100%)	0	100	100
1	M	360/368 (98%)	360 (100%)	0	100	100
1	O	360/368 (98%)	360 (100%)	0	100	100
1	Q	360/368 (98%)	360 (100%)	0	100	100
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%)	6543 (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. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	31	GLN
1	K	31	GLN
1	Q	35	GLN
1	I	35	GLN
2	J	96	GLN

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 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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	1.35	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	B	501	-	24,30,30	2.77	8 (33%)	26,47,47	3.32	10 (38%)
6	TA1	B	502	-	68,68,68	1.94	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	C	501	4	26,34,34	1.35	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	D	501	-	24,30,30	2.77	8 (33%)	26,47,47	3.32	10 (38%)
6	TA1	D	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	E	501	4	26,34,34	1.35	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	F	501	-	24,30,30	2.78	8 (33%)	26,47,47	3.33	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TA1	F	502	-	68,68,68	1.94	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	G	501	4	26,34,34	1.35	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	H	501	-	24,30,30	2.77	8 (33%)	26,47,47	3.32	10 (38%)
6	TA1	H	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	I	501	4	26,34,34	1.34	1 (3%)	29,54,54	2.26	4 (13%)
5	GDP	J	501	-	24,30,30	2.78	8 (33%)	26,47,47	3.32	10 (38%)
6	TA1	J	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	K	501	4	26,34,34	1.35	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	L	501	-	24,30,30	2.77	8 (33%)	26,47,47	3.32	10 (38%)
6	TA1	L	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	M	501	4	26,34,34	1.34	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	N	501	-	24,30,30	2.77	8 (33%)	26,47,47	3.33	10 (38%)
6	TA1	N	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
3	GTP	O	501	4	26,34,34	1.34	2 (7%)	29,54,54	2.28	4 (13%)
5	GDP	P	501	-	24,30,30	2.78	8 (33%)	26,47,47	3.32	10 (38%)
6	TA1	P	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.30	8 (7%)
3	GTP	Q	501	4	26,34,34	1.34	2 (7%)	29,54,54	2.27	4 (13%)
5	GDP	R	501	-	24,30,30	2.78	8 (33%)	26,47,47	3.31	10 (38%)
6	TA1	R	502	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)

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
6	TA1	B	502	-	-	0/41/127/127	0/5/7/7
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
6	TA1	D	502	-	-	0/41/127/127	0/5/7/7
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
6	TA1	F	502	-	-	0/41/127/127	0/5/7/7
3	GTP	G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	H	501	-	-	0/12/32/32	0/3/3/3
6	TA1	H	502	-	-	0/41/127/127	0/5/7/7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	I	501	4	-	0/18/38/38	0/3/3/3
5	GDP	J	501	-	-	0/12/32/32	0/3/3/3
6	TA1	J	502	-	-	0/41/127/127	0/5/7/7
3	GTP	K	501	4	-	0/18/38/38	0/3/3/3
5	GDP	L	501	-	-	0/12/32/32	0/3/3/3
6	TA1	L	502	-	-	0/41/127/127	0/5/7/7
3	GTP	M	501	4	-	0/18/38/38	0/3/3/3
5	GDP	N	501	-	-	0/12/32/32	0/3/3/3
6	TA1	N	502	-	-	0/41/127/127	0/5/7/7
3	GTP	O	501	4	-	0/18/38/38	0/3/3/3
5	GDP	P	501	-	-	0/12/32/32	0/3/3/3
6	TA1	P	502	-	-	0/41/127/127	0/5/7/7
3	GTP	Q	501	4	-	0/18/38/38	0/3/3/3
5	GDP	R	501	-	-	0/12/32/32	0/3/3/3
6	TA1	R	502	-	-	0/41/127/127	0/5/7/7

The worst 5 of 269 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TA1	C07-C06	-4.97	1.25	1.38
6	F	502	TA1	C07-C06	-4.97	1.25	1.38
6	N	502	TA1	C07-C06	-4.97	1.25	1.38
6	H	502	TA1	C07-C06	-4.96	1.25	1.38
6	P	502	TA1	C07-C06	-4.96	1.25	1.38

The worst 5 of 198 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	501	GDP	C6-C5-C4	-10.06	109.37	120.86
5	F	501	GDP	C6-C5-C4	-10.05	109.38	120.86
5	P	501	GDP	C6-C5-C4	-10.03	109.40	120.86
5	J	501	GDP	C6-C5-C4	-10.03	109.40	120.86
5	D	501	GDP	C6-C5-C4	-10.03	109.40	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 54 short contacts:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502	TA1	4	0
5	D	501	GDP	2	0
6	D	502	TA1	4	0
5	F	501	GDP	2	0
6	F	502	TA1	4	0
5	H	501	GDP	2	0
6	H	502	TA1	4	0
5	J	501	GDP	2	0
6	J	502	TA1	4	0
5	L	501	GDP	2	0
6	L	502	TA1	4	0
5	N	501	GDP	2	0
6	N	502	TA1	4	0
5	P	501	GDP	2	0
6	P	502	TA1	4	0
5	R	501	GDP	2	0
6	R	502	TA1	4	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.