



## wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:10 pm BST

PDB ID : 5ND3 / pdb\_00005nd3  
EMDB ID : EMD-3621  
Title : Microtubule-bound MKLP2 motor domain in the with no nucleotide  
Authors : Atherton, J.; Yu, I.M.; Cook, A.; Muretta, J.M.; Joseph, A.P.; Major, J.; Sourigues, Y.; Clause, J.; Topf, M.; Rosenfeld, S.S.; Houdusse, A.; Moores, C.A.  
Deposited on : 2017-03-07  
Resolution : 6.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

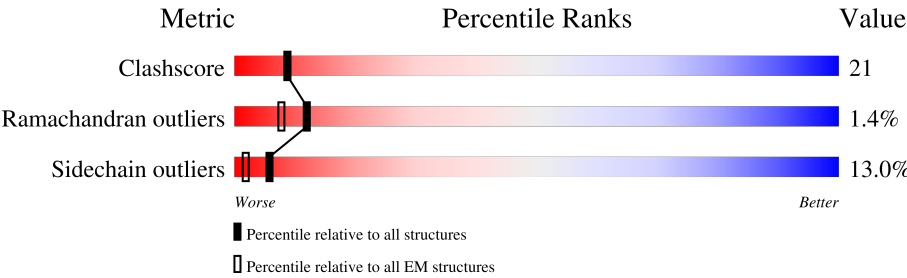
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	1-C	501	<div> <div>24%</div> <div>30%</div> <div>5%</div> <div>41%</div> </div>
1	2-C	501	<div> <div>25%</div> <div>29%</div> <div>5%</div> <div>41%</div> </div>
1	3-C	501	<div> <div>25%</div> <div>29%</div> <div>5%</div> <div>41%</div> </div>
1	4-C	501	<div> <div>24%</div> <div>30%</div> <div>5%</div> <div>41%</div> </div>
1	5-C	501	<div> <div>25%</div> <div>29%</div> <div>6%</div> <div>41%</div> </div>
2	1-A	451	<div> <div>57%</div> <div>32%</div> <div>•</div> <div>9%</div> </div>
2	2-A	451	<div> <div>57%</div> <div>32%</div> <div>•</div> <div>9%</div> </div>
2	3-A	451	<div> <div>57%</div> <div>32%</div> <div>•</div> <div>9%</div> </div>
2	4-A	451	<div> <div>57%</div> <div>32%</div> <div>•</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	5-A	451	
3	1-B	445	
3	2-B	445	
3	3-B	445	
3	4-B	445	
3	5-B	445	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	1-A	500	-	-	X	-
4	GTP	2-A	500	-	-	X	-
4	GTP	3-A	500	-	-	X	-
4	GTP	4-A	500	-	-	X	-
4	GTP	5-A	500	-	-	X	-
6	GDP	1-B	600	-	-	X	-
6	GDP	2-B	600	-	-	X	-
6	GDP	3-B	600	-	-	X	-
6	GDP	4-B	600	-	-	X	-
6	GDP	5-B	600	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 45371 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 KIF20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-C	296	Total	C	N	O	S	0	0
			2375	1508	420	436	11		
1	2-C	296	Total	C	N	O	S	0	0
			2375	1508	420	436	11		
1	3-C	295	Total	C	N	O	S	0	0
			2366	1502	418	435	11		
1	4-C	296	Total	C	N	O	S	0	0
			2375	1508	420	436	11		
1	5-C	296	Total	C	N	O	S	0	0
			2375	1508	420	436	11		

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	2-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	3-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	4-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	5-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

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

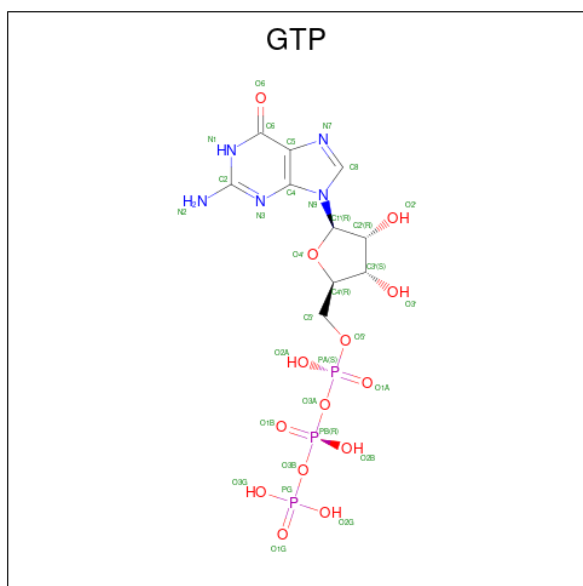
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	2-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	3-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	4-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		
3	5-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	ALA	THR	conflict	UNP Q6B856
B	172	VAL	MET	conflict	UNP Q6B856
B	298	ALA	SER	conflict	UNP Q6B856
B	318	VAL	ILE	conflict	UNP Q6B856

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



Mol	Chain	Residues	Atoms					AltConf
4	1-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	2-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	3-A	1	Total	C	N	O	P	0
			32	10	5	14	3	

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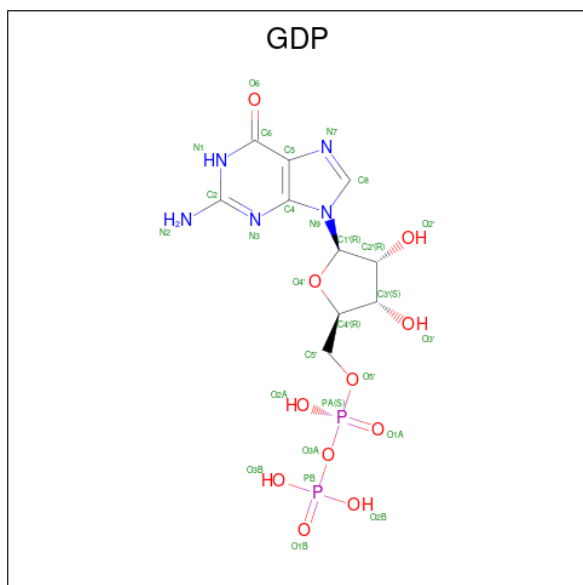
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Mol	Chain	Residues	Atoms					AltConf
4	4-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	5-A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	1-A	1	Total	Mg	0
			1	1	
5	2-A	1	Total	Mg	0
			1	1	
5	3-A	1	Total	Mg	0
			1	1	
5	4-A	1	Total	Mg	0
			1	1	
5	5-A	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



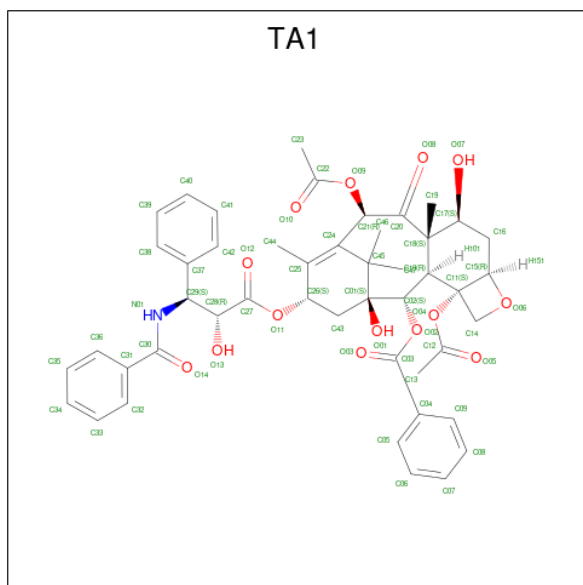
Mol	Chain	Residues	Atoms					AltConf
6	1-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	2-B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
6	3-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	4-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
6	5-B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (CCD ID: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).

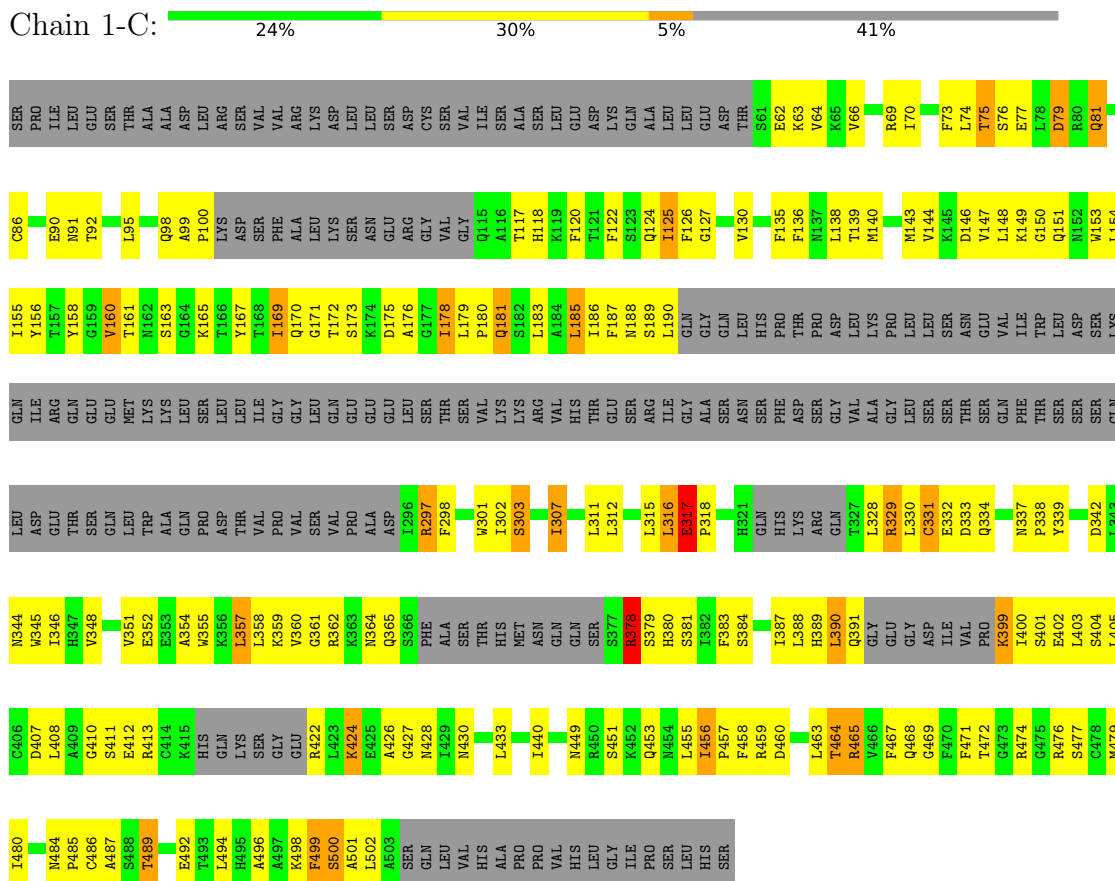


Mol	Chain	Residues	Atoms				AltConf
7	1-B	1	Total	C	N	O	0
			62	47	1	14	
7	2-B	1	Total	C	N	O	0
			62	47	1	14	
7	3-B	1	Total	C	N	O	0
			62	47	1	14	
7	4-B	1	Total	C	N	O	0
			62	47	1	14	
7	5-B	1	Total	C	N	O	0
			62	47	1	14	

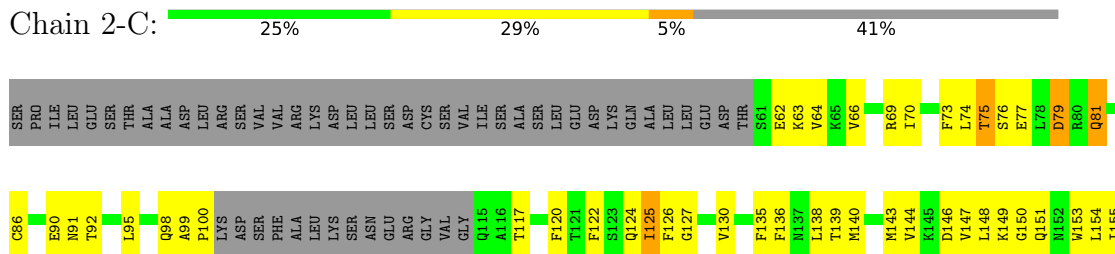
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 KIF20A

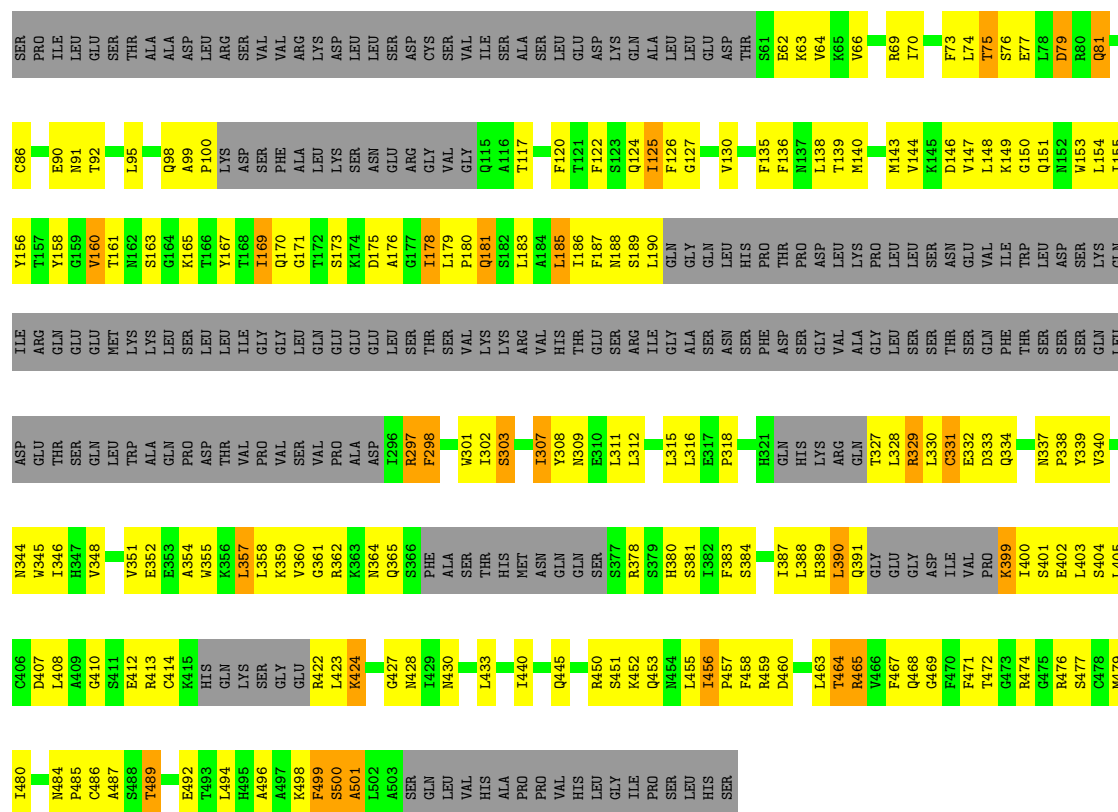


#### • Molecule 1: Kinesin-like protein KIF20A



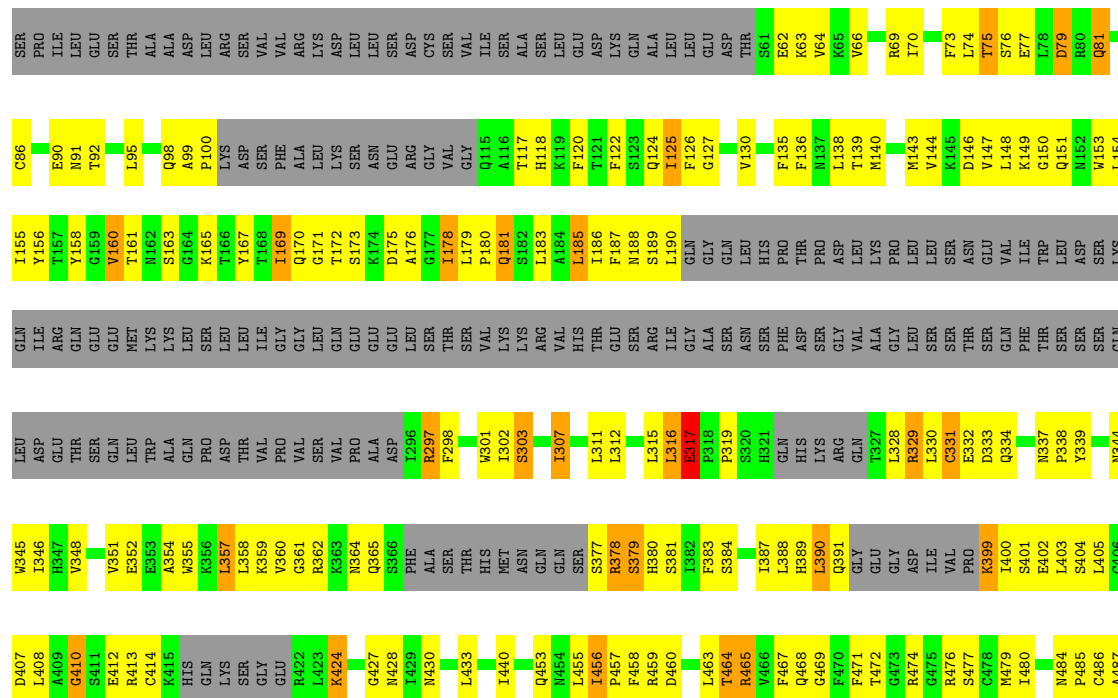






• Molecule 1: Kinesin-like protein KIF20A

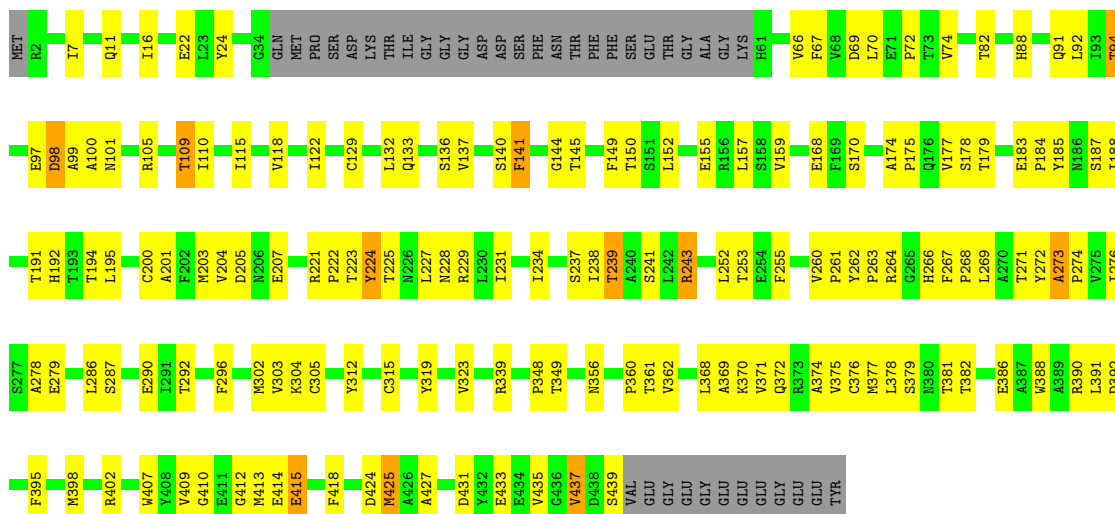
Chain 5-C: 25% 29% 6% 41%





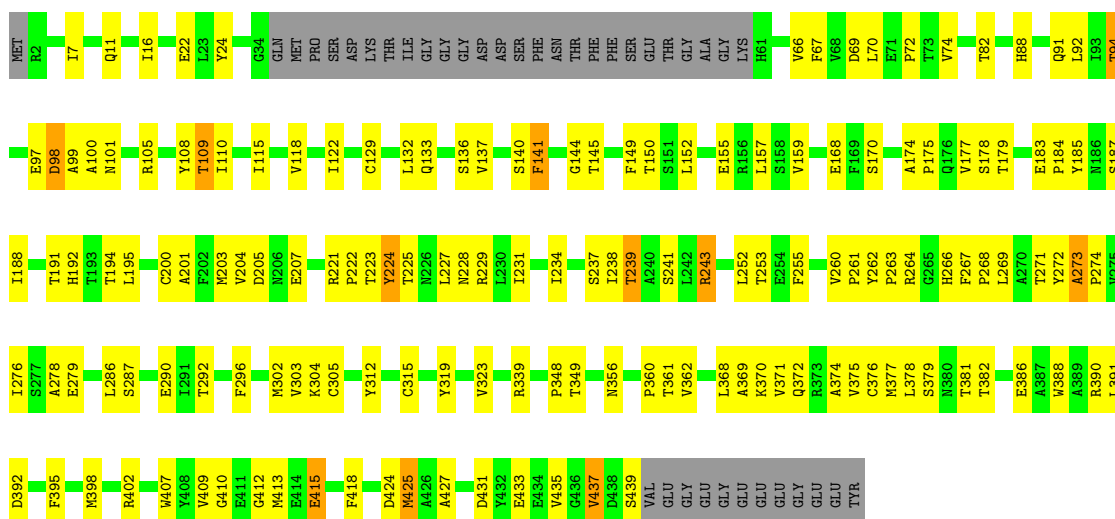
• Molecule 2: Tubulin alpha chain

Chain 1-A: 57% 32% 9%



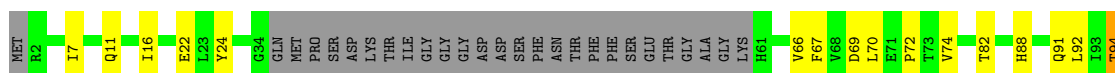
• Molecule 2: Tubulin alpha chain

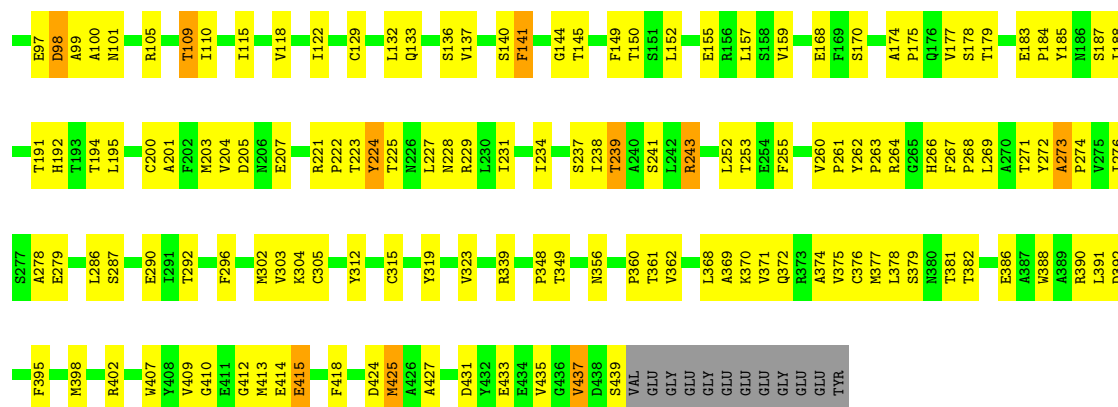
Chain 2-A: 57% 32% 9%



• Molecule 2: Tubulin alpha chain

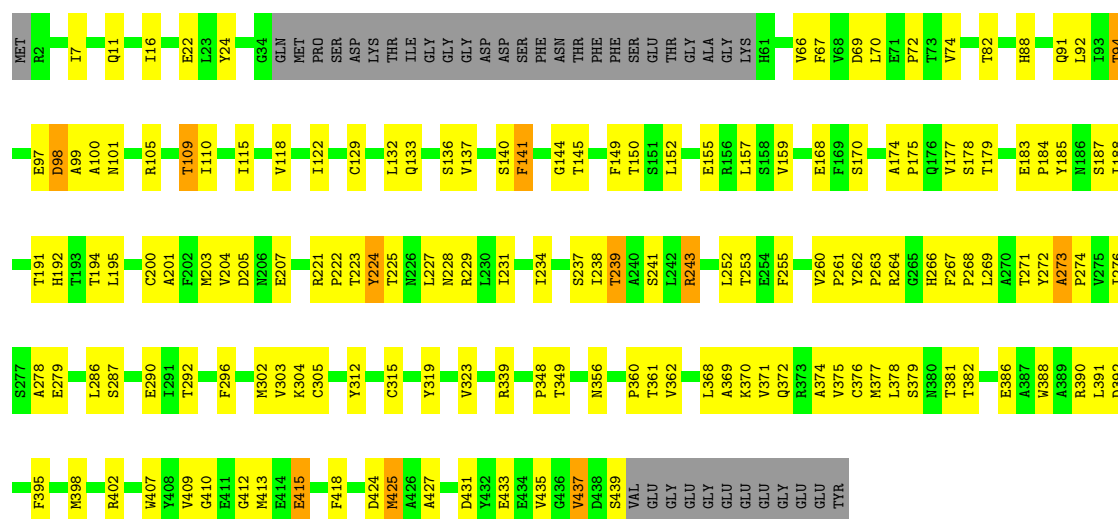
Chain 3-A: 57% 32% 9%





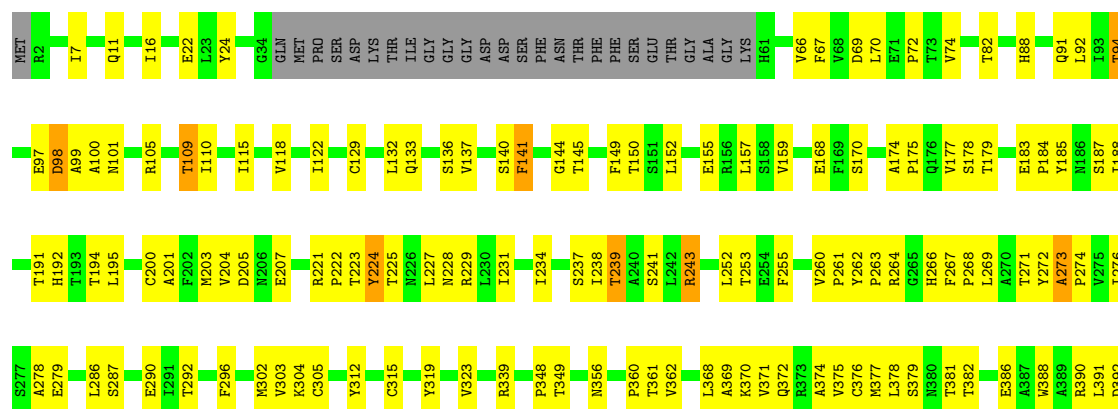
• Molecule 2: Tubulin alpha chain

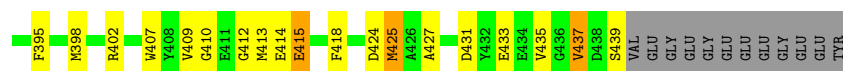
Chain 4-A: 57% 32% 9%



• Molecule 2: Tubulin alpha chain

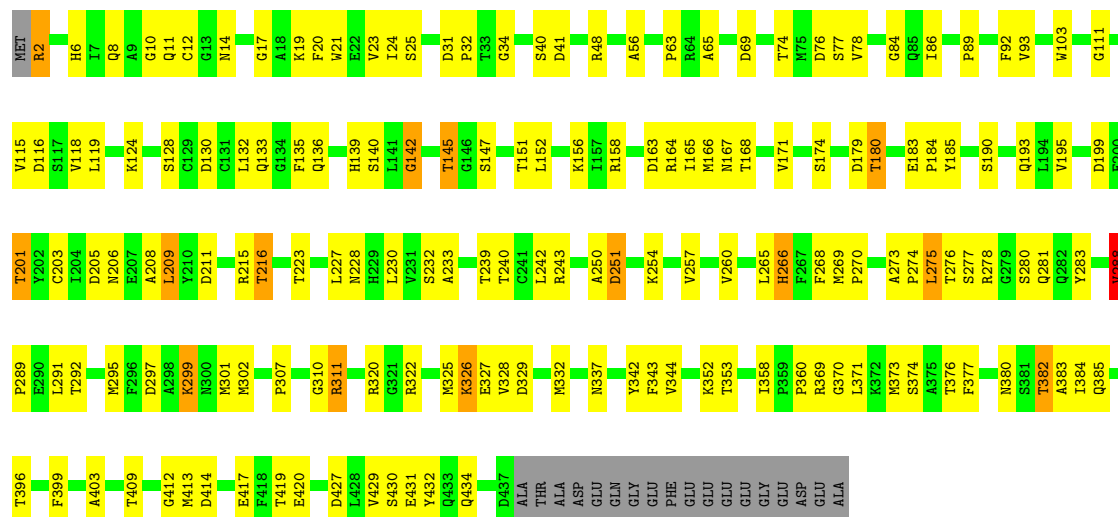
Chain 5-A: 57% 32% 9%





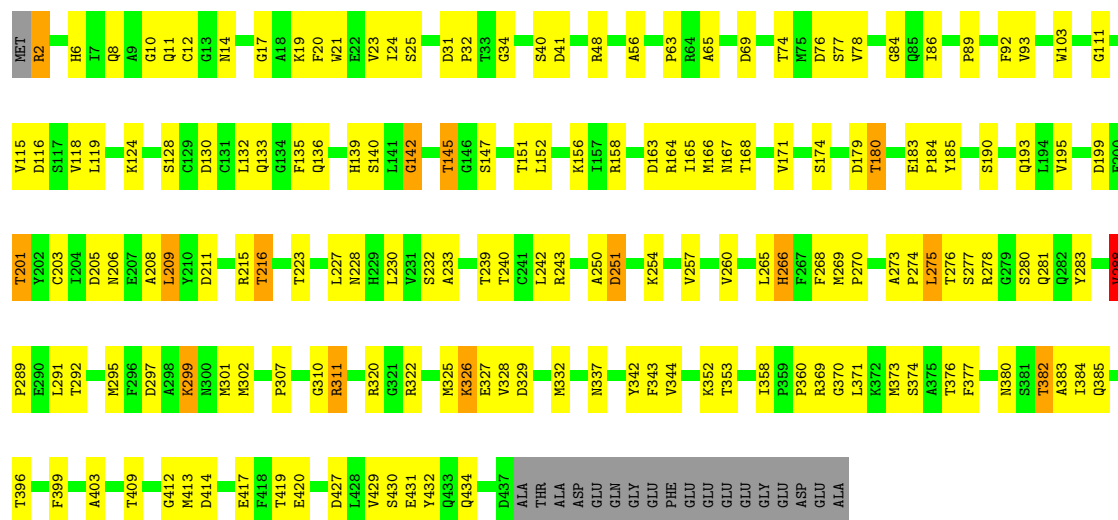
• Molecule 3: Tubulin beta-2B chain

Chain 1-B: 58% 34%



• Molecule 3: Tubulin beta-2B chain

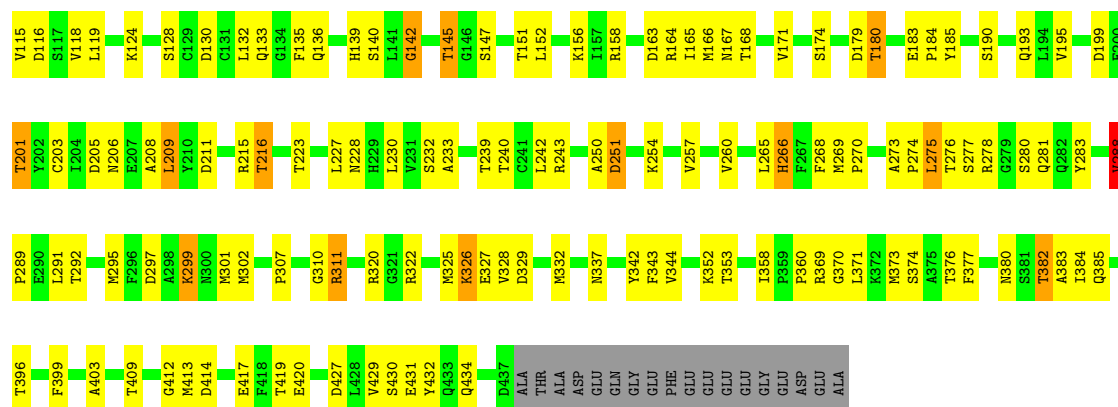
Chain 2-B: 58% 34%



• Molecule 3: Tubulin beta-2B chain

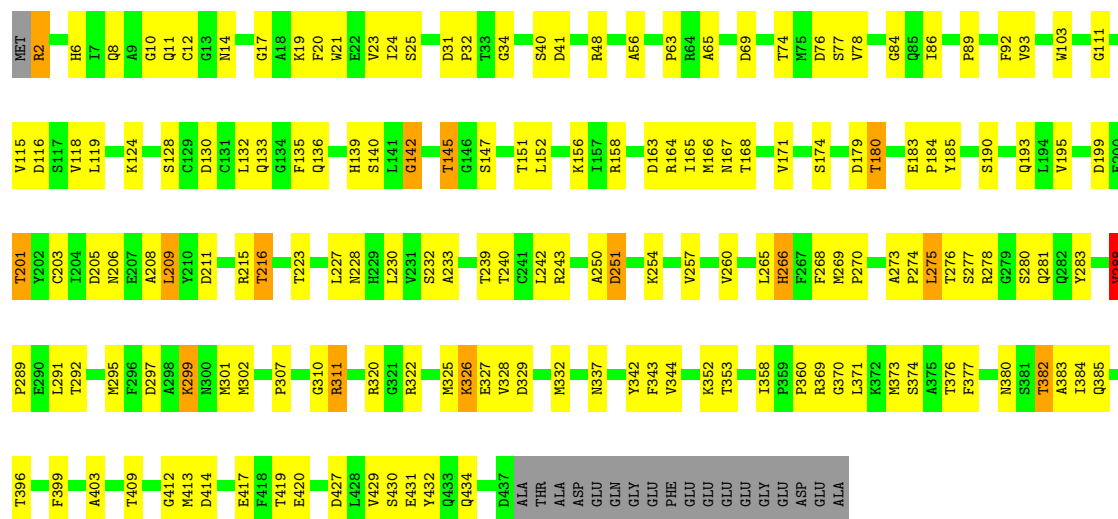
Chain 3-B: 58% 34%





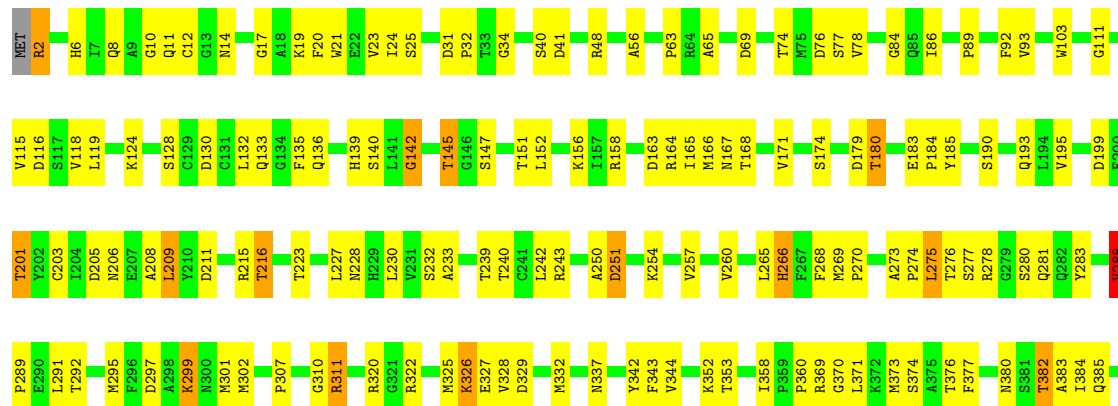
• Molecule 3: Tubulin beta-2B chain

Chain 4-B: 58% 34%



• Molecule 3: Tubulin beta-2B chain

Chain 5-B: 58% 34%



T396					G412	E417	D427	V429	Q433	D437	ALA	THR	ALA	ASP	GLU	GLN	GLY	PHE	GLU	GLU	GLU	GLY	GLY	ASP	GLU	ALA
F399					M413	F418	I428	S430	Q434		ALA		ALA													
A403					D414	T419		E431																		
T409						E420		Y432																		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9257	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 ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0321	Depositor
Map size (Å)	244.79999, 212.67, 246.33	wwPDB
Map dimensions	160, 139, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.53, 1.53, 1.53	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: TA1, GDP, MG, GTP

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  > 5$	RMSZ	# $ Z  > 5$
1	1-C	0.59	2/2416 (0.1%)	0.81	7/3254 (0.2%)
1	2-C	0.58	2/2416 (0.1%)	0.80	6/3254 (0.2%)
1	3-C	0.58	2/2407 (0.1%)	0.75	6/3243 (0.2%)
1	4-C	0.58	2/2416 (0.1%)	0.79	6/3254 (0.2%)
1	5-C	0.60	2/2416 (0.1%)	0.80	6/3254 (0.2%)
2	1-A	0.26	0/3300	0.39	0/4482
2	2-A	0.26	0/3300	0.39	0/4482
2	3-A	0.26	0/3300	0.39	0/4482
2	4-A	0.26	0/3300	0.39	0/4482
2	5-A	0.26	0/3300	0.39	0/4482
3	1-B	0.28	0/3426	0.42	0/4642
3	2-B	0.28	0/3426	0.42	0/4642
3	3-B	0.28	0/3426	0.42	0/4642
3	4-B	0.28	0/3426	0.42	0/4642
3	5-B	0.28	0/3426	0.42	0/4642
All	All	0.38	10/45701 (0.0%)	0.53	31/61879 (0.1%)

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	1-C	1	4
1	2-C	1	3
1	3-C	1	2
1	4-C	1	1
1	5-C	1	4
All	All	5	14

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-C	465	ARG	CZ-NH1	6.06	1.41	1.33
1	4-C	465	ARG	CZ-NH1	6.03	1.40	1.33
1	2-C	465	ARG	CZ-NH1	6.01	1.40	1.33
1	3-C	465	ARG	CZ-NH1	6.01	1.40	1.33
1	5-C	465	ARG	CZ-NH1	5.98	1.40	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-C	378	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	2-C	320	SER	C-N-CA	11.17	149.63	121.70
1	3-C	465	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	5-C	465	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	4-C	465	ARG	NE-CZ-NH2	-10.36	115.12	120.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1-C	297	ARG	CA
1	2-C	297	ARG	CA
1	3-C	297	ARG	CA
1	4-C	297	ARG	CA
1	5-C	297	ARG	CA

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-C	316	LEU	Mainchain
1	1-C	317	GLU	Peptide
1	1-C	378	ARG	Sidechain
1	1-C	459	ARG	Sidechain
1	2-C	410	GLY	Mainchain

## 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	1-C	2375	0	2385	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-C	2375	0	2385	144	0
1	3-C	2366	0	2372	144	0
1	4-C	2375	0	2385	158	0
1	5-C	2375	0	2385	148	0
2	1-A	3227	0	3141	121	0
2	2-A	3227	0	3141	122	0
2	3-A	3227	0	3141	124	0
2	4-A	3227	0	3141	119	0
2	5-A	3227	0	3141	121	0
3	1-B	3351	0	3229	115	0
3	2-B	3351	0	3229	114	0
3	3-B	3351	0	3229	115	0
3	4-B	3351	0	3229	119	0
3	5-B	3351	0	3229	116	0
4	1-A	32	0	12	26	0
4	2-A	32	0	12	26	0
4	3-A	32	0	12	26	0
4	4-A	32	0	12	26	0
4	5-A	32	0	12	26	0
5	1-A	1	0	0	0	0
5	2-A	1	0	0	0	0
5	3-A	1	0	0	0	0
5	4-A	1	0	0	0	0
5	5-A	1	0	0	0	0
6	1-B	28	0	12	11	0
6	2-B	28	0	12	11	0
6	3-B	28	0	12	11	0
6	4-B	28	0	12	11	0
6	5-B	28	0	12	11	0
7	1-B	62	0	51	19	0
7	2-B	62	0	51	19	0
7	3-B	62	0	51	19	0
7	4-B	62	0	51	19	0
7	5-B	62	0	51	19	0
All	All	45371	0	44137	1851	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 21.

The worst 5 of 1851 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:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34
2:A:179:THR:OG1	4:A:500:GTP:C3'	1.73	1.34

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	1-C	282/501 (56%)	267 (95%)	10 (4%)	5 (2%)	7	34
1	2-C	282/501 (56%)	265 (94%)	14 (5%)	3 (1%)	12	47
1	3-C	281/501 (56%)	266 (95%)	10 (4%)	5 (2%)	7	34
1	4-C	282/501 (56%)	266 (94%)	12 (4%)	4 (1%)	9	40
1	5-C	282/501 (56%)	265 (94%)	11 (4%)	6 (2%)	5	30
2	1-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	13	49
2	2-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	13	49
2	3-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	13	49
2	4-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	13	49
2	5-A	408/451 (90%)	366 (90%)	38 (9%)	4 (1%)	13	49
3	1-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	7	36
3	2-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	7	36
3	3-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	7	36
3	4-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	7	36
3	5-B	424/445 (95%)	379 (89%)	38 (9%)	7 (2%)	7	36
All	All	5569/6985 (80%)	5054 (91%)	437 (8%)	78 (1%)	12	40

5 of 78 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	317	GLU
3	1-B	288	VAL
3	2-B	288	VAL
1	3-C	379	SER
3	3-B	288	VAL

### 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	1-C	265/447 (59%)	224 (84%)	41 (16%)	2	11
1	2-C	265/447 (59%)	225 (85%)	40 (15%)	2	11
1	3-C	264/447 (59%)	221 (84%)	43 (16%)	2	10
1	4-C	265/447 (59%)	225 (85%)	40 (15%)	2	11
1	5-C	265/447 (59%)	225 (85%)	40 (15%)	2	11
2	1-A	347/377 (92%)	311 (90%)	36 (10%)	5	20
2	2-A	347/377 (92%)	311 (90%)	36 (10%)	5	20
2	3-A	347/377 (92%)	311 (90%)	36 (10%)	5	20
2	4-A	347/377 (92%)	311 (90%)	36 (10%)	5	20
2	5-A	347/377 (92%)	311 (90%)	36 (10%)	5	20
3	1-B	367/381 (96%)	317 (86%)	50 (14%)	3	13
3	2-B	367/381 (96%)	317 (86%)	50 (14%)	3	13
3	3-B	367/381 (96%)	317 (86%)	50 (14%)	3	13
3	4-B	367/381 (96%)	317 (86%)	50 (14%)	3	13
3	5-B	367/381 (96%)	317 (86%)	50 (14%)	3	13
All	All	4894/6025 (81%)	4260 (87%)	634 (13%)	6	14

5 of 634 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4-B	76	ASP
2	5-A	315	CYS
3	4-B	185	TYR
3	4-B	48	ARG
1	5-C	169	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-C	365	GLN
1	5-C	84	GLN
1	4-C	445	GLN
3	4-B	206	ASN
1	5-C	365	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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
6	GDP	4-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
4	GTP	5-A	500	5,2	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
6	GDP	3-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
6	GDP	5-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
7	TA1	3-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
6	GDP	1-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
4	GTP	1-A	500	5,2	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
7	TA1	1-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
4	GTP	3-A	500	5,2	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
7	TA1	2-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
4	GTP	2-A	500	5,2	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
7	TA1	4-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
7	TA1	5-B	601	-	68,68,68	2.00	19 (27%)	105,105,105	1.39	11 (10%)
6	GDP	2-B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
4	GTP	4-A	500	5,2	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)

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
6	GDP	4-B	600	-	-	4/12/32/32	0/3/3/3
4	GTP	5-A	500	5,2	-	3/18/38/38	0/3/3/3
6	GDP	3-B	600	-	-	4/12/32/32	0/3/3/3
6	GDP	5-B	600	-	-	4/12/32/32	0/3/3/3
7	TA1	3-B	601	-	-	9/41/127/127	0/7/7/7
6	GDP	1-B	600	-	-	4/12/32/32	0/3/3/3
4	GTP	1-A	500	5,2	-	3/18/38/38	0/3/3/3
7	TA1	1-B	601	-	-	9/41/127/127	0/7/7/7
4	GTP	3-A	500	5,2	-	3/18/38/38	0/3/3/3
7	TA1	2-B	601	-	-	9/41/127/127	0/7/7/7
4	GTP	2-A	500	5,2	-	3/18/38/38	0/3/3/3
7	TA1	4-B	601	-	-	9/41/127/127	0/7/7/7
7	TA1	5-B	601	-	-	9/41/127/127	0/7/7/7
6	GDP	2-B	600	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	4-A	500	5,2	-	3/18/38/38	0/3/3/3

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	2-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	3-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	4-B	600	GDP	O4'-C1'	6.36	1.50	1.41
6	5-B	600	GDP	O4'-C1'	6.36	1.50	1.41

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	2-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	3-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	4-B	600	GDP	C8-N7-C5	9.30	120.71	102.99
6	5-B	600	GDP	C8-N7-C5	9.30	120.71	102.99

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1-B	600	GDP	PA-O3A-PB-O2B
6	1-B	600	GDP	C5'-O5'-PA-O3A
6	1-B	600	GDP	C5'-O5'-PA-O1A
6	2-B	600	GDP	PA-O3A-PB-O2B
6	2-B	600	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

15 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	4-B	600	GDP	11	0
4	5-A	500	GTP	26	0
6	3-B	600	GDP	11	0
6	5-B	600	GDP	11	0
7	3-B	601	TA1	19	0
6	1-B	600	GDP	11	0
4	1-A	500	GTP	26	0

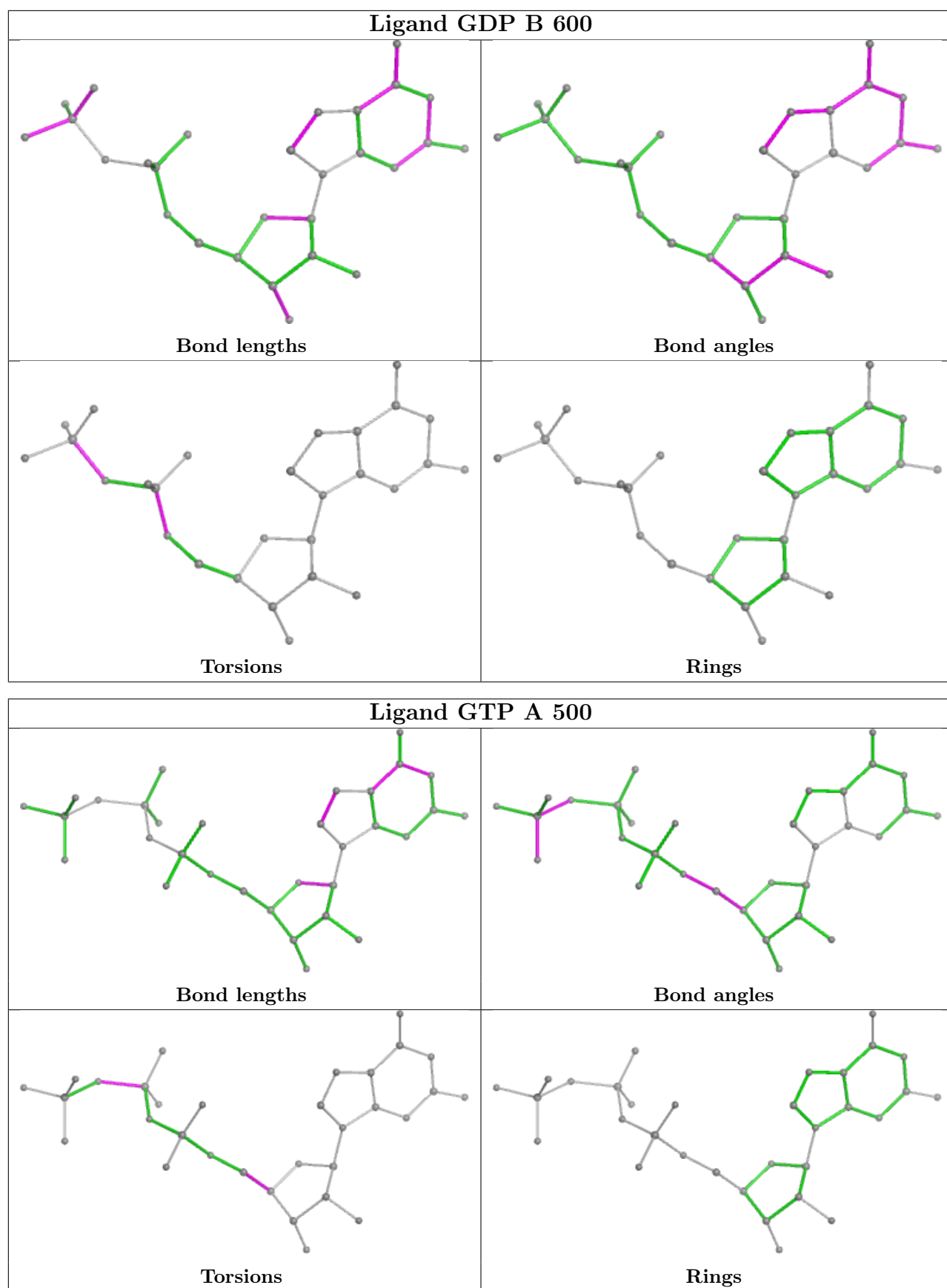
*Continued on next page...*

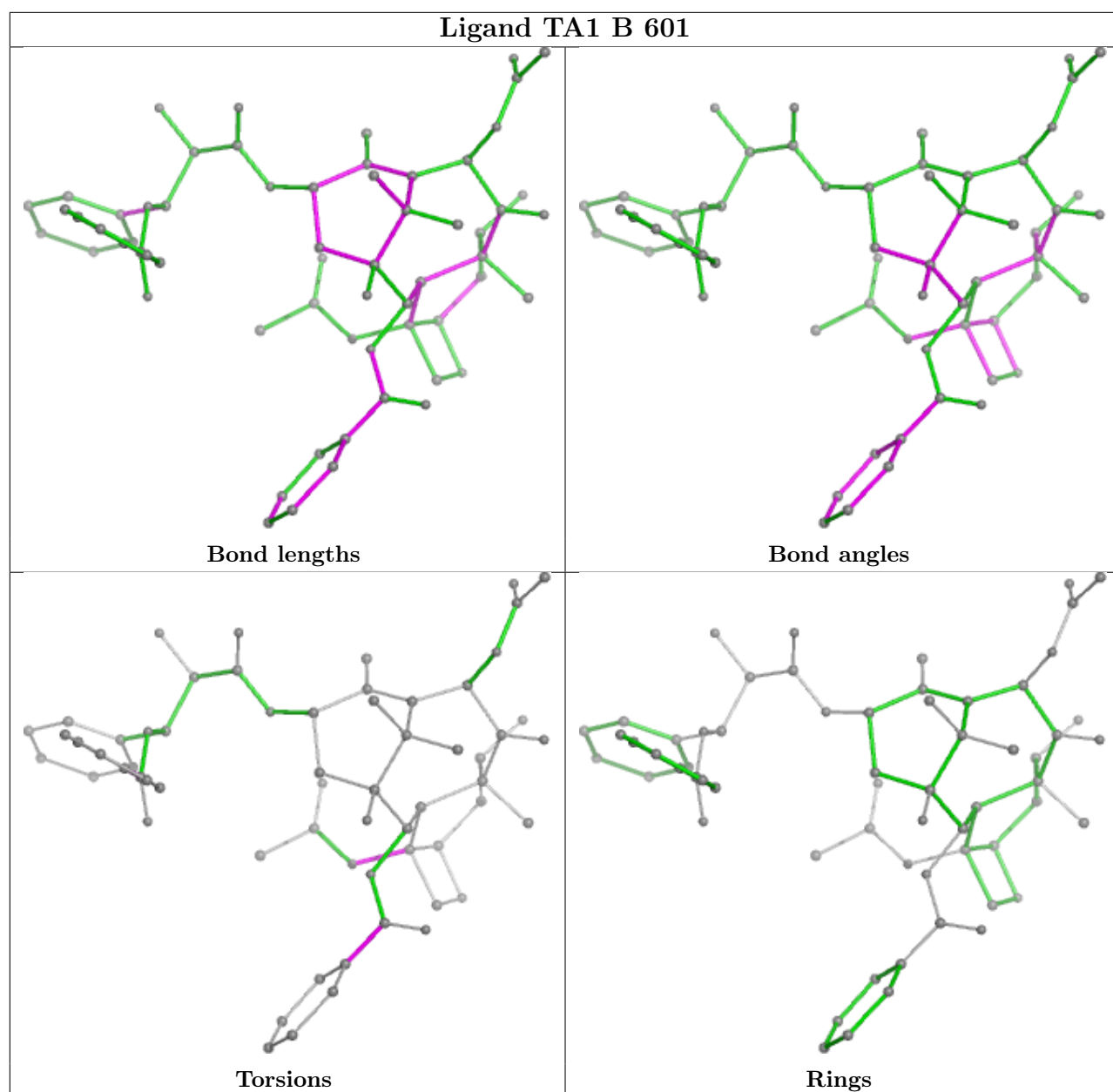


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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1-B	601	TA1	19	0
4	3-A	500	GTP	26	0
7	2-B	601	TA1	19	0
4	2-A	500	GTP	26	0
7	4-B	601	TA1	19	0
7	5-B	601	TA1	19	0
6	2-B	600	GDP	11	0
4	4-A	500	GTP	26	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.

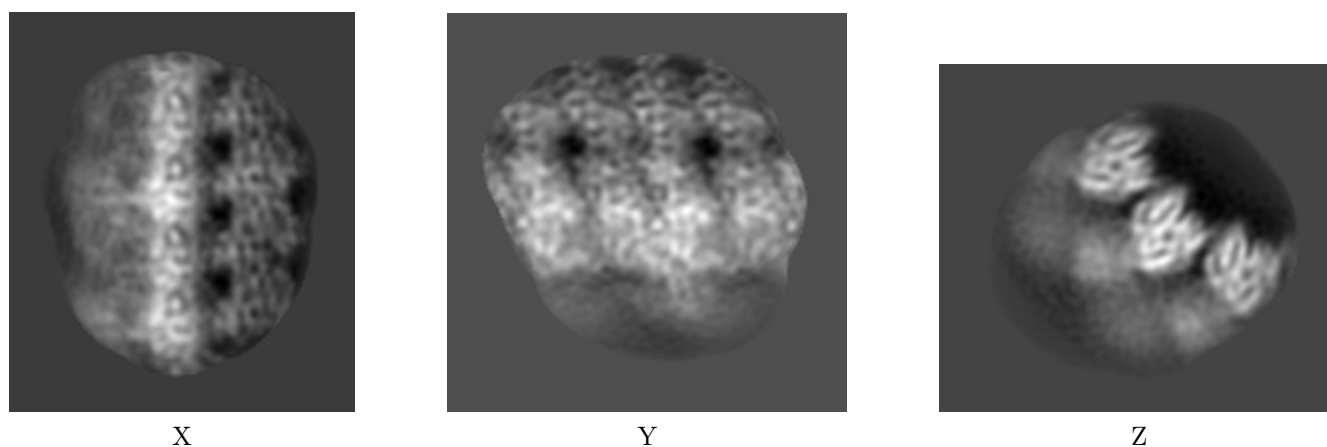
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3621. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

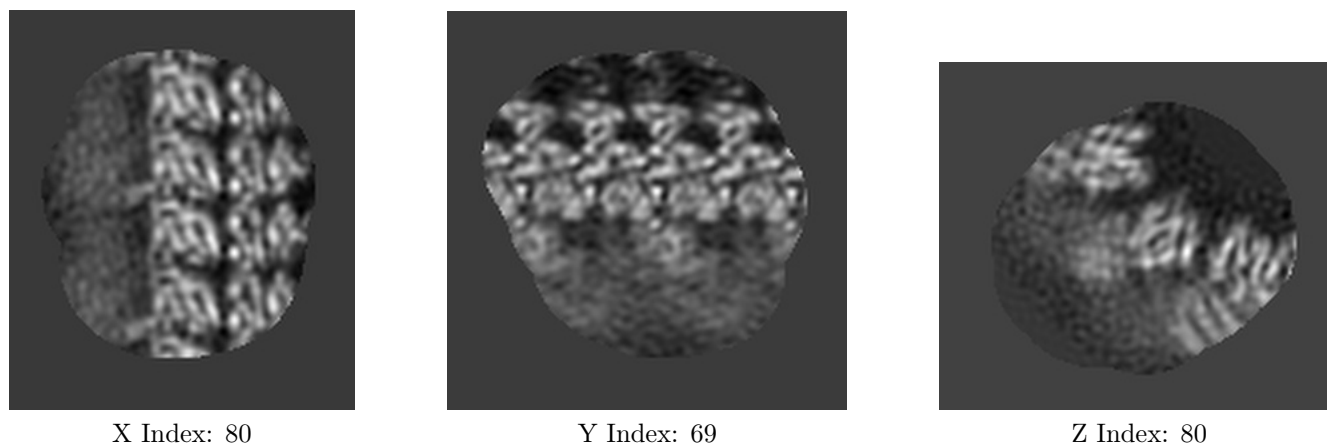
#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

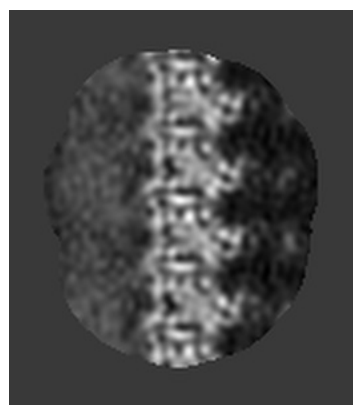
#### 6.2.1 Primary map



The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

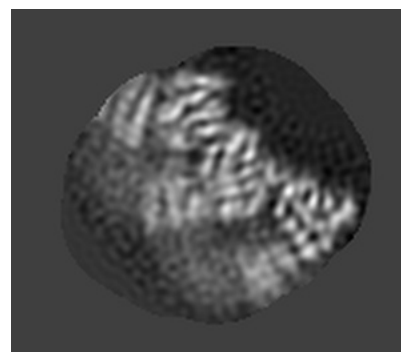
### 6.3.1 Primary map



X Index: 87



Y Index: 59

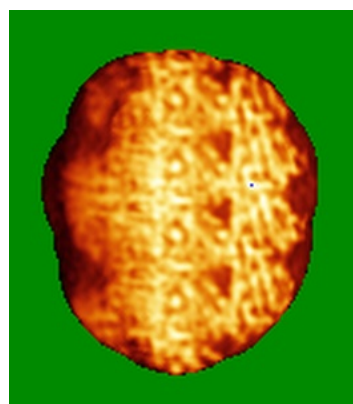


Z Index: 91

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

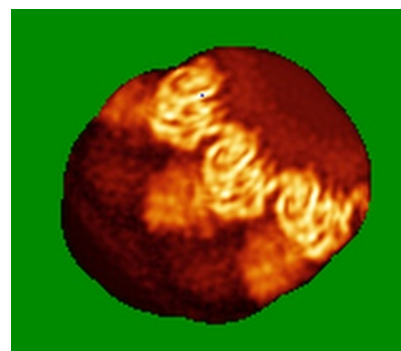
### 6.4.1 Primary map



X



Y

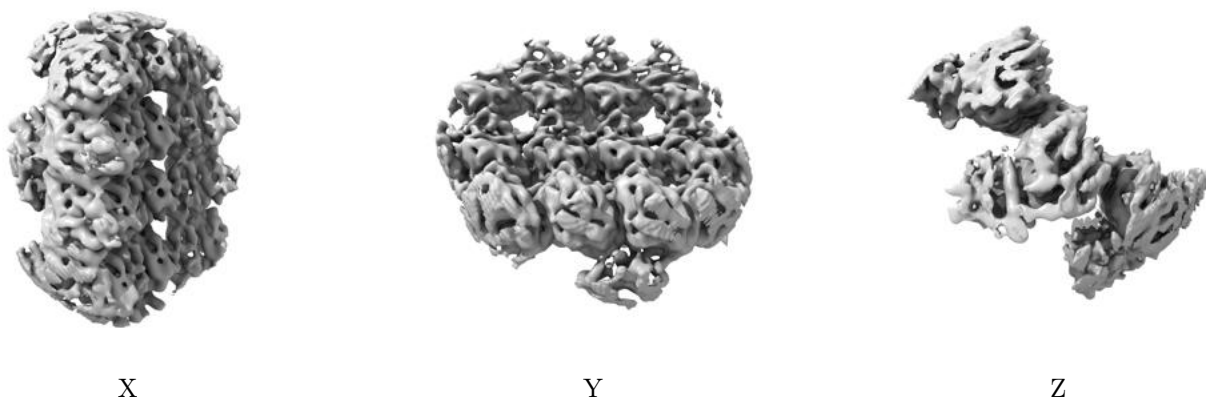


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0321. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

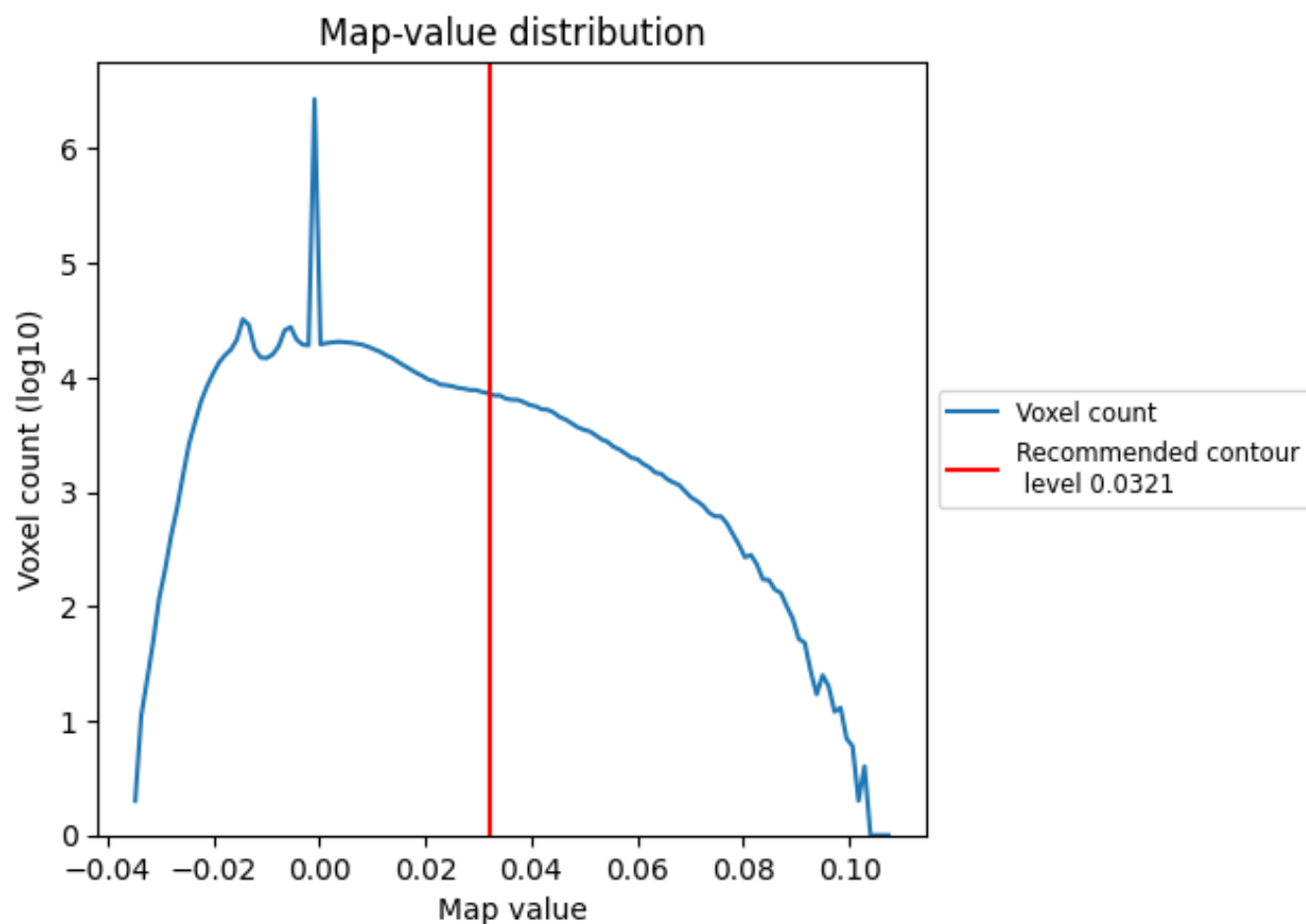
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

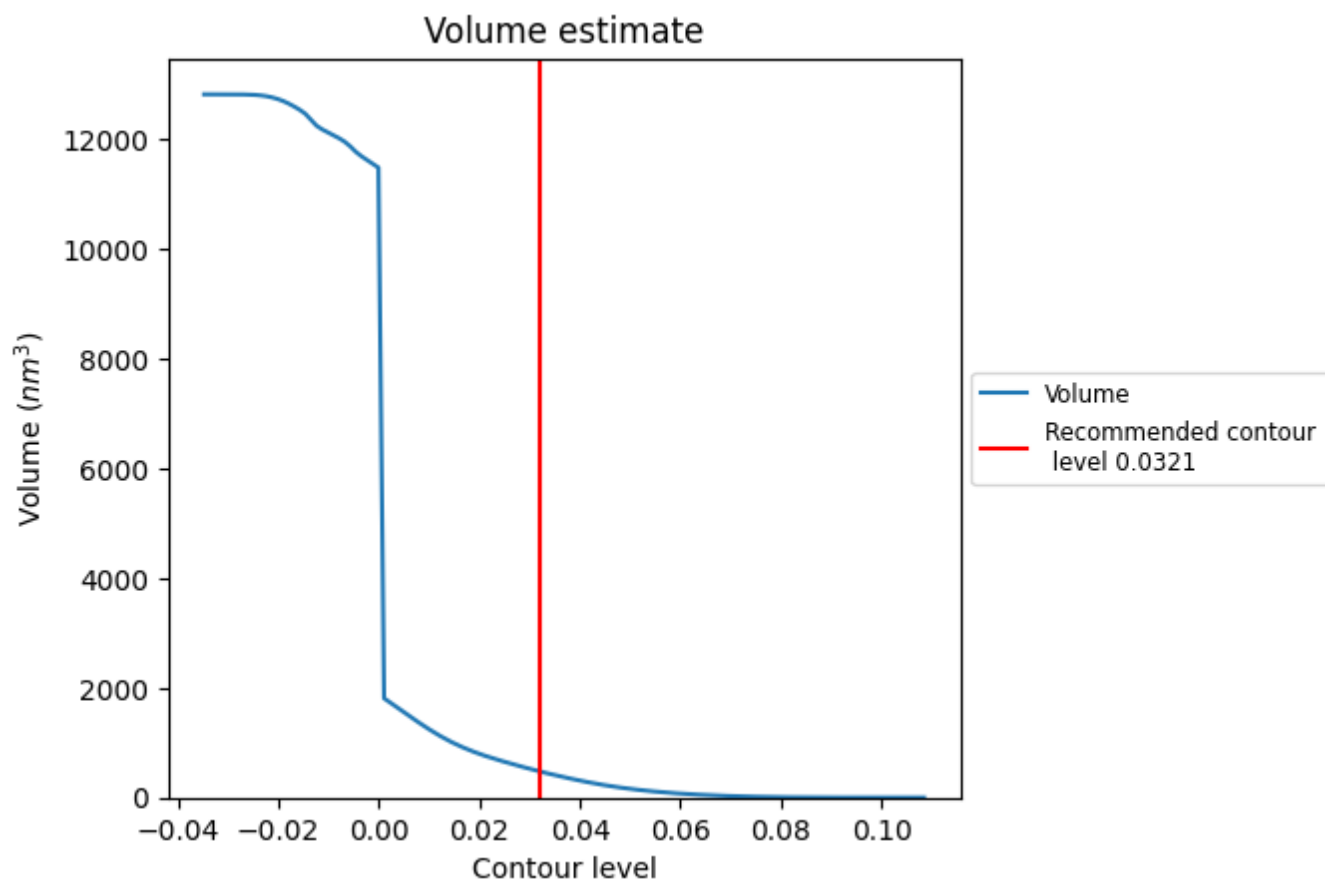
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 476 nm<sup>3</sup>; this corresponds to an approximate mass of 430 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.