



## wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:44 pm BST

PDB ID : 5ND7 / pdb\_00005nd7  
EMDB ID : EMD-3623  
Title : Microtubule-bound MKLP2 motor domain in the presence of AMPPNP  
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 : 7.90 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

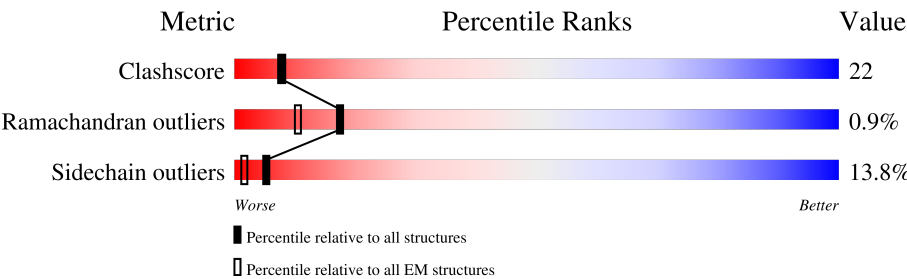
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.90 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	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	
1	2-C	501	
1	3-C	501	
1	4-C	501	
1	5-C	501	
2	1-A	451	
2	2-A	451	
2	3-A	451	
2	4-A	451	

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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
6	GTP	1-A	500	-	-	X	-
6	GTP	2-A	500	-	-	X	-
6	GTP	3-A	500	-	-	X	-
6	GTP	4-A	500	-	-	X	-
6	GTP	5-A	500	-	-	X	-
7	GDP	1-B	600	-	-	X	-
7	GDP	2-B	600	-	-	X	-
7	GDP	3-B	600	-	-	X	-
7	GDP	4-B	600	-	-	X	-
7	GDP	5-B	600	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 45700 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	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	2-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	3-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	4-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	11		
1	5-C	300	Total	C	N	O	S	0	0
			2407	1531	425	440	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		

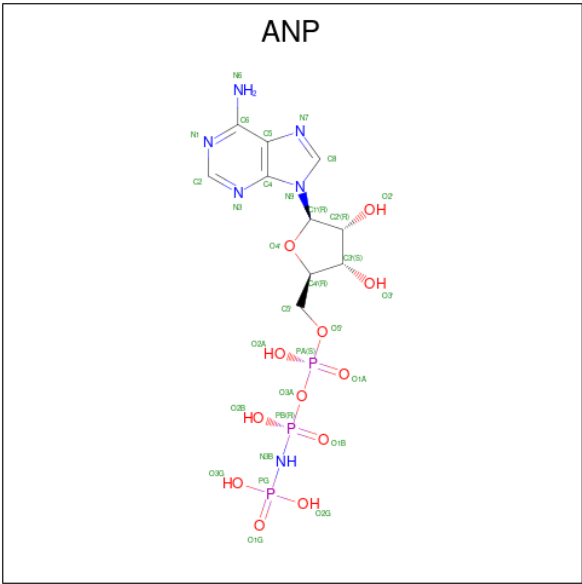
There are 4 discrepancies between the modelled and reference sequences:

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



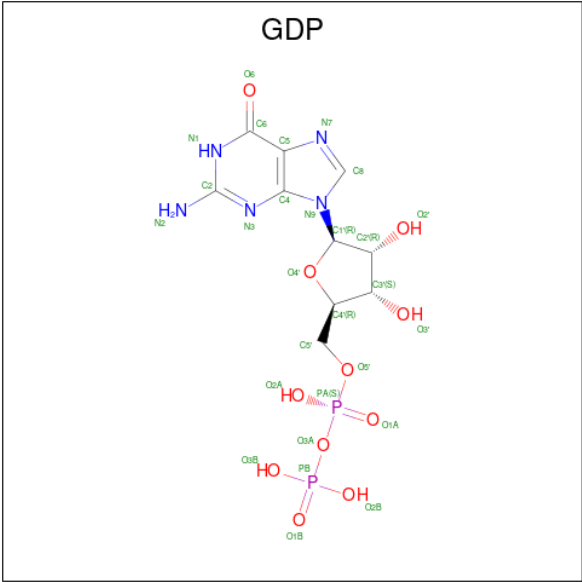
Mol	Chain	Residues	Atoms					AltConf
5	1-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	2-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	3-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	4-C	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	5-C	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



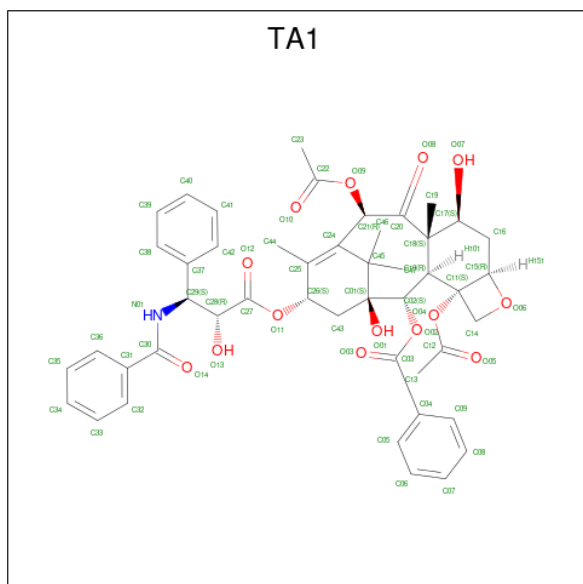
Mol	Chain	Residues	Atoms					AltConf
6	1-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	2-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	3-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	4-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	5-A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 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
7	1-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	2-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	3-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	4-B	1	Total	C	N	O	P	0
			28	10	5	11	2	
7	5-B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 8 is TAXOL (CCD ID: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).



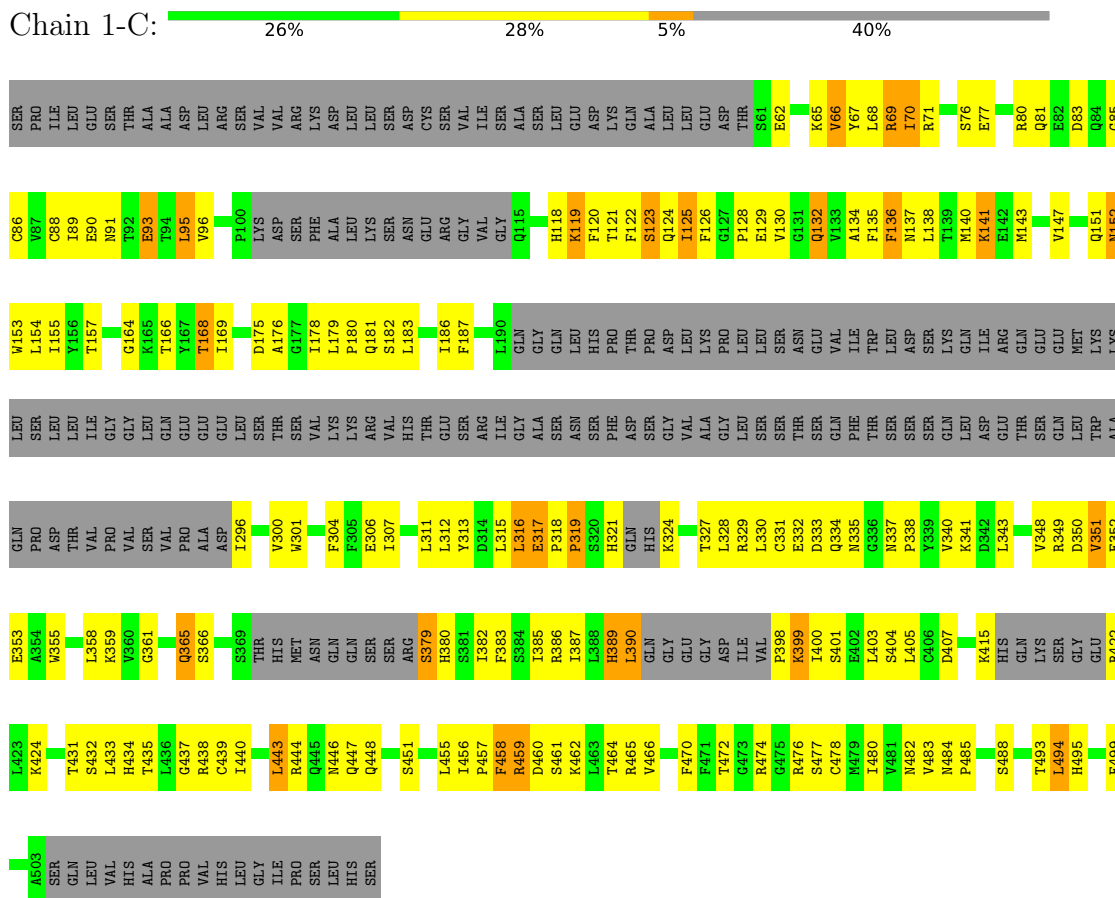
Mol	Chain	Residues	Atoms				AltConf
8	1-B	1	Total	C	N	O	0
			62	47	1	14	
8	2-B	1	Total	C	N	O	0
			62	47	1	14	
8	3-B	1	Total	C	N	O	0
			62	47	1	14	
8	4-B	1	Total	C	N	O	0
			62	47	1	14	
8	5-B	1	Total	C	N	O	0
			62	47	1	14	



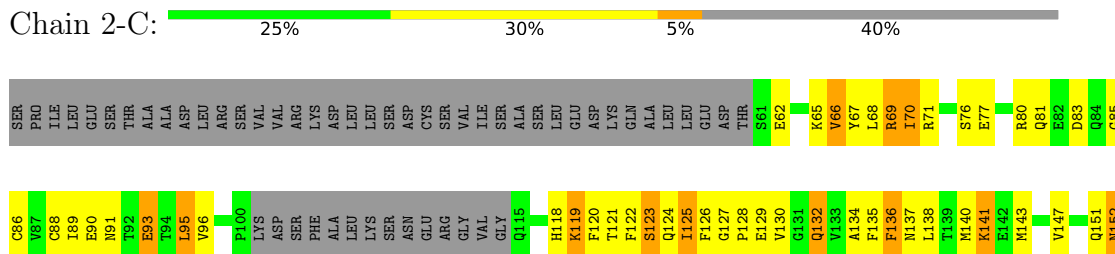
### 3 Residue-property plots

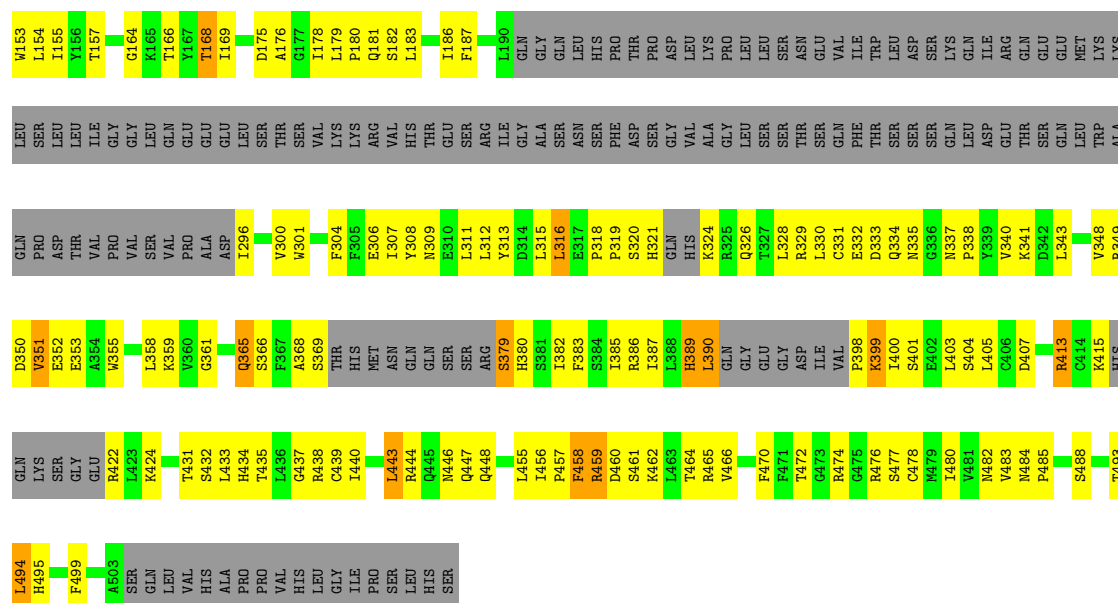
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



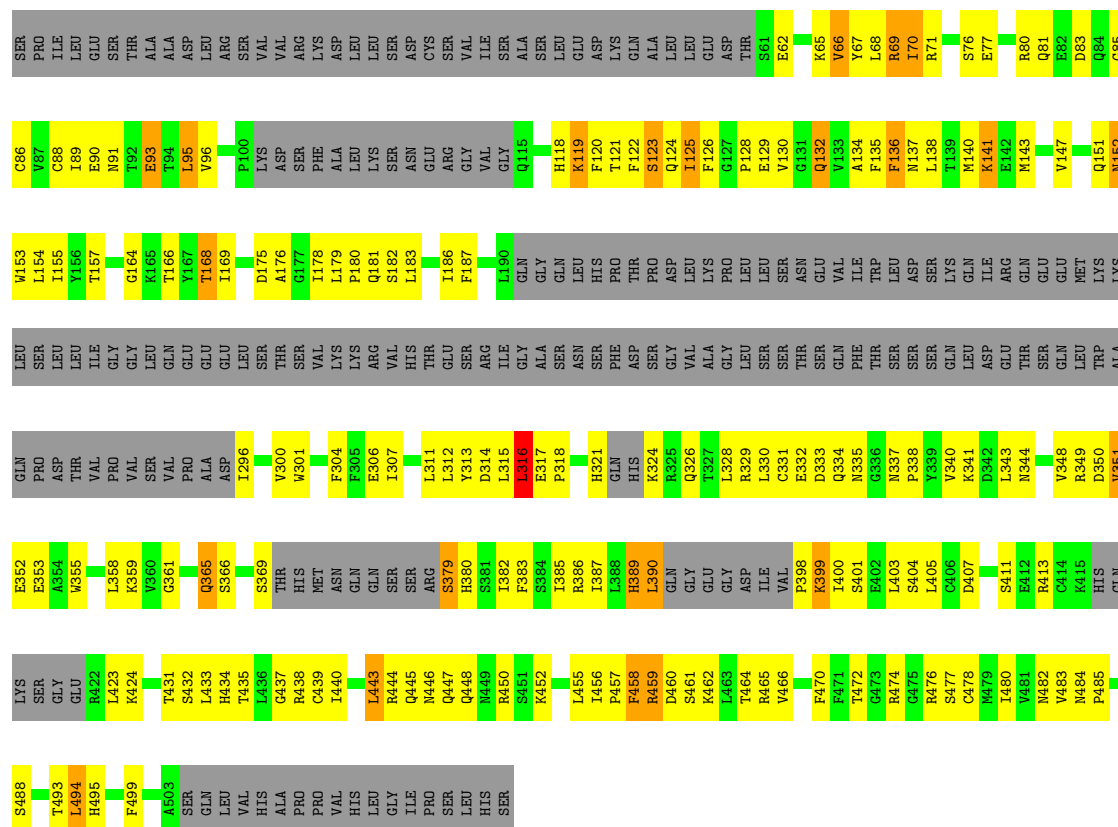
#### • Molecule 1: Kinesin-like protein KIF20A





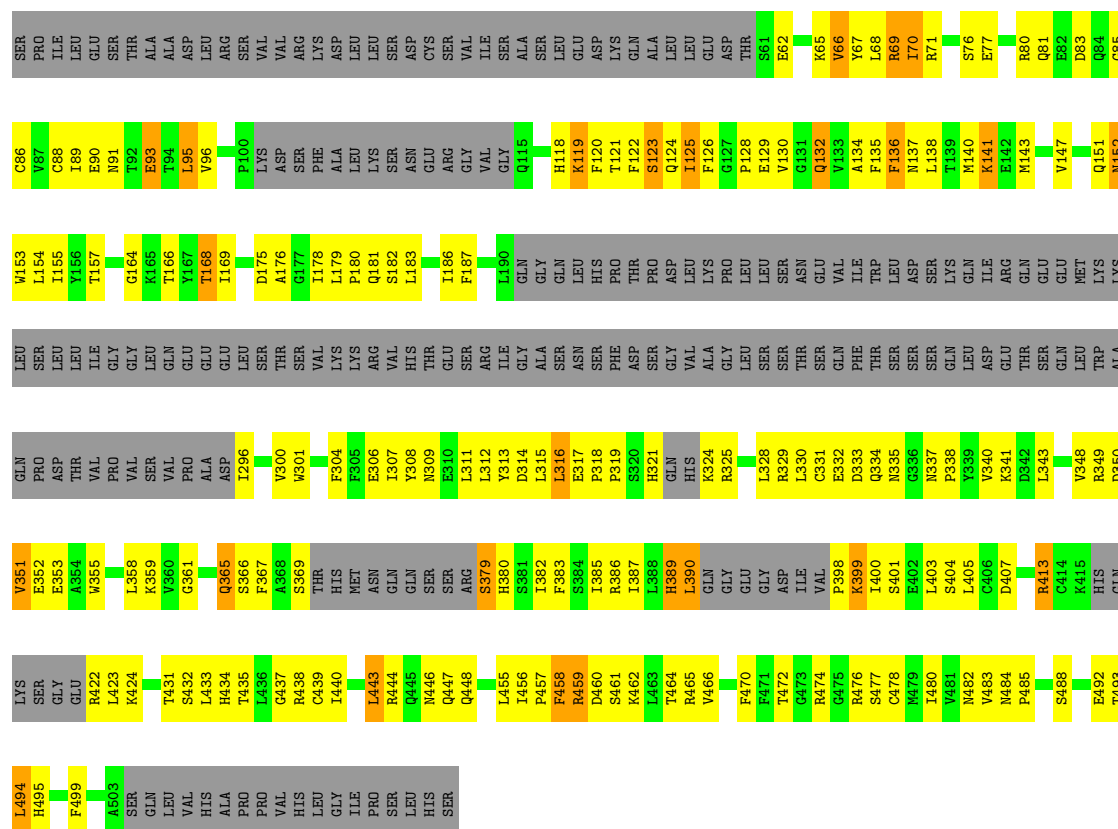
• Molecule 1: Kinesin-like protein KIF20A

Chain 3-C: 25% 30% 5% 40%



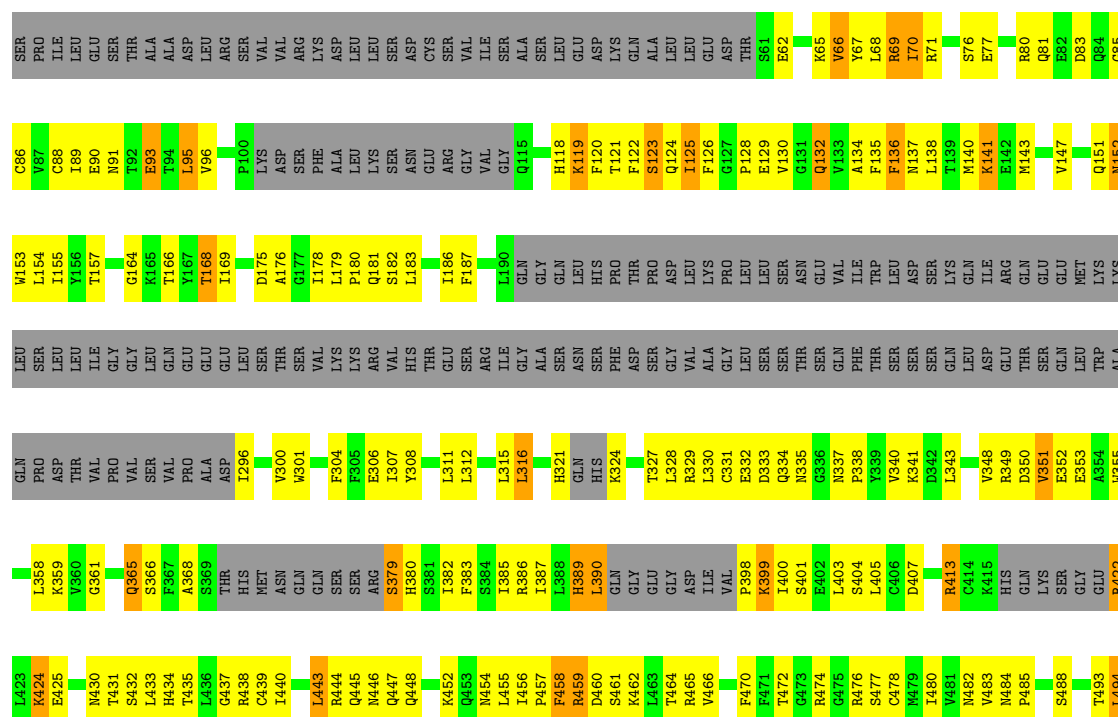
• Molecule 1: Kinesin-like protein KIF20A

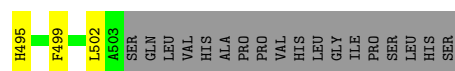
Chain 4-C: 25% 30% 5% 40%



• Molecule 1: Kinesin-like protein KIF20A

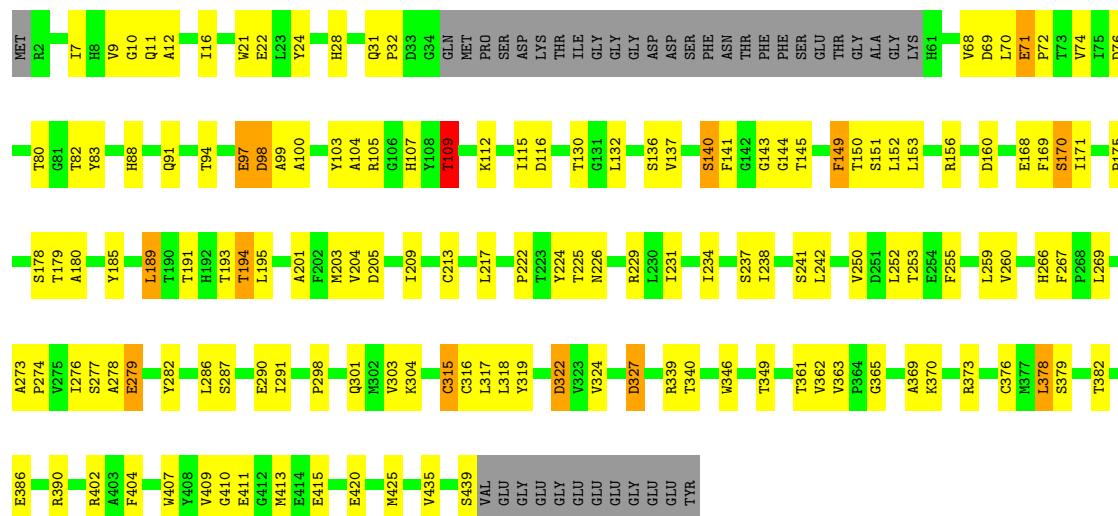
Chain 5-C: 26% 29% 5% 40%





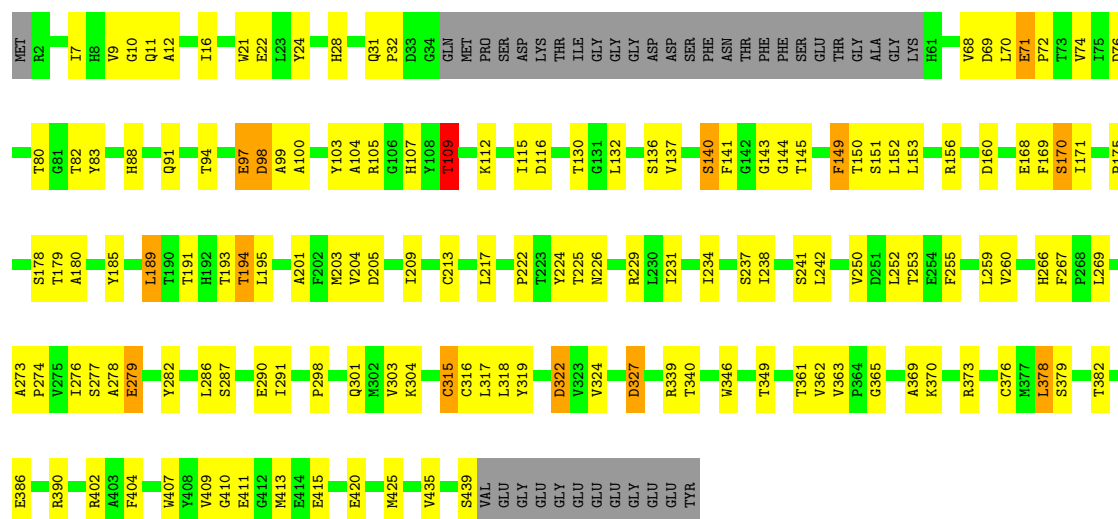
• Molecule 2: Tubulin alpha chain

Chain 1-A: 59% 29% 9%



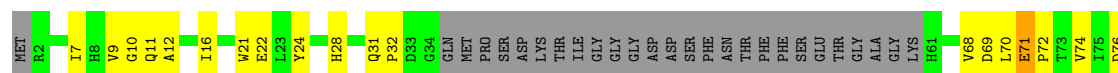
• Molecule 2: Tubulin alpha chain

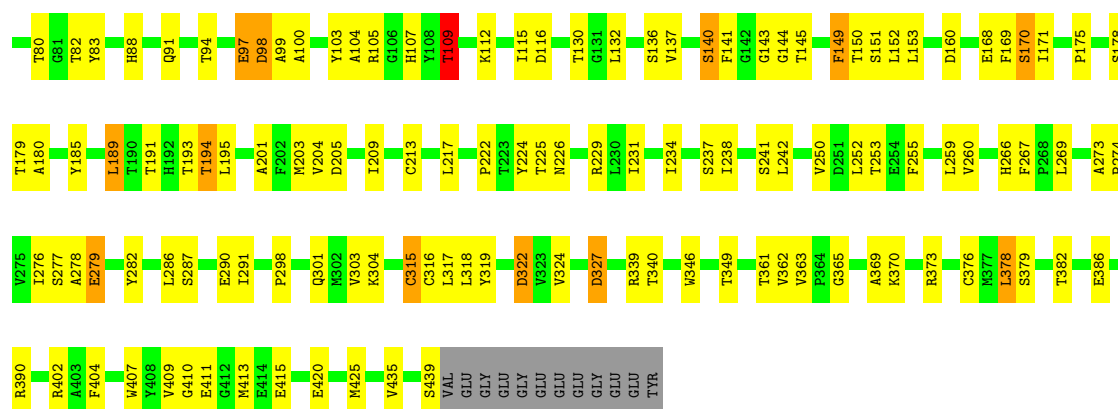
Chain 2-A: 59% 29% 9%



• Molecule 2: Tubulin alpha chain

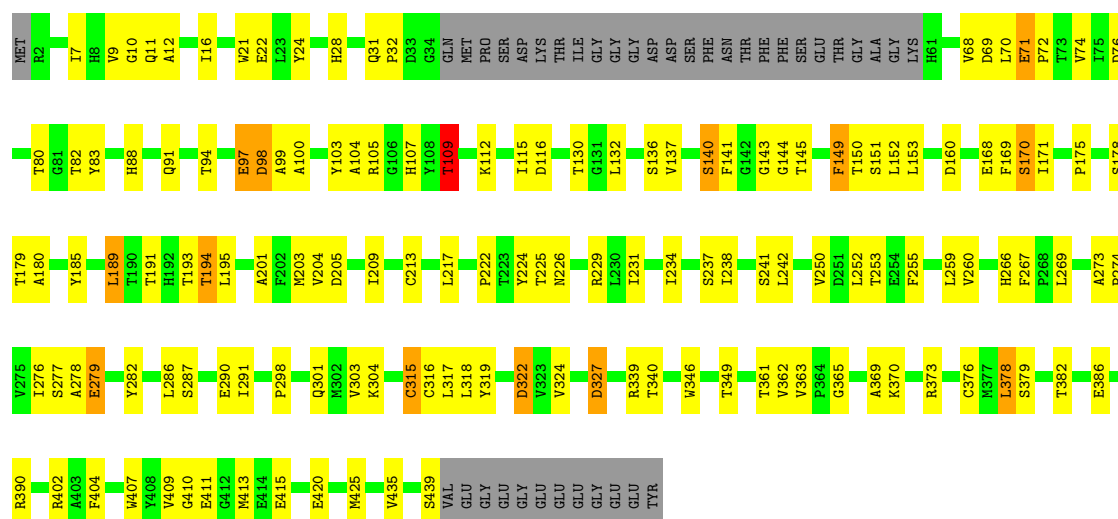
Chain 3-A: 59% 29% 9%





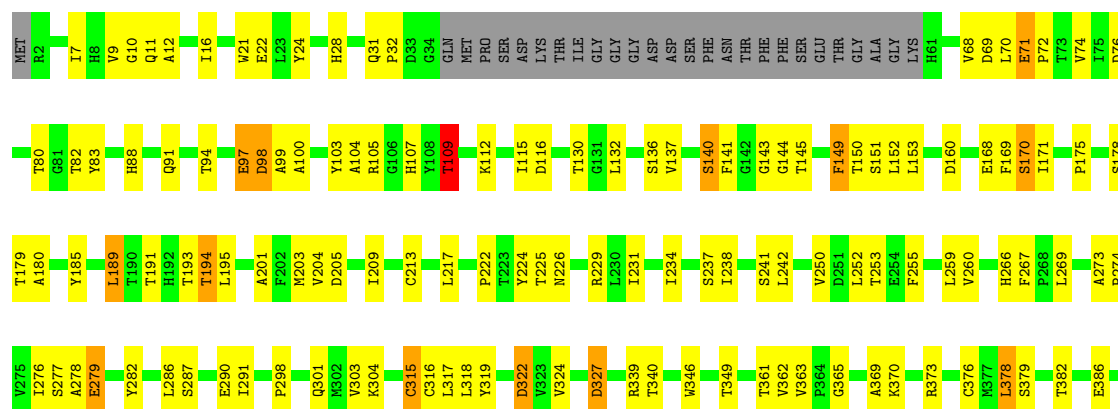
• Molecule 2: Tubulin alpha chain

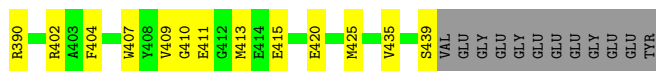
Chain 4-A: 59% 29% 9%



• Molecule 2: Tubulin alpha chain

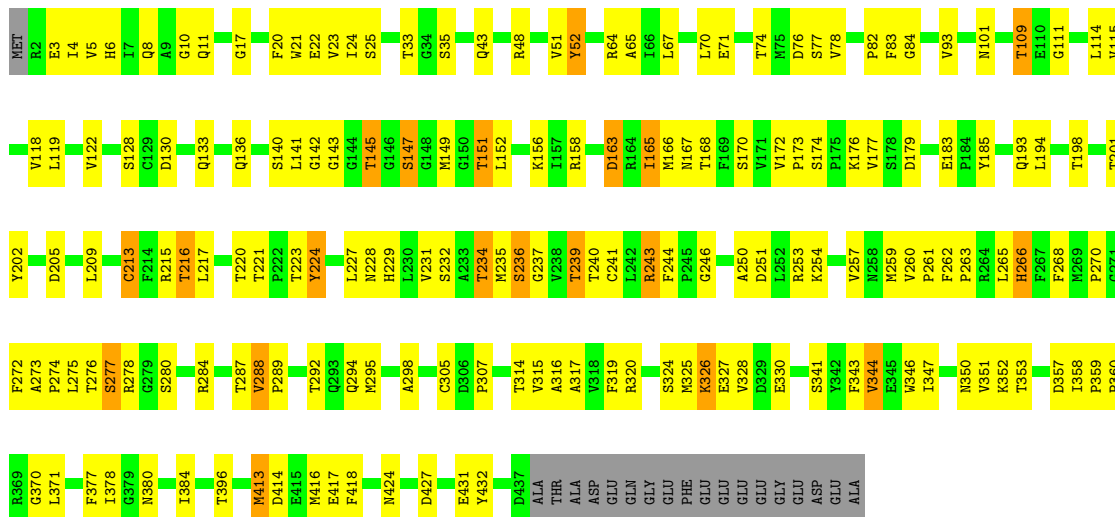
Chain 5-A: 59% 29% 9%





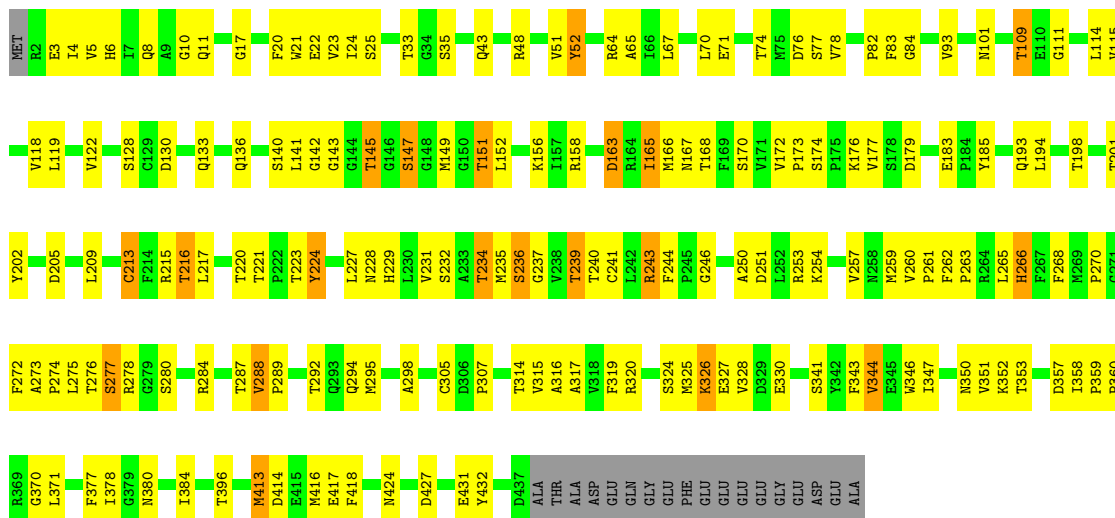
• Molecule 3: Tubulin beta-2B chain

Chain 1-B: 57% 34%



• Molecule 3: Tubulin beta-2B chain

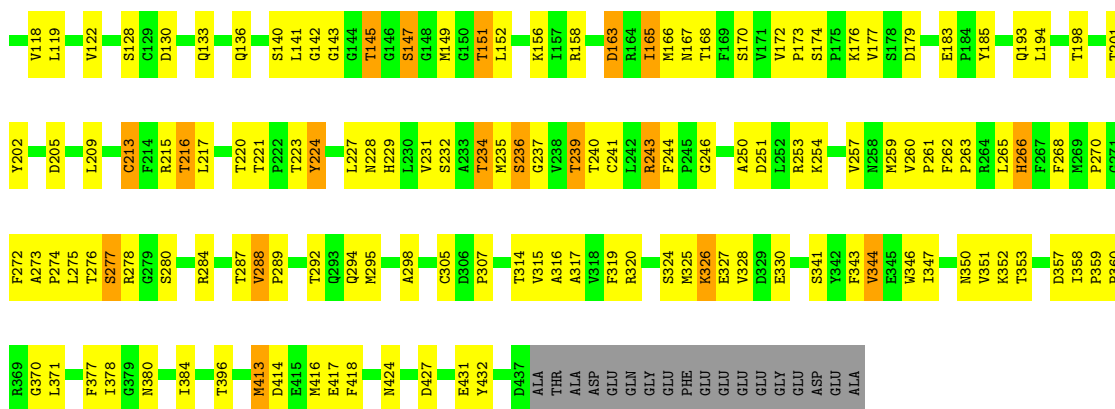
Chain 2-B: 57% 34%



• Molecule 3: Tubulin beta-2B chain

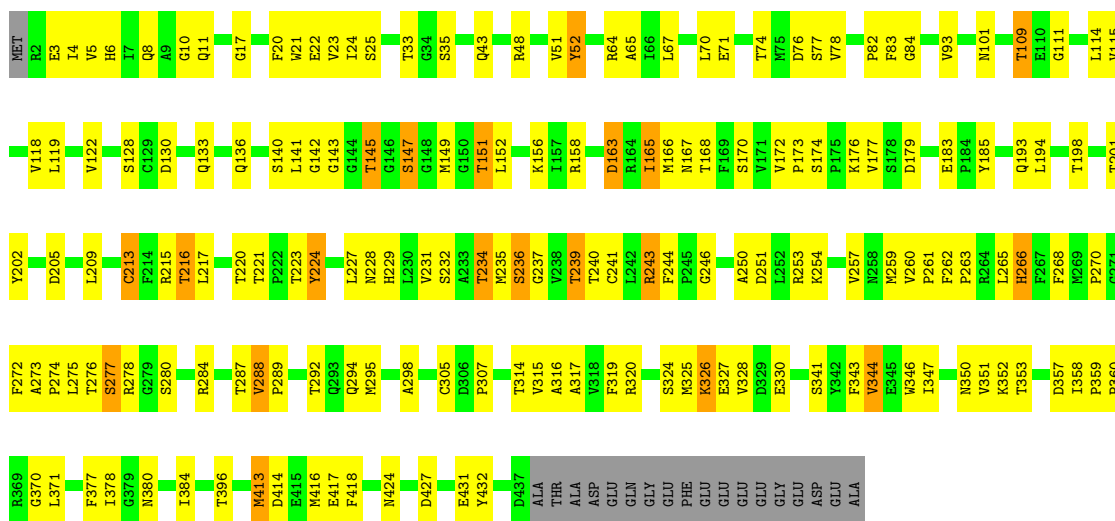
Chain 3-B: 57% 34%





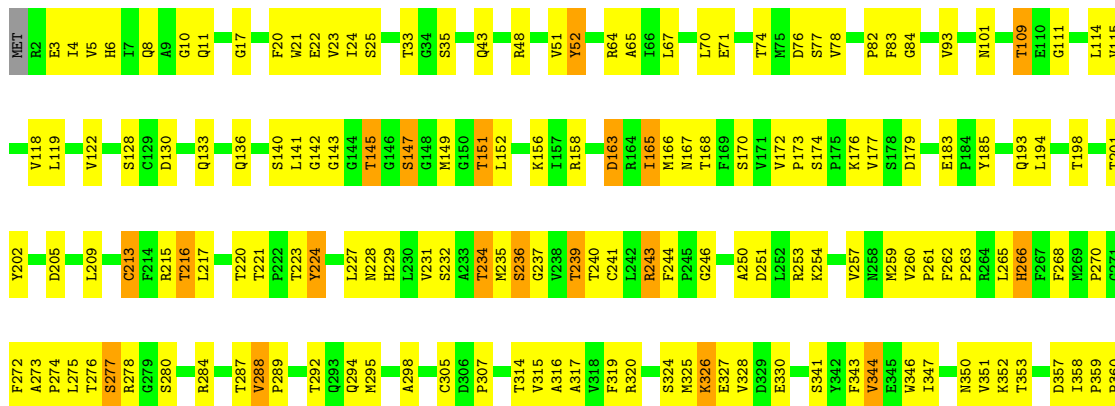
• Molecule 3: Tubulin beta-2B chain

Chain 4-B: 57% 34%



• Molecule 3: Tubulin beta-2B chain

Chain 5-B: 57% 34%



E369	G370	L371	F377	I378	G379	N380	I384	I396	M413	D414	E415	M416	E417	F418	N424	D427	E431	Y432	D437	ALA	THR	ALA	ASP	GLU	GLN	GLY	GLU	PHE	GLU	GLU	GLU	GLY	GLY	GLU	ASP	GLU	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	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	0.084	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0322	Depositor
Map size (Å)	246.4, 214.06, 247.93999	wwPDB
Map dimensions	160, 139, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.54, 1.54, 1.54	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, ANP, 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  >5	RMSZ	# Z  >5
1	1-C	0.55	0/2450	0.71	3/3299 (0.1%)
1	2-C	0.56	0/2450	0.74	4/3299 (0.1%)
1	3-C	0.56	0/2450	0.73	3/3299 (0.1%)
1	4-C	0.57	0/2450	0.76	3/3299 (0.1%)
1	5-C	0.57	0/2450	0.73	2/3299 (0.1%)
2	1-A	0.27	0/3300	0.40	0/4482
2	2-A	0.27	0/3300	0.40	0/4482
2	3-A	0.27	0/3300	0.40	0/4482
2	4-A	0.27	0/3300	0.40	0/4482
2	5-A	0.27	0/3300	0.40	0/4482
3	1-B	0.29	0/3426	0.43	0/4642
3	2-B	0.29	0/3426	0.43	0/4642
3	3-B	0.29	0/3426	0.43	0/4642
3	4-B	0.29	0/3426	0.43	0/4642
3	5-B	0.29	0/3426	0.43	0/4642
All	All	0.38	0/45880	0.52	15/62115 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5-C	0	2

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-C	459	ARG	NE-CZ-NH1	9.50	125.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-C	459	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	2-C	459	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	4-C	459	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	3-C	459	ARG	NE-CZ-NH1	9.35	124.97	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	5-C	413	ARG	Sidechain
1	5-C	422	ARG	Sidechain

## 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	1-C	2407	0	2419	181	0
1	2-C	2407	0	2419	191	0
1	3-C	2407	0	2419	185	0
1	4-C	2407	0	2419	189	0
1	5-C	2407	0	2419	182	0
2	1-A	3227	0	3141	121	0
2	2-A	3227	0	3141	124	0
2	3-A	3227	0	3141	119	0
2	4-A	3227	0	3141	118	0
2	5-A	3227	0	3141	118	0
3	1-B	3351	0	3229	147	0
3	2-B	3351	0	3229	143	0
3	3-B	3351	0	3229	141	0
3	4-B	3351	0	3229	144	0
3	5-B	3351	0	3229	144	0
4	1-A	1	0	0	0	0
4	1-C	1	0	0	0	0
4	2-A	1	0	0	0	0
4	2-C	1	0	0	0	0
4	3-A	1	0	0	0	0
4	3-C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4-A	1	0	0	0	0
4	4-C	1	0	0	0	0
4	5-A	1	0	0	0	0
4	5-C	1	0	0	0	0
5	1-C	31	0	13	2	0
5	2-C	31	0	13	2	0
5	3-C	31	0	13	2	0
5	4-C	31	0	13	2	0
5	5-C	31	0	13	2	0
6	1-A	32	0	12	28	0
6	2-A	32	0	12	27	0
6	3-A	32	0	12	28	0
6	4-A	32	0	12	27	0
6	5-A	32	0	12	27	0
7	1-B	28	0	12	9	0
7	2-B	28	0	12	9	0
7	3-B	28	0	12	9	0
7	4-B	28	0	12	9	0
7	5-B	28	0	12	9	0
8	1-B	62	0	51	14	0
8	2-B	62	0	51	14	0
8	3-B	62	0	51	14	0
8	4-B	62	0	51	14	0
8	5-B	62	0	51	14	0
All	All	45700	0	44385	2005	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 22.

The worst 5 of 2005 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:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27
2:A:179:THR:CB	6:A:500:GTP:H3'	1.62	1.27

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	1-C	286/501 (57%)	273 (96%)	11 (4%)	2 (1%)	19	57
1	2-C	286/501 (57%)	272 (95%)	12 (4%)	2 (1%)	19	57
1	3-C	286/501 (57%)	270 (94%)	15 (5%)	1 (0%)	37	73
1	4-C	286/501 (57%)	270 (94%)	15 (5%)	1 (0%)	37	73
1	5-C	286/501 (57%)	271 (95%)	13 (4%)	2 (1%)	19	57
2	1-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	25	64
2	2-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	25	64
2	3-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	25	64
2	4-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	25	64
2	5-A	408/451 (90%)	367 (90%)	39 (10%)	2 (0%)	25	64
3	1-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	41
3	2-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	41
3	3-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	41
3	4-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	41
3	5-B	424/445 (95%)	384 (91%)	34 (8%)	6 (1%)	9	41
All	All	5590/6985 (80%)	5111 (91%)	431 (8%)	48 (1%)	17	52

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	123	SER
1	1-C	451	SER
1	2-C	123	SER
1	3-C	123	SER
1	4-C	123	SER

### 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	268/447 (60%)	223 (83%)	45 (17%)	1	9
1	2-C	268/447 (60%)	224 (84%)	44 (16%)	2	10
1	3-C	268/447 (60%)	225 (84%)	43 (16%)	2	10
1	4-C	268/447 (60%)	224 (84%)	44 (16%)	2	10
1	5-C	268/447 (60%)	225 (84%)	43 (16%)	2	10
2	1-A	347/377 (92%)	307 (88%)	40 (12%)	4	16
2	2-A	347/377 (92%)	307 (88%)	40 (12%)	4	16
2	3-A	347/377 (92%)	307 (88%)	40 (12%)	4	16
2	4-A	347/377 (92%)	307 (88%)	40 (12%)	4	16
2	5-A	347/377 (92%)	307 (88%)	40 (12%)	4	16
3	1-B	367/381 (96%)	315 (86%)	52 (14%)	2	12
3	2-B	367/381 (96%)	315 (86%)	52 (14%)	2	12
3	3-B	367/381 (96%)	315 (86%)	52 (14%)	2	12
3	4-B	367/381 (96%)	315 (86%)	52 (14%)	2	12
3	5-B	367/381 (96%)	315 (86%)	52 (14%)	2	12
All	All	4910/6025 (82%)	4231 (86%)	679 (14%)	5	13

5 of 679 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4-A	136	SER
1	5-C	400	ILE
2	4-A	253	THR
2	4-A	132	LEU
3	4-B	221	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
3	4-B	11	GLN
2	5-A	192	HIS
3	4-B	300	ASN
1	5-C	170	GLN
3	5-B	337	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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	$\# Z  > 2$
5	ANP	5-C	602	4	29,33,33	2.10	8 (27%)	31,52,52	3.42	15 (48%)
5	ANP	1-C	602	4	29,33,33	2.10	9 (31%)	31,52,52	3.42	15 (48%)
7	GDP	5-B	600	-	24,30,30	2.58	9 (37%)	30,47,47	2.92	8 (26%)
6	GTP	1-A	500	2,4	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
6	GTP	2-A	500	2,4	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
8	TA1	3-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
8	TA1	4-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
7	GDP	2-B	600	-	24,30,30	2.58	9 (37%)	30,47,47	2.92	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GDP	4-B	600	-	24,30,30	2.58	9 (37%)	30,47,47	2.92	8 (26%)
5	ANP	3-C	602	4	29,33,33	2.09	8 (27%)	31,52,52	3.42	15 (48%)
8	TA1	2-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
5	ANP	2-C	602	4	29,33,33	2.09	9 (31%)	31,52,52	3.42	15 (48%)
7	GDP	3-B	600	-	24,30,30	2.58	9 (37%)	30,47,47	2.92	8 (26%)
5	ANP	4-C	602	4	29,33,33	2.10	9 (31%)	31,52,52	3.42	15 (48%)
6	GTP	4-A	500	2,4	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
6	GTP	5-A	500	2,4	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
8	TA1	1-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
7	GDP	1-B	600	-	24,30,30	2.58	9 (37%)	30,47,47	2.92	8 (26%)
6	GTP	3-A	500	2,4	26,34,34	1.33	4 (15%)	32,54,54	1.02	2 (6%)
8	TA1	5-B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)

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
5	ANP	5-C	602	4	-	9/14/38/38	0/3/3/3
5	ANP	1-C	602	4	-	9/14/38/38	0/3/3/3
7	GDP	5-B	600	-	-	4/12/32/32	0/3/3/3
6	GTP	1-A	500	2,4	-	3/18/38/38	0/3/3/3
6	GTP	2-A	500	2,4	-	3/18/38/38	0/3/3/3
8	TA1	3-B	601	-	-	9/41/127/127	0/7/7/7
8	TA1	4-B	601	-	-	9/41/127/127	0/7/7/7
7	GDP	2-B	600	-	-	4/12/32/32	0/3/3/3
7	GDP	4-B	600	-	-	4/12/32/32	0/3/3/3
5	ANP	3-C	602	4	-	9/14/38/38	0/3/3/3
8	TA1	2-B	601	-	-	9/41/127/127	0/7/7/7
5	ANP	2-C	602	4	-	9/14/38/38	0/3/3/3
7	GDP	3-B	600	-	-	4/12/32/32	0/3/3/3
5	ANP	4-C	602	4	-	9/14/38/38	0/3/3/3
6	GTP	4-A	500	2,4	-	3/18/38/38	0/3/3/3
6	GTP	5-A	500	2,4	-	3/18/38/38	0/3/3/3
8	TA1	1-B	601	-	-	9/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GDP	1-B	600	-	-	4/12/32/32	0/3/3/3
6	GTP	3-A	500	2,4	-	3/18/38/38	0/3/3/3
8	TA1	5-B	601	-	-	9/41/127/127	0/7/7/7

The worst 5 of 203 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4-C	602	ANP	PB-O2B	-6.23	1.40	1.56
5	2-C	602	ANP	PB-O2B	-6.21	1.40	1.56
5	5-C	602	ANP	PB-O2B	-6.21	1.40	1.56
5	1-C	602	ANP	PB-O2B	-6.19	1.40	1.56
7	1-B	600	GDP	O4'-C1'	6.18	1.49	1.41

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1-B	600	GDP	C8-N7-C5	9.26	120.62	102.99
7	2-B	600	GDP	C8-N7-C5	9.26	120.62	102.99
7	3-B	600	GDP	C8-N7-C5	9.26	120.62	102.99
7	4-B	600	GDP	C8-N7-C5	9.26	120.62	102.99
7	5-B	600	GDP	C8-N7-C5	9.26	120.62	102.99

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1-C	602	ANP	PG-N3B-PB-O1B
5	1-C	602	ANP	PA-O3A-PB-O1B
5	1-C	602	ANP	PA-O3A-PB-O2B
5	1-C	602	ANP	C5'-O5'-PA-O1A
5	1-C	602	ANP	C5'-O5'-PA-O2A

There are no ring outliers.

20 monomers are involved in 262 short contacts:

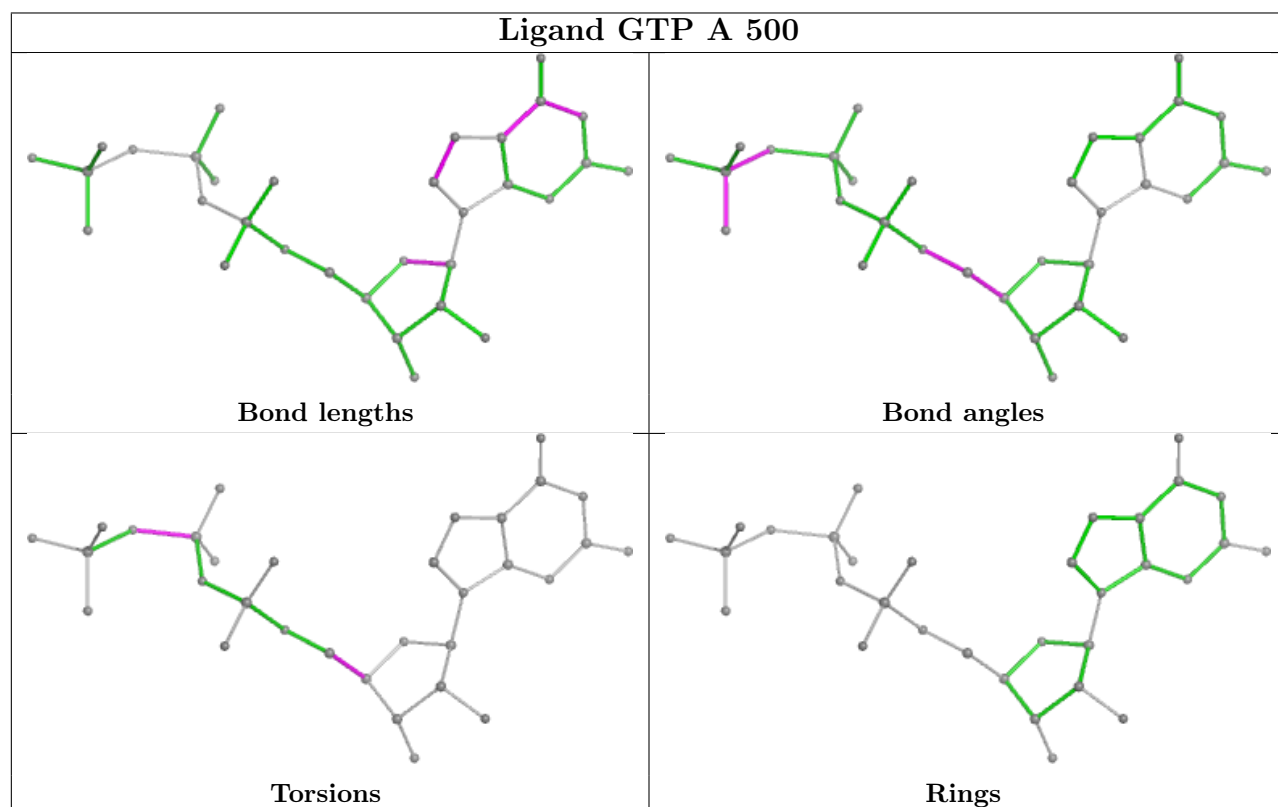
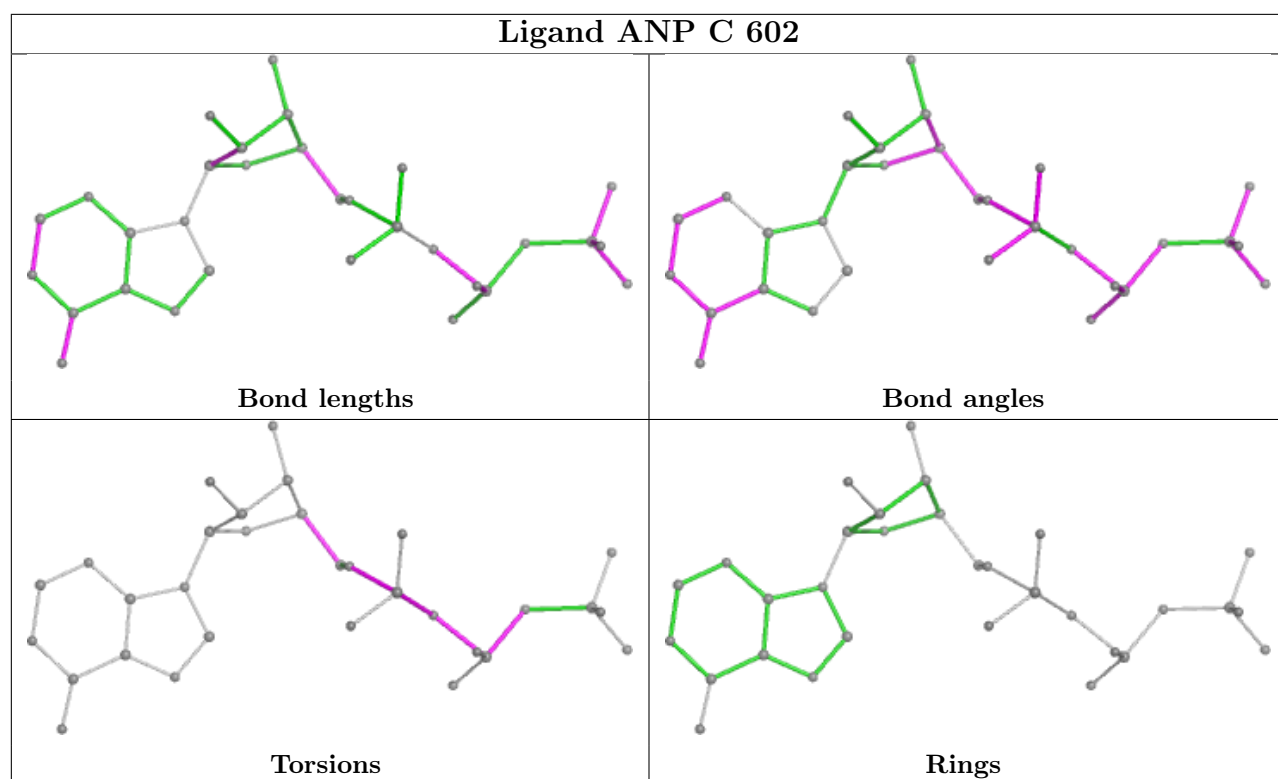
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5-C	602	ANP	2	0
5	1-C	602	ANP	2	0
7	5-B	600	GDP	9	0
6	1-A	500	GTP	28	0

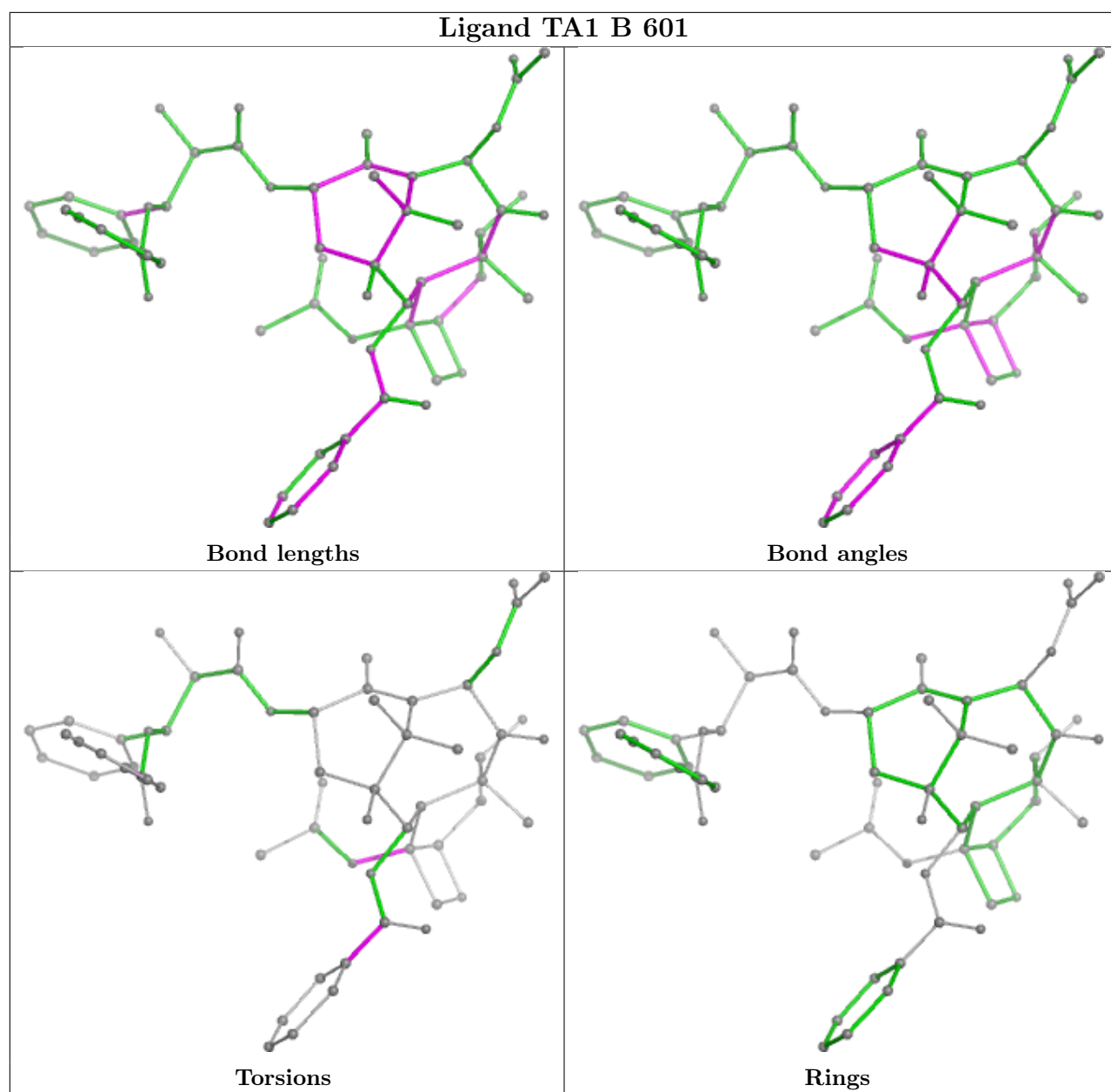
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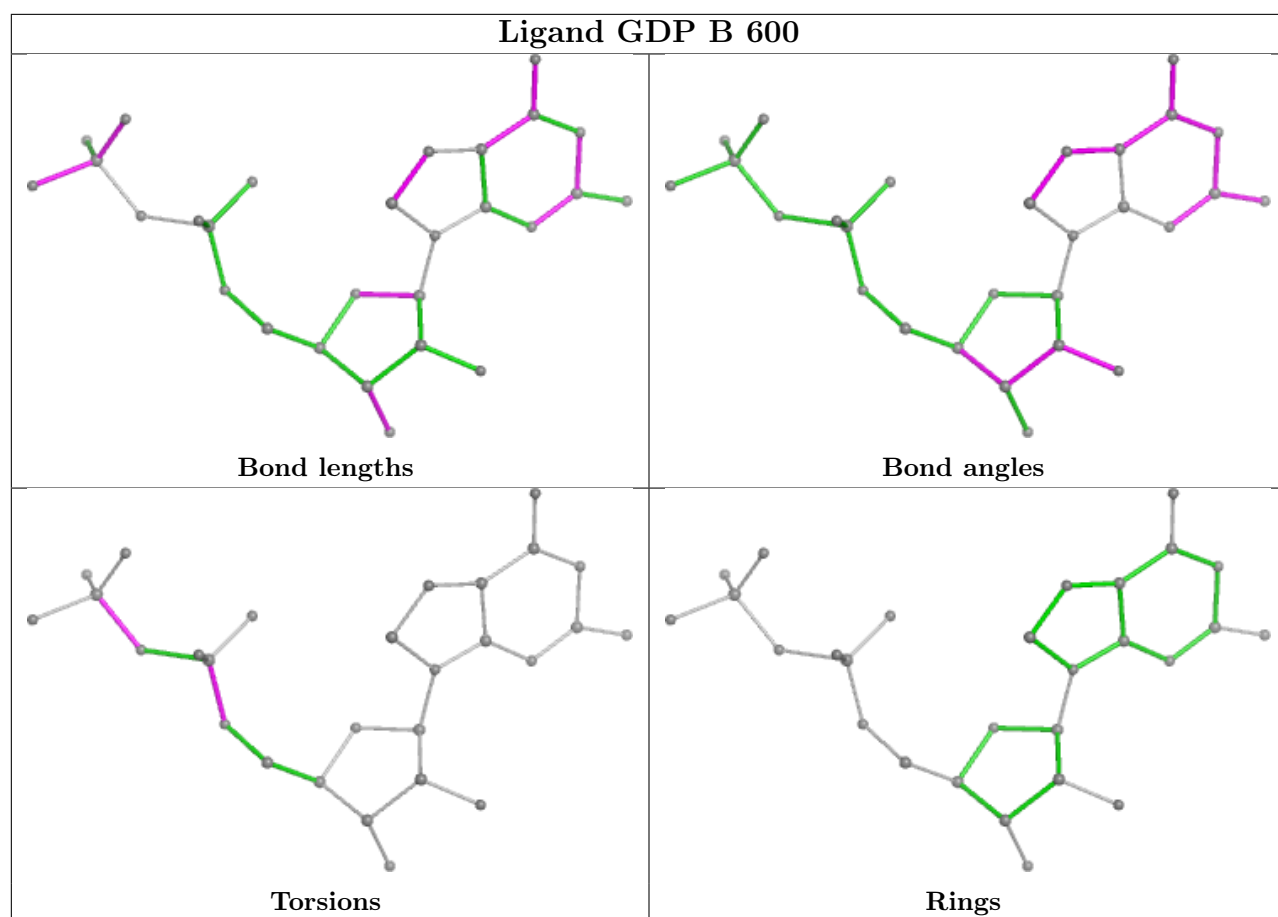
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2-A	500	GTP	27	0
8	3-B	601	TA1	14	0
8	4-B	601	TA1	14	0
7	2-B	600	GDP	9	0
7	4-B	600	GDP	9	0
5	3-C	602	ANP	2	0
8	2-B	601	TA1	14	0
5	2-C	602	ANP	2	0
7	3-B	600	GDP	9	0
5	4-C	602	ANP	2	0
6	4-A	500	GTP	27	0
6	5-A	500	GTP	27	0
8	1-B	601	TA1	14	0
7	1-B	600	GDP	9	0
6	3-A	500	GTP	28	0
8	5-B	601	TA1	14	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.

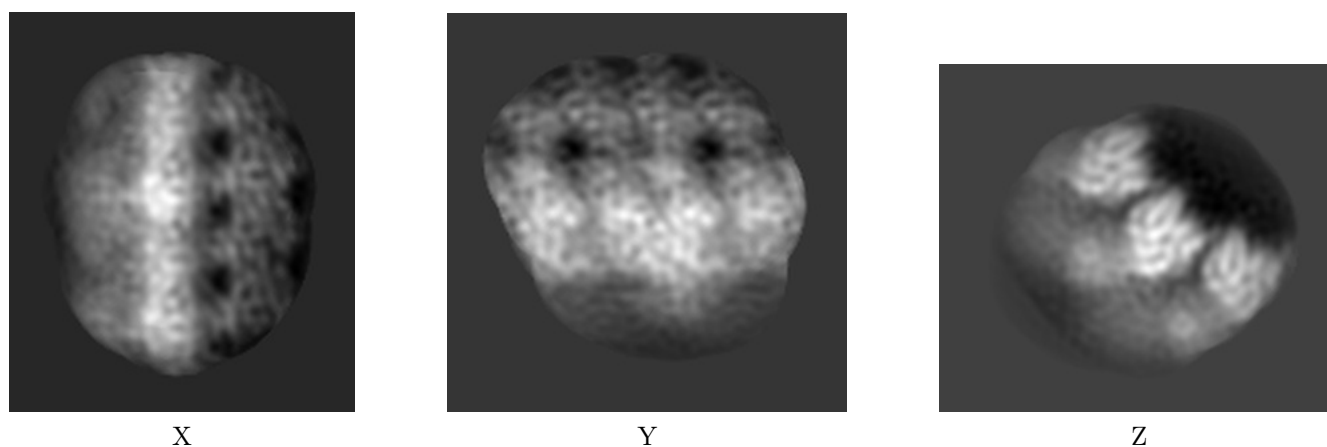
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3623. 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](#)

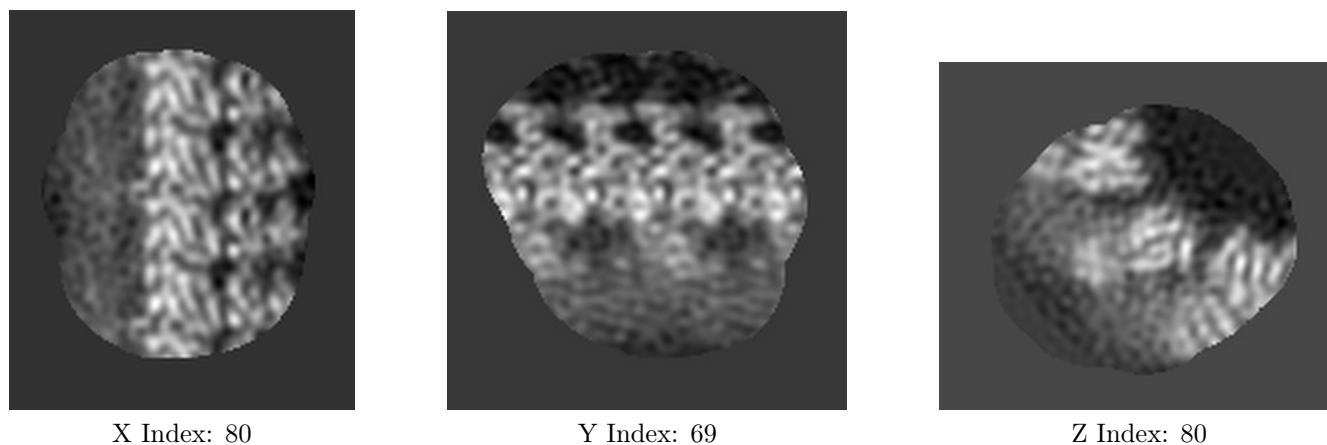
#### 6.1.1 Primary map



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

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

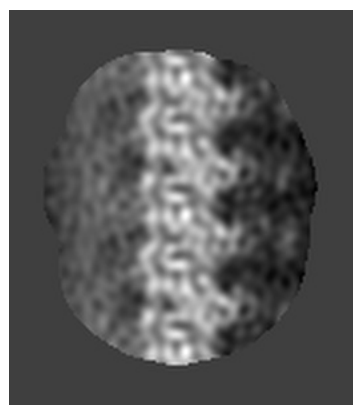
#### 6.2.1 Primary map



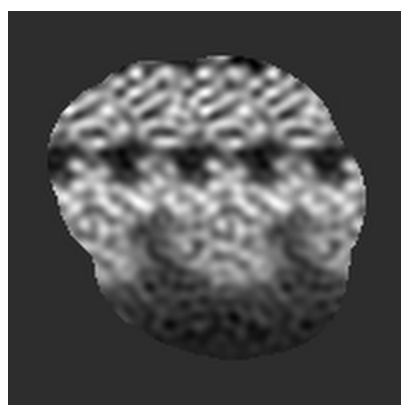
The images above show central slices of the map in three orthogonal directions.

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

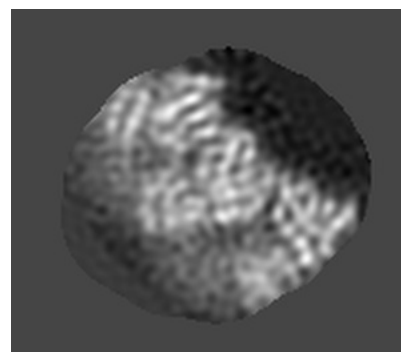
### 6.3.1 Primary map



X Index: 85



Y Index: 57

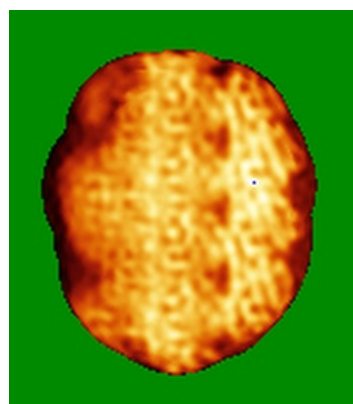


Z Index: 92

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

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

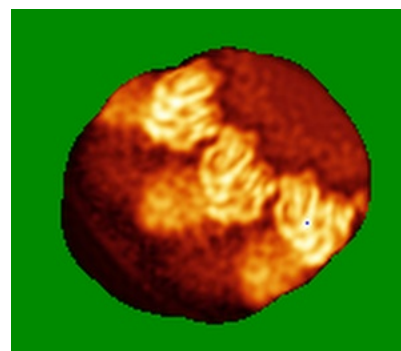
### 6.4.1 Primary map



X



Y

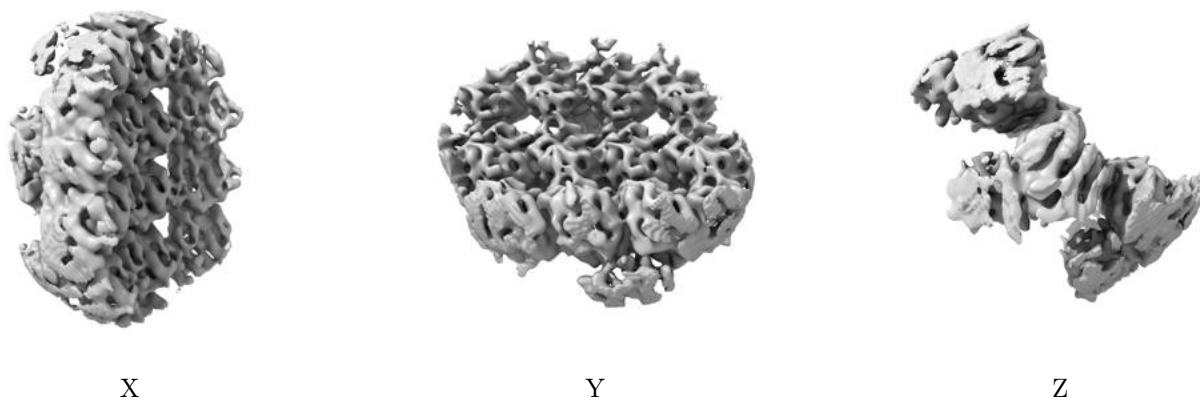


Z

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 0.0322. 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](#)

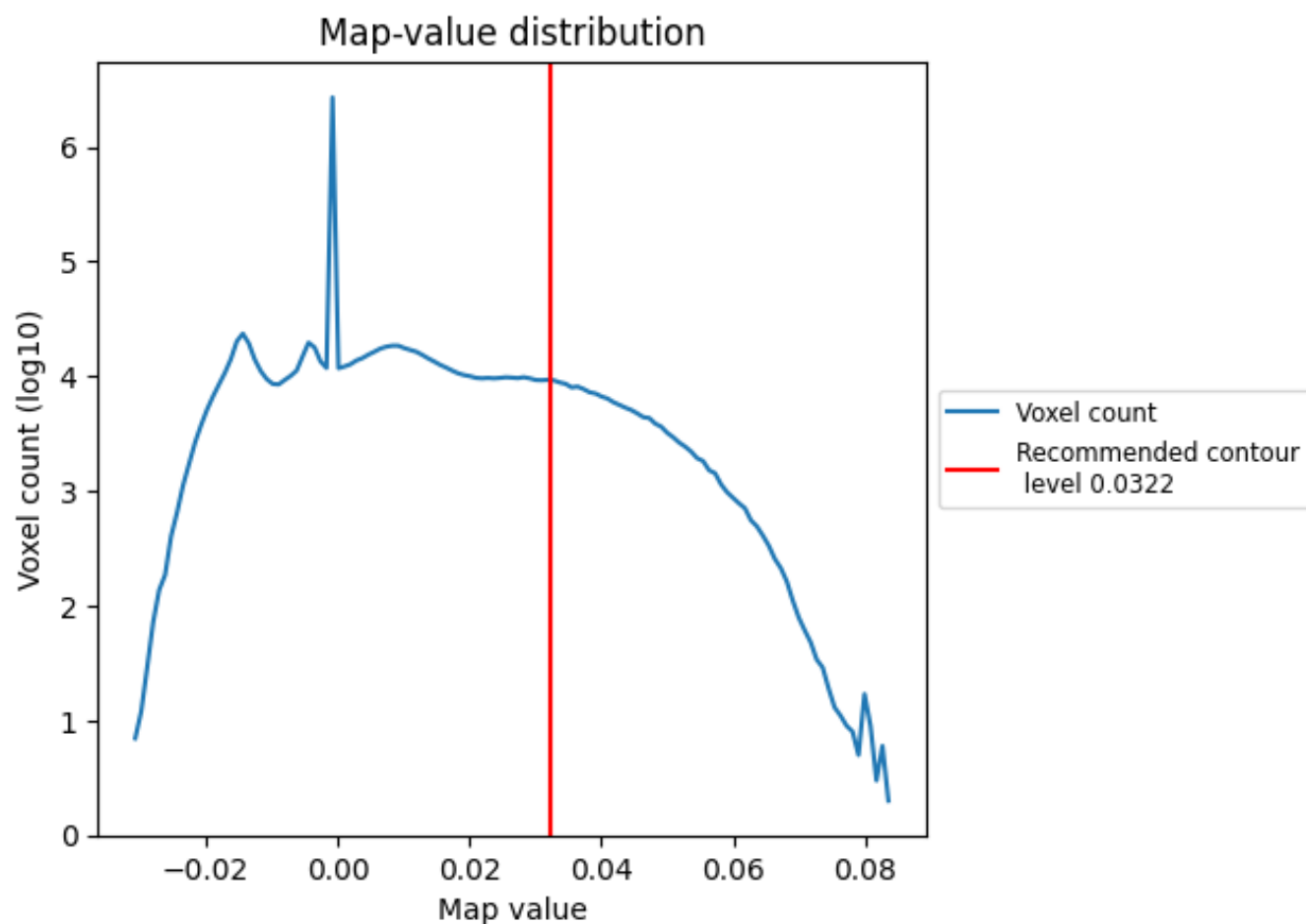
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

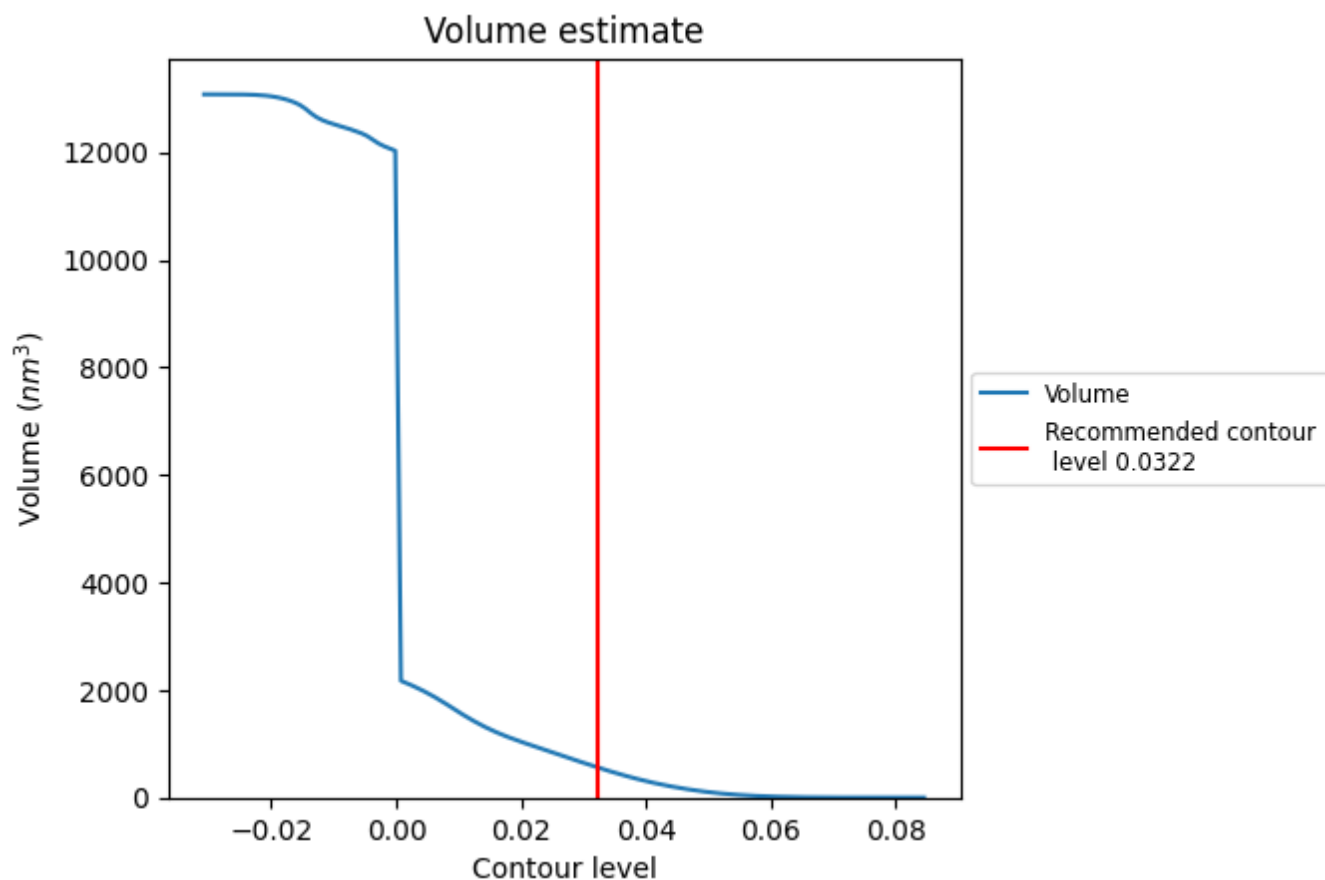
This section contains the results of statistical analysis of the map.

### 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 563 nm<sup>3</sup>; this corresponds to an approximate mass of 509 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.