



## wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 12:16 PM EST

PDB ID : 6BJC  
EMDB ID : EMD-7101  
Title : TPX2\_mini decorated GMPCPP-microtubule  
Authors : Zhang, R.; Nogales, E.  
Deposited on : 2017-11-05  
Resolution : 3.30 Å(reported)

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

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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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

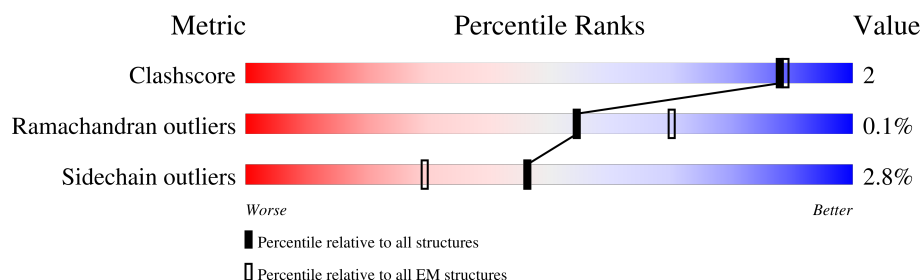
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
1	E	451	
1	J	451	
1	K	451	
1	L	451	
2	B	445	
2	D	445	

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Mol	Chain	Length	Quality of chain
2	F	445	 88% 8% .
2	G	445	 88% 8% .
2	H	445	 88% 8% .
2	I	445	 88% 8% .
3	P	747	 96% .
3	T	747	 96% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 41136 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3356	2129	573	633	21		
1	C	430	Total	C	N	O	S	0	0
			3356	2129	573	633	21		
1	E	430	Total	C	N	O	S	0	0
			3356	2129	573	633	21		
1	J	430	Total	C	N	O	S	0	0
			3356	2129	573	633	21		
1	L	430	Total	C	N	O	S	0	0
			3356	2129	573	633	21		
1	K	430	Total	C	N	O	S	0	0
			3356	2129	573	633	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	427	Total	C	N	O	S	0	0
			3353	2107	573	647	26		
2	D	427	Total	C	N	O	S	0	0
			3353	2107	573	647	26		
2	F	427	Total	C	N	O	S	0	0
			3353	2107	573	647	26		
2	H	427	Total	C	N	O	S	0	0
			3353	2107	573	647	26		
2	G	427	Total	C	N	O	S	0	0
			3353	2107	573	647	26		
2	I	427	Total	C	N	O	S	0	0
			3353	2107	573	647	26		

- Molecule 3 is a protein called Targeting protein for Xklp2.

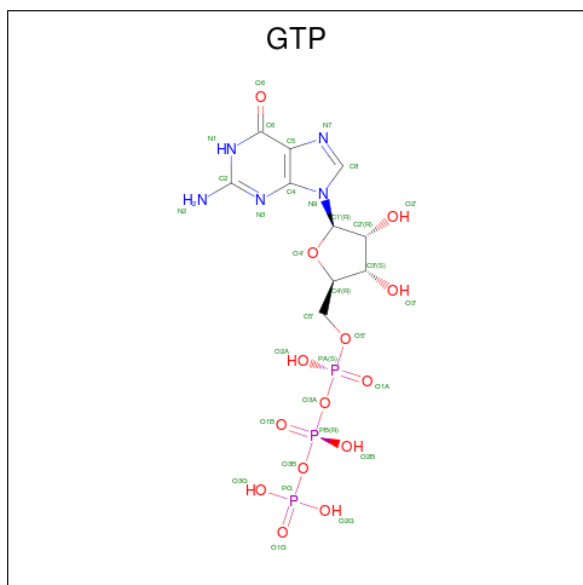
Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	31	Total	C	N	O	S	0	0
			243	156	42	44	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	31	Total	C	N	O	S	0	0
			243	156	42	44	1		

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



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

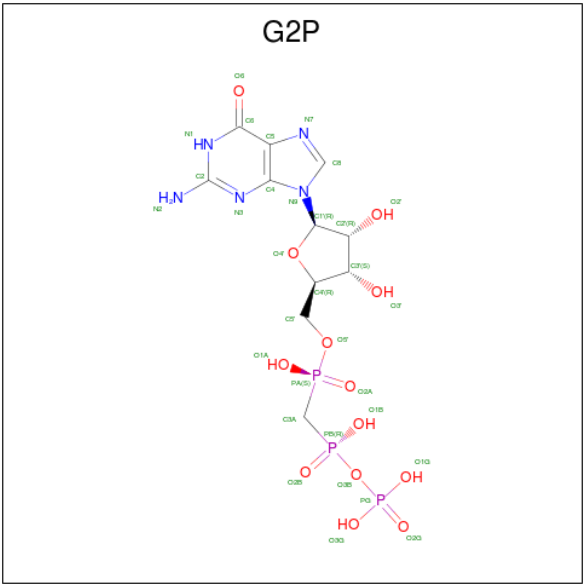
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	
5	J	1	Total	Mg	0
			1	1	
5	H	1	Total	Mg	0
			1	1	
5	L	1	Total	Mg	0
			1	1	
5	G	1	Total	Mg	0
			1	1	
5	K	1	Total	Mg	0
			1	1	
5	I	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			32	11	5	13	3	

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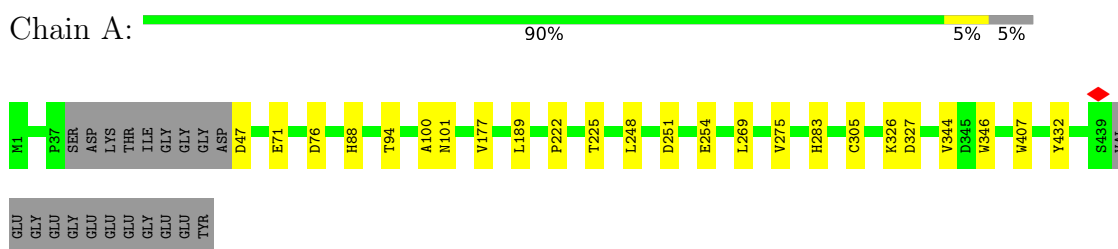
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Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			32	11	5	13	3	
6	F	1	Total	C	N	O	P	0
			32	11	5	13	3	
6	H	1	Total	C	N	O	P	0
			32	11	5	13	3	
6	G	1	Total	C	N	O	P	0
			32	11	5	13	3	
6	I	1	Total	C	N	O	P	0
			32	11	5	13	3	

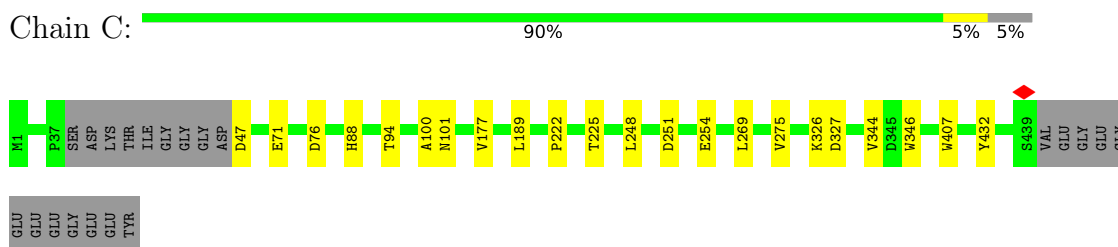
### 3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

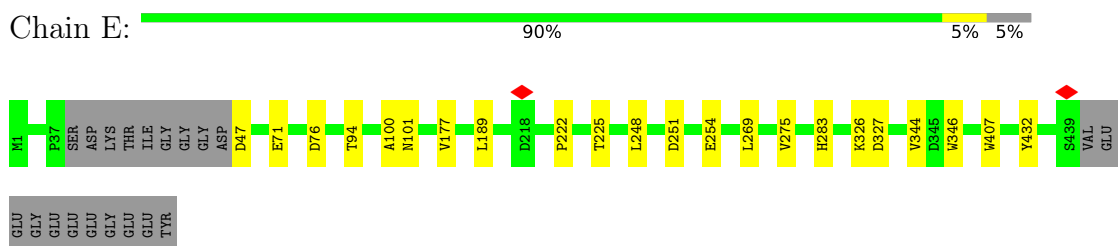
- Molecule 1: Tubulin alpha-1B chain



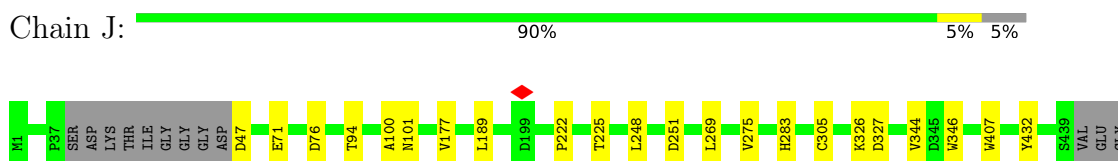
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain




- Molecule 1: Tubulin alpha-1B chain

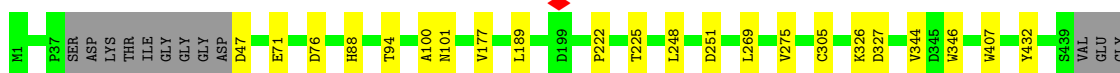




GLU  
GLY  
GLU  
GLU  
GLU  
GLY  
GLY  
GLU  
GLU  
TYR

• Molecule 1: Tubulin alpha-1B chain

Chain L:  90% 5% 5%



GLU  
GLY  
GLU  
GLU  
GLU  
GLY  
GLY  
GLU  
GLU  
TYR


• Molecule 1: Tubulin alpha-1B chain

Chain K:  90% 5% 5%

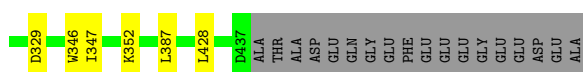


GLU  
GLU  
GLY  
GLY  
GLU  
GLU  
TYR


• Molecule 2: Tubulin beta chain

Chain B:  88% 8% .

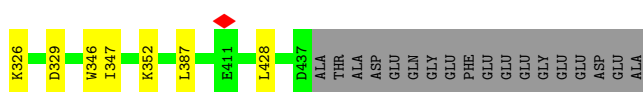





• Molecule 2: Tubulin beta chain

Chain D:  87% 8% .

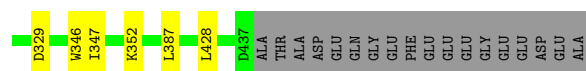




• Molecule 2: Tubulin beta chain

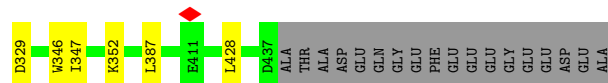
Chain F:  88% 8% .





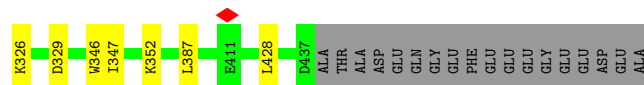
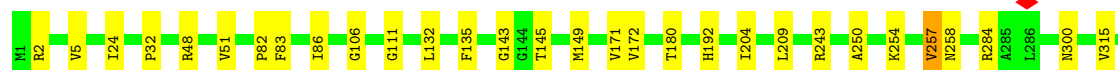
- Molecule 2: Tubulin beta chain

Chain H: 88% 8% .



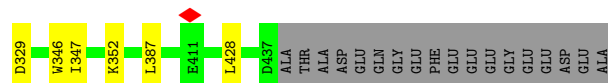
- Molecule 2: Tubulin beta chain

Chain G: 88% 8% .



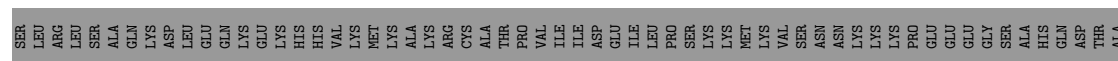
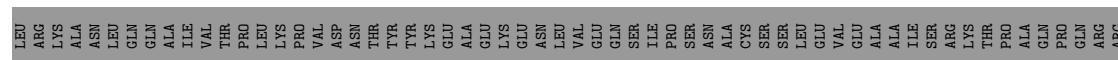
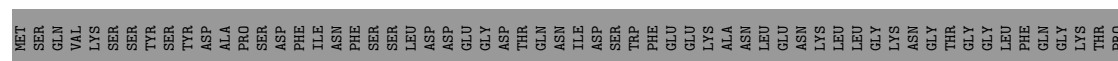
- Molecule 2: Tubulin beta chain

Chain I: 88% 8% .



- Molecule 3: Targeting protein for Xklp2

Chain T: 96% .



[illegible]

- Molecule 3: Targeting protein for Xklp2

Chain P:  96%

[illegible]

PRO	GLN	LEU	GLY
LEU	GLU	GLU	LYS
THR	LEU	GLU	ILE
VAL	GLU	LEU	LYS
PRO	LYS	ARG	GLU
VAL	MET	GLN	LEU
SER	ALA	GLY	GLN
PRO	VAL	GLU	LYS
LYS	VAL	GLU	GLY
PHE	GLU	ALA	VAL
SER	GLU	ALA	VAL
THR	GLN	CYS	PRO
ARG	LYS	PHE	LYS
PHE	ALA	LYS	PHE
HIS	GLN	ALA	LYS
CYS	GLN	ARG	ALA
	LEU	PRO	LEU
	GLU	ASN	PRO
	GLU	THR	LEU
	ALA	VAL	PRO
	ARG	ILE	HIS
	LEU	SER	PHE
	GLN	GLN	ASP
	GLU	GLU	THR
	GLU	PRO	ILE
	GLU	PHE	ASN
	GLN	VAL	LEU
	LYS	PRO	PRO
	LYS	LYS	GLU
	GLU	GLU	LYS
	LEU	LYS	VAL
	ALA	LYS	LYS
	ARG	SER	ASN
	LEU	VAL	VAL
	ARG	ALA	THR
	ARG	GLY	GLN
	GLU	LEU	GLU
	LEU	SER	GLU
	VAL	GLY	PRO
	HIS	PHE	PHE
	LYS	SER	CYS
	ALA	LEU	LEU
	ASN	VAL	GLU
	PRO	GLN	THR
	ILE	GLU	ASP
	ARG	PRO	ARG
	LYS	PHE	ARG
	TYR	GLN	GLY
	GLN	LEU	ALA
	GLY	ALA	LEU
	LEU	THR	LYS
	GLU	GLU	ALA
	ILE	LYS	GLN
	LYS	ARG	THR
	SER	ALA	TRP
	SER	LYS	LYS
	ASP	GLU	HIS
	GLN	ARG	ARG

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.74°, rise=9.03 Å, axial sym=C1	Depositor
Number of segments used	85000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	27.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.346	Depositor
Minimum map value	-12.165	Depositor
Average map value	-0.016	Depositor
Map value standard deviation	0.932	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	680.96, 680.96, 680.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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: MG, G2P, 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	A	0.43	0/3433	0.71	0/4662
1	C	0.42	0/3433	0.71	0/4662
1	E	0.43	0/3433	0.71	0/4662
1	J	0.42	0/3433	0.71	0/4662
1	K	0.43	0/3433	0.71	0/4662
1	L	0.43	0/3433	0.71	0/4662
2	B	0.43	0/3428	0.70	0/4645
2	D	0.43	0/3428	0.70	0/4645
2	F	0.43	0/3428	0.70	0/4645
2	G	0.43	0/3428	0.70	0/4645
2	H	0.43	0/3428	0.70	0/4645
2	I	0.43	0/3428	0.70	0/4645
3	P	0.48	0/248	0.67	0/336
3	T	0.46	0/248	0.65	0/336
All	All	0.43	0/41662	0.71	0/56514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3356	0	3264	18	0
1	C	3356	0	3264	17	0
1	E	3356	0	3264	16	0
1	J	3356	0	3264	12	0
1	K	3356	0	3264	13	0
1	L	3356	0	3264	13	0
2	B	3353	0	3230	24	0
2	D	3353	0	3230	25	0
2	F	3353	0	3230	23	0
2	G	3353	0	3230	23	0
2	H	3353	0	3230	23	0
2	I	3353	0	3230	23	0
3	P	243	0	235	0	0
3	T	243	0	235	0	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	E	32	0	12	0	0
4	J	32	0	12	0	0
4	K	32	0	12	0	0
4	L	32	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	B	32	0	14	1	0
6	D	32	0	14	1	0
6	F	32	0	14	1	0
6	G	32	0	14	1	0
6	H	32	0	14	1	0
6	I	32	0	14	1	0
All	All	41136	0	39590	157	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 2.

The worst 5 of 157 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:A:177:VAL:HG13	2:H:329:ASP:HB3	1.66	0.76
2:B:329:ASP:HB3	1:K:177:VAL:HG13	1.66	0.76
2:F:329:ASP:HB3	1:J:177:VAL:HG13	1.66	0.76
1:E:177:VAL:HG13	2:G:329:ASP:HB3	1.66	0.75
2:D:329:ASP:HB3	1:L:177:VAL:HG13	1.67	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/451 (94%)	412 (97%)	13 (3%)	1 (0%)	47	77
1	C	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
1	E	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
1	J	426/451 (94%)	412 (97%)	13 (3%)	1 (0%)	47	77
1	K	426/451 (94%)	412 (97%)	14 (3%)	0	100	100
1	L	426/451 (94%)	412 (97%)	13 (3%)	1 (0%)	47	77
2	B	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	D	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	F	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	G	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	H	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
2	I	425/445 (96%)	413 (97%)	12 (3%)	0	100	100
3	P	27/747 (4%)	25 (93%)	2 (7%)	0	100	100
3	T	27/747 (4%)	25 (93%)	2 (7%)	0	100	100
All	All	5160/6870 (75%)	5000 (97%)	157 (3%)	3 (0%)	54	81



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	CYS
1	J	305	CYS
1	L	305	CYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/379 (95%)	350 (98%)	9 (2%)	47	72
1	C	359/379 (95%)	350 (98%)	9 (2%)	47	72
1	E	359/379 (95%)	350 (98%)	9 (2%)	47	72
1	J	359/379 (95%)	350 (98%)	9 (2%)	47	72
1	K	359/379 (95%)	350 (98%)	9 (2%)	47	72
1	L	359/379 (95%)	350 (98%)	9 (2%)	47	72
2	B	367/381 (96%)	356 (97%)	11 (3%)	41	68
2	D	367/381 (96%)	356 (97%)	11 (3%)	41	68
2	F	367/381 (96%)	356 (97%)	11 (3%)	41	68
2	G	367/381 (96%)	356 (97%)	11 (3%)	41	68
2	H	367/381 (96%)	356 (97%)	11 (3%)	41	68
2	I	367/381 (96%)	356 (97%)	11 (3%)	41	68
3	P	27/680 (4%)	26 (96%)	1 (4%)	34	63
3	T	27/680 (4%)	26 (96%)	1 (4%)	34	63
All	All	4410/5920 (74%)	4288 (97%)	122 (3%)	46	70

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	300	ASN
2	I	24	ILE
2	H	132	LEU

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Mol	Chain	Res	Type
1	K	432	TYR
2	I	315	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	6	HIS
1	L	300	ASN
2	I	436	GLN
2	H	14	ASN
2	H	385	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GTP	A	501	5	26,34,34	0.95	2 (7%)	32,54,54	1.12	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GTP	J	501	5	26,34,34	0.93	1 (3%)	32,54,54	1.15	4 (12%)
6	G2P	H	501	5	27,34,34	2.00	9 (33%)	33,54,54	2.35	14 (42%)
4	GTP	E	501	5	26,34,34	0.94	2 (7%)	32,54,54	1.13	4 (12%)
4	GTP	L	501	5	26,34,34	0.91	1 (3%)	32,54,54	1.14	3 (9%)
4	GTP	K	501	5	26,34,34	0.92	1 (3%)	32,54,54	1.15	5 (15%)
6	G2P	F	501	5	27,34,34	1.98	8 (29%)	33,54,54	2.50	16 (48%)
6	G2P	D	501	5	27,34,34	1.94	8 (29%)	33,54,54	2.46	14 (42%)
6	G2P	B	501	5	27,34,34	1.95	8 (29%)	33,54,54	2.48	15 (45%)
6	G2P	G	501	5	27,34,34	1.99	9 (33%)	33,54,54	2.34	14 (42%)
6	G2P	I	501	5	27,34,34	2.04	9 (33%)	33,54,54	2.50	15 (45%)
4	GTP	C	501	5	26,34,34	0.94	2 (7%)	32,54,54	1.12	4 (12%)

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
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3
4	GTP	J	501	5	-	6/18/38/38	0/3/3/3
6	G2P	H	501	5	-	2/15/38/38	0/3/3/3
4	GTP	E	501	5	-	7/18/38/38	0/3/3/3
4	GTP	L	501	5	-	6/18/38/38	0/3/3/3
4	GTP	K	501	5	-	6/18/38/38	0/3/3/3
6	G2P	F	501	5	-	4/15/38/38	0/3/3/3
6	G2P	D	501	5	-	2/15/38/38	0/3/3/3
6	G2P	B	501	5	-	4/15/38/38	0/3/3/3
6	G2P	G	501	5	-	2/15/38/38	0/3/3/3
6	G2P	I	501	5	-	3/15/38/38	0/3/3/3
4	GTP	C	501	5	-	7/18/38/38	0/3/3/3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	501	G2P	C5-C6	4.25	1.48	1.41
6	H	501	G2P	PB-O2B	4.25	1.61	1.51
6	G	501	G2P	PB-O2B	4.24	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	501	G2P	PB-O2B	4.23	1.61	1.51
6	H	501	G2P	C5-C6	4.22	1.48	1.41

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	501	G2P	C2-N3-C4	5.15	121.24	115.36
6	H	501	G2P	C2-N3-C4	5.15	121.24	115.36
6	G	501	G2P	C2-N3-C4	5.11	121.20	115.36
6	D	501	G2P	C2-N3-C4	5.08	121.16	115.36
6	I	501	G2P	C2-N3-C4	5.06	121.14	115.36

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O1A

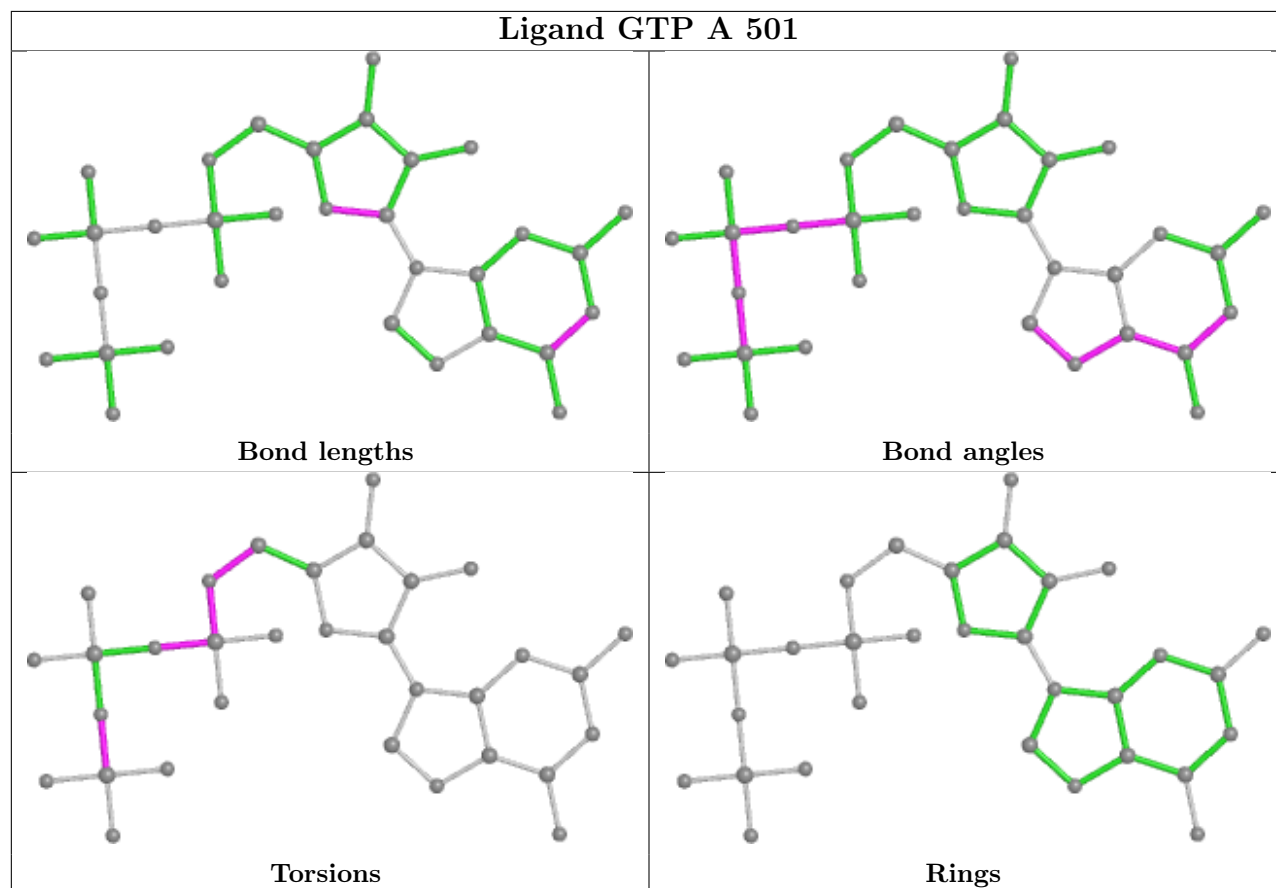
There are no ring outliers.

6 monomers are involved in 6 short contacts:

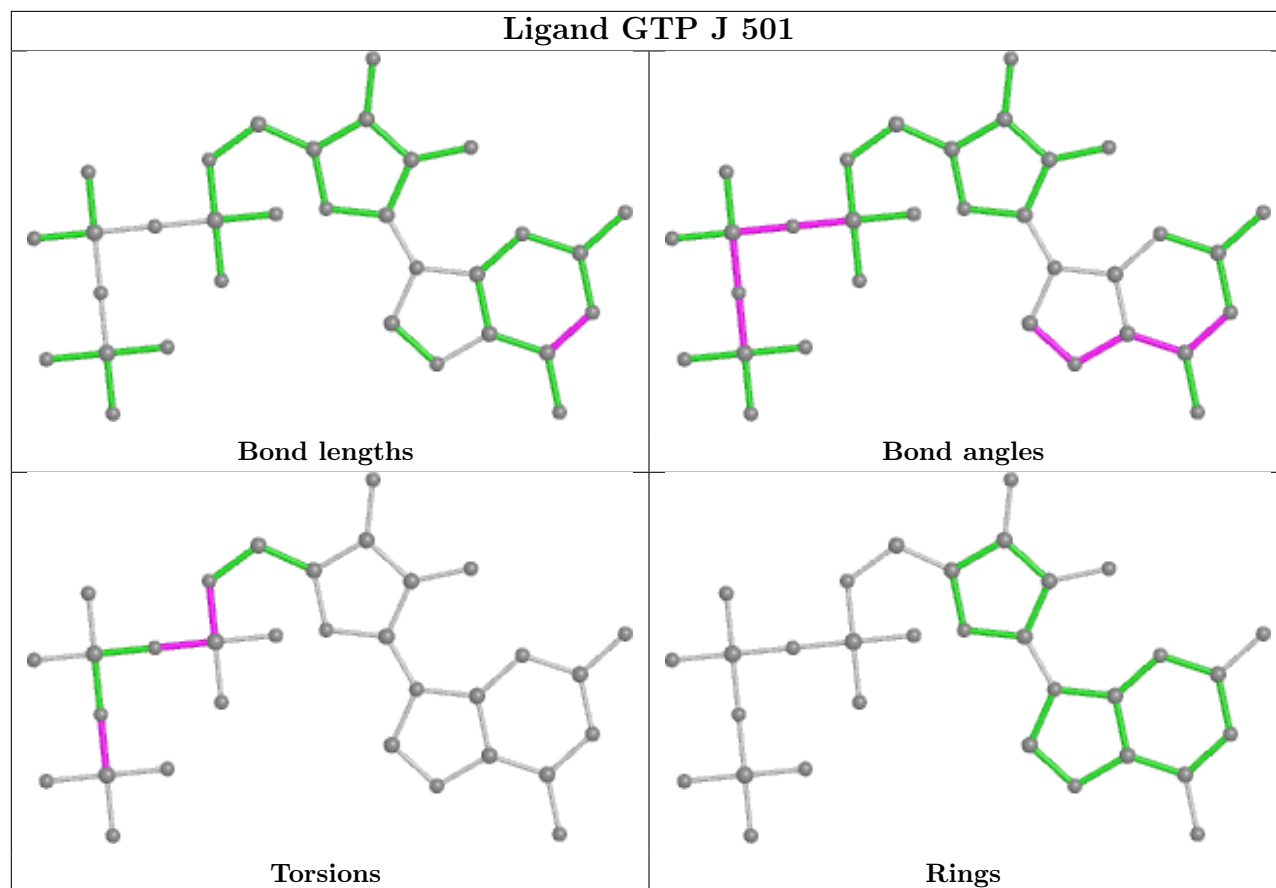
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	501	G2P	1	0
6	F	501	G2P	1	0
6	D	501	G2P	1	0
6	B	501	G2P	1	0
6	G	501	G2P	1	0
6	I	501	G2P	1	0

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

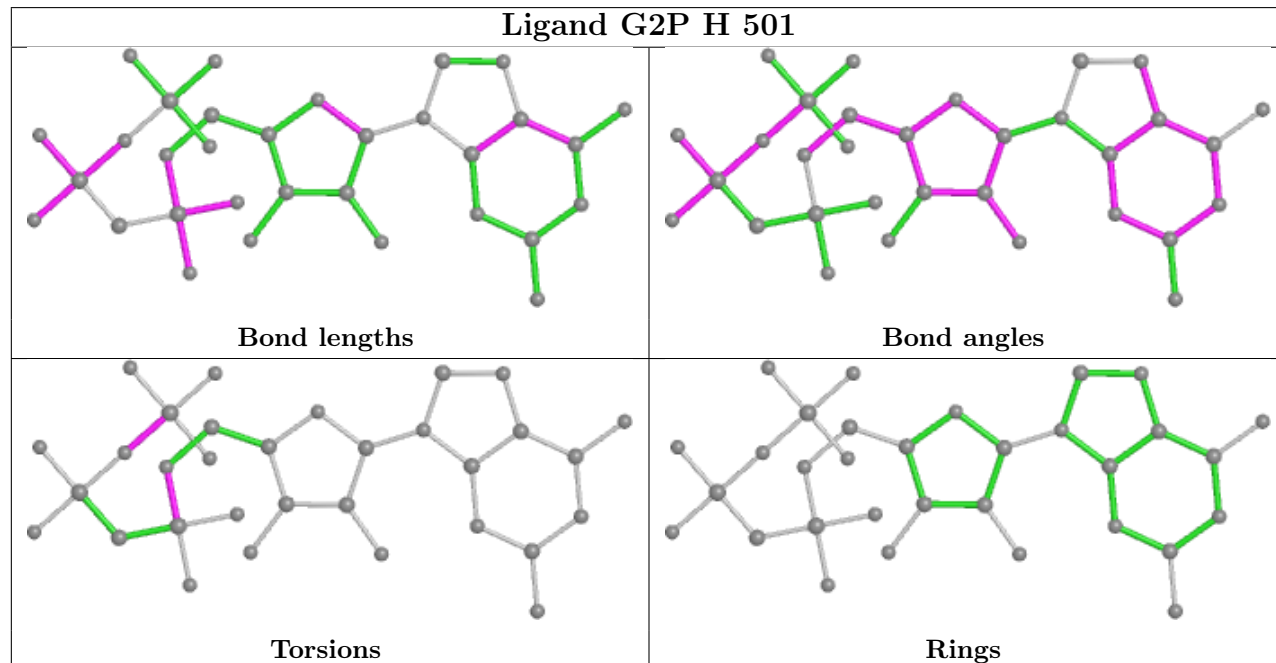
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



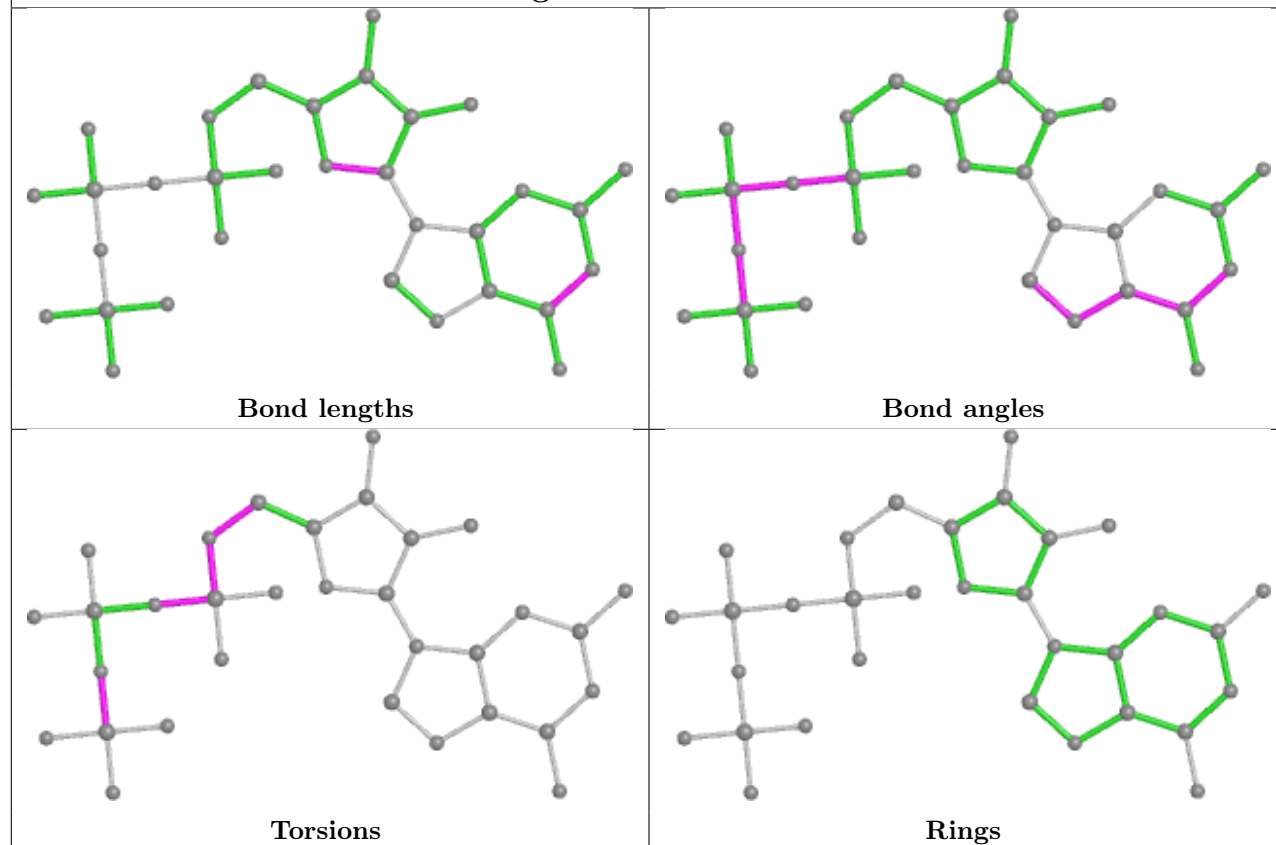
## Ligand GTP J 501



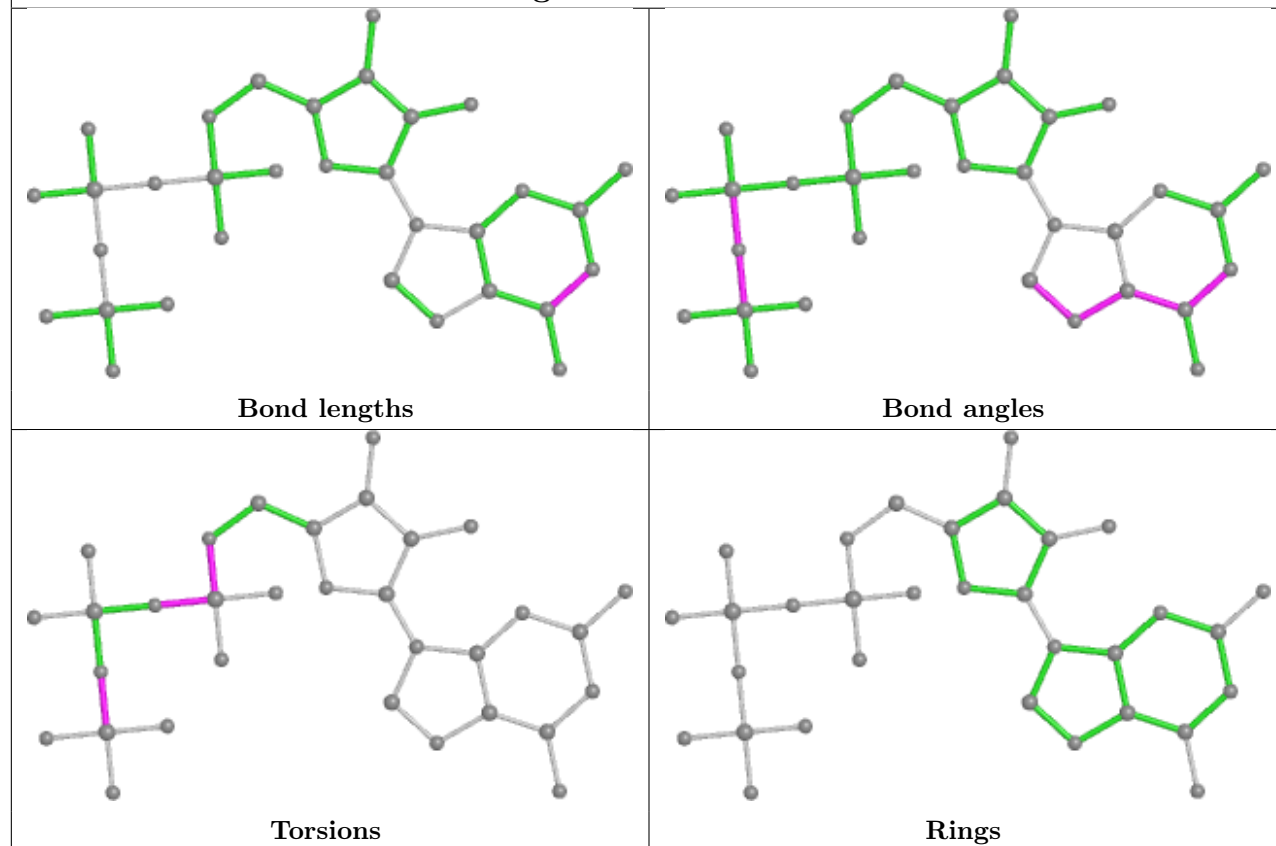
## Ligand G2P H 501

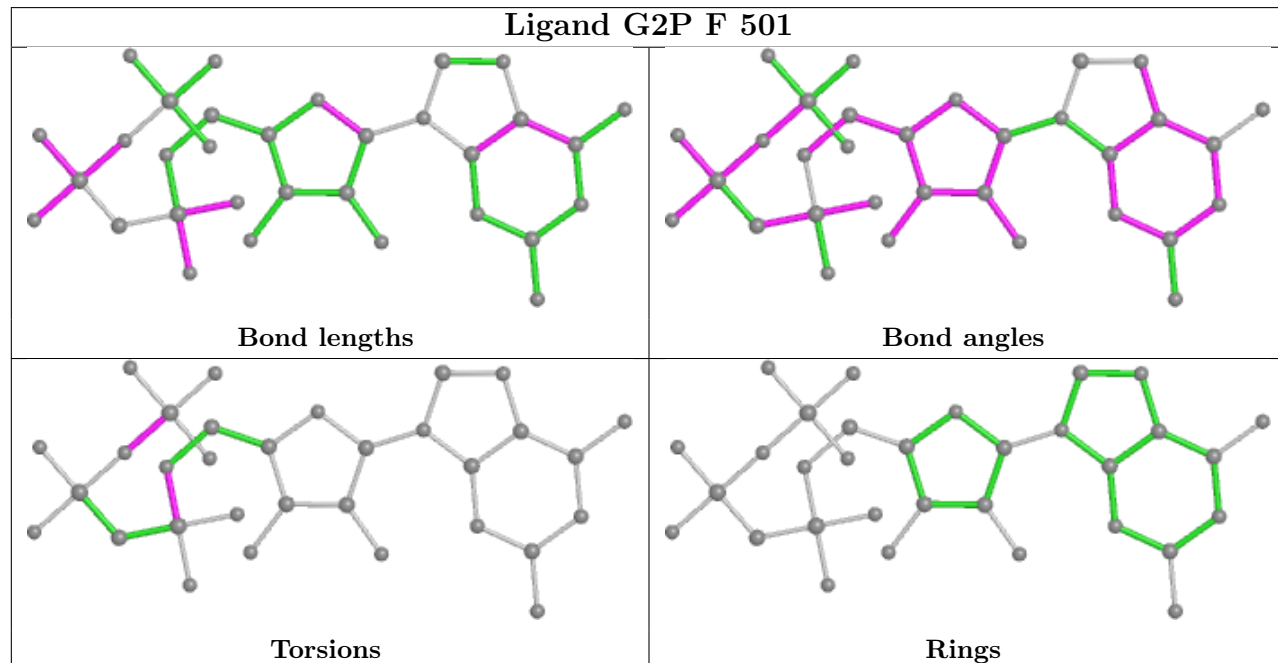
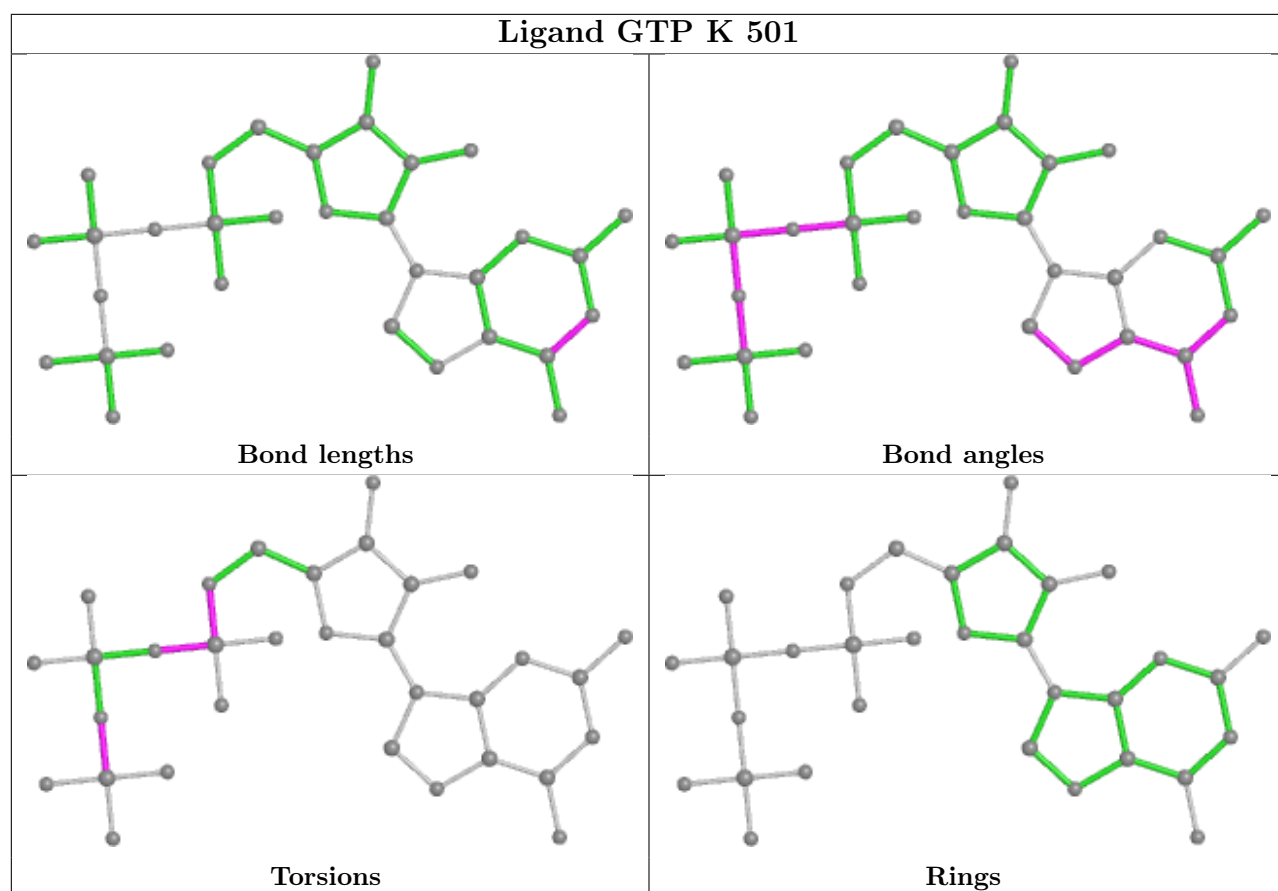


## Ligand GTP E 501

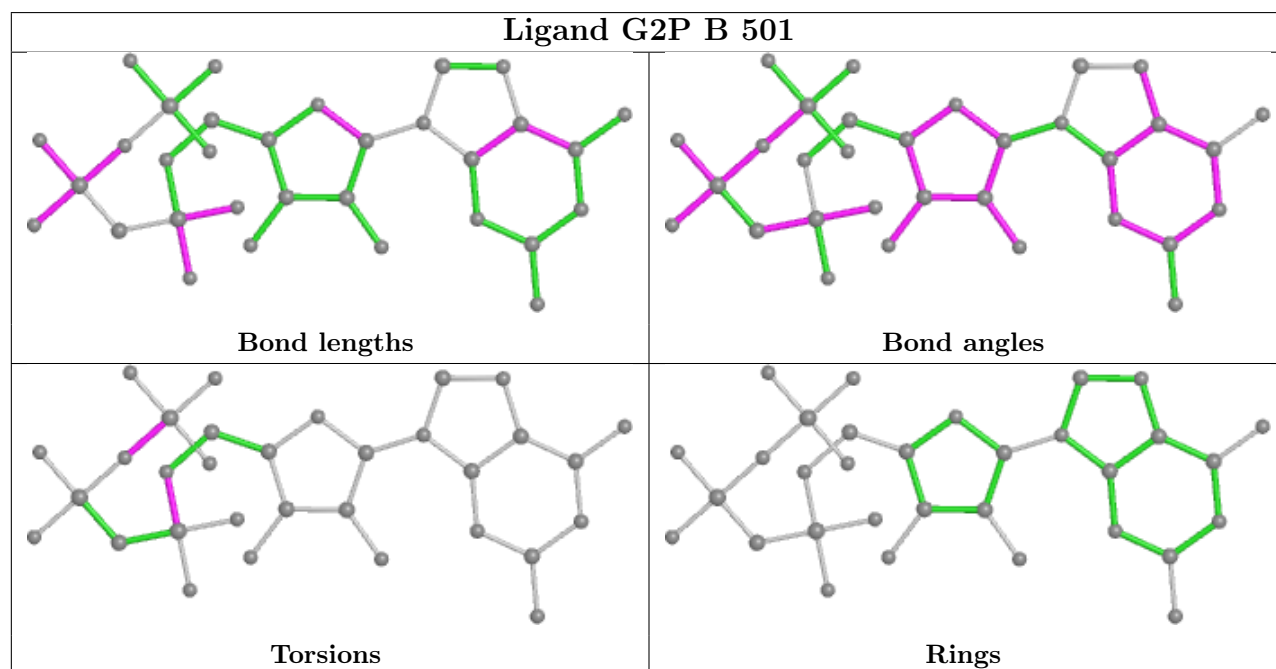
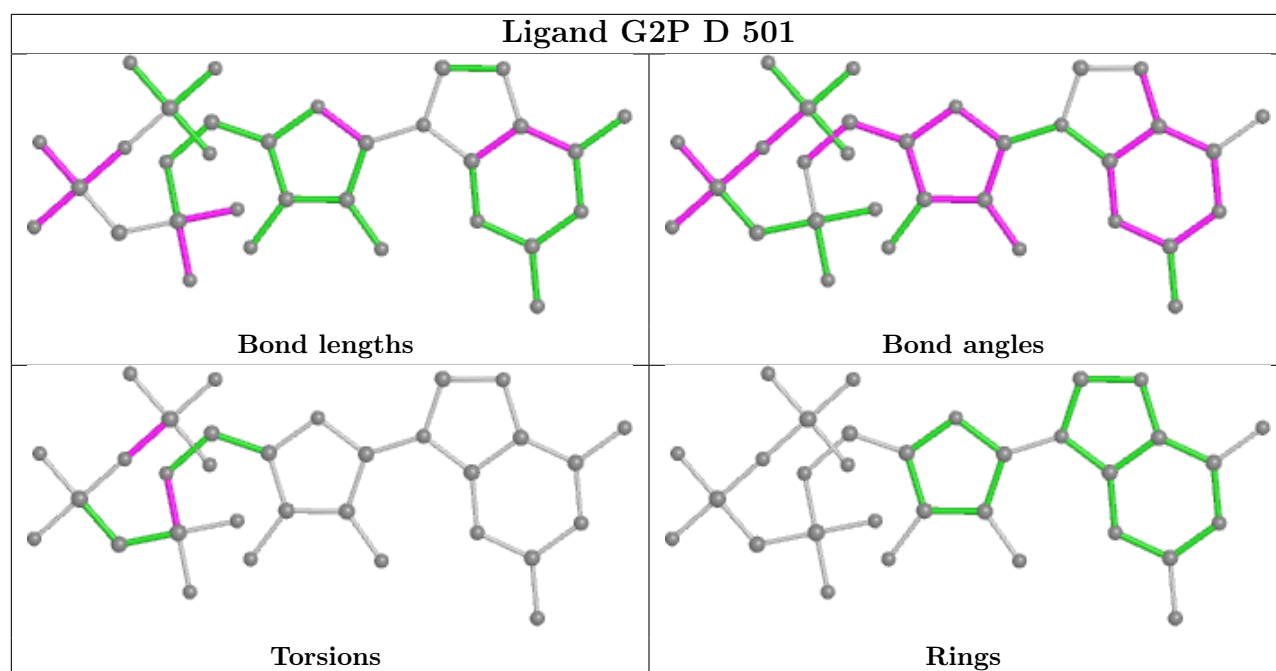


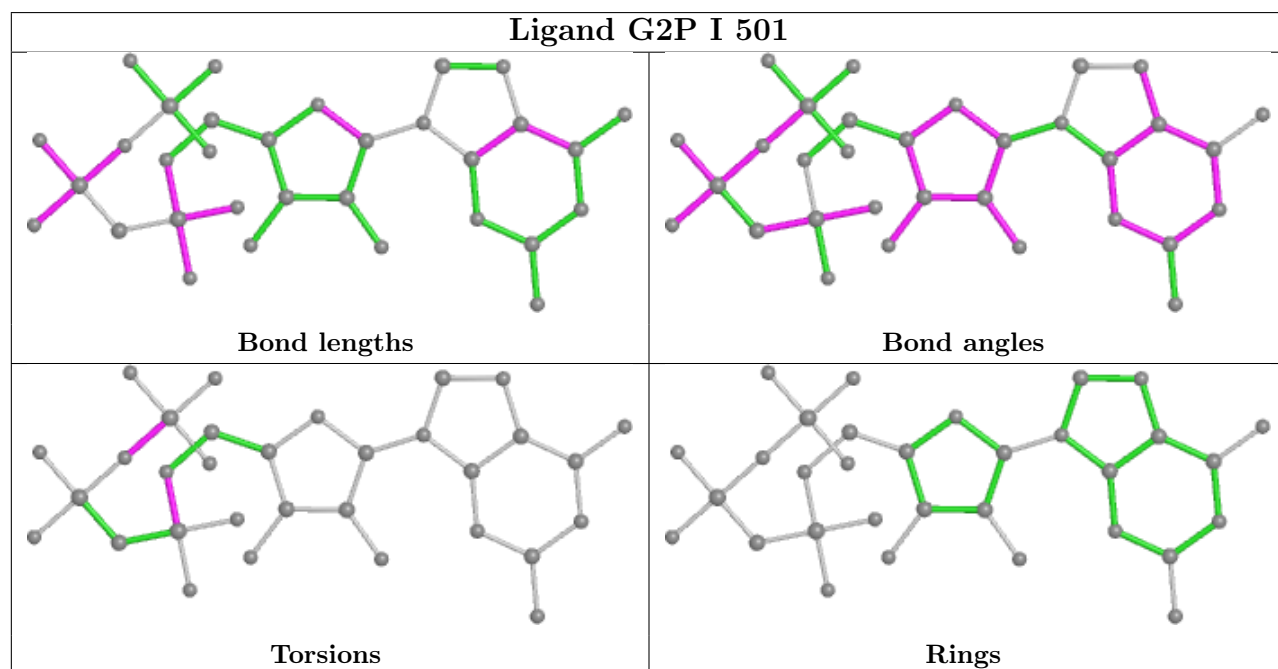
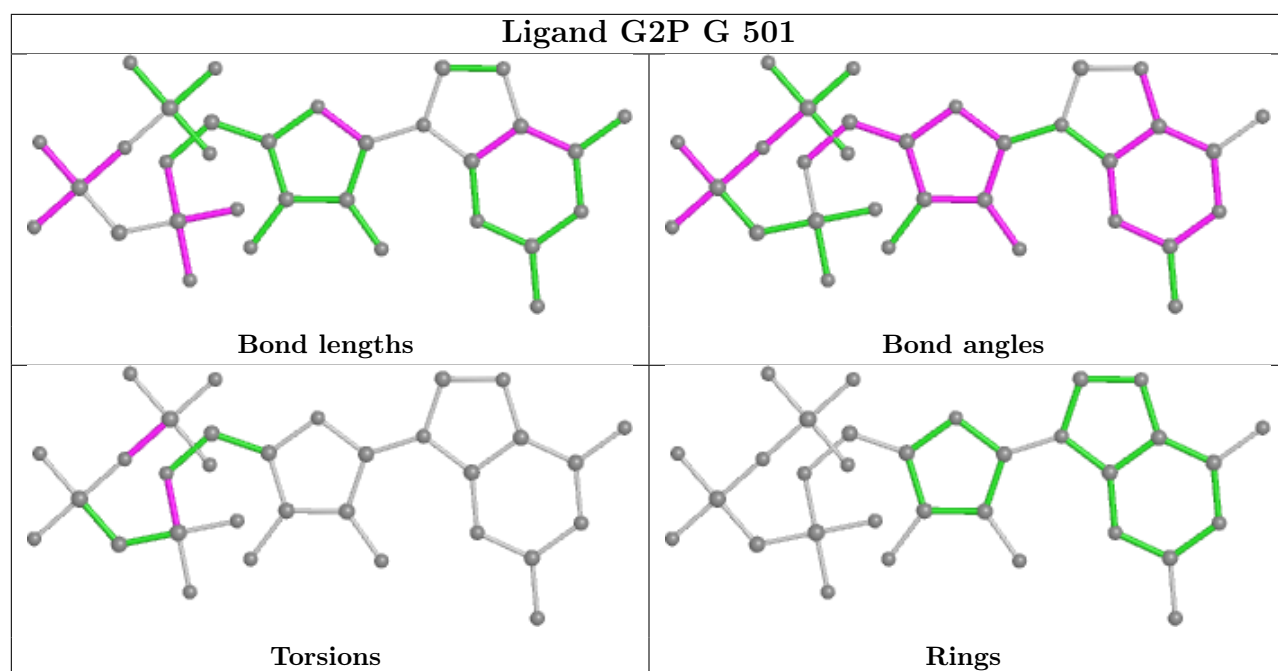
## Ligand GTP L 501

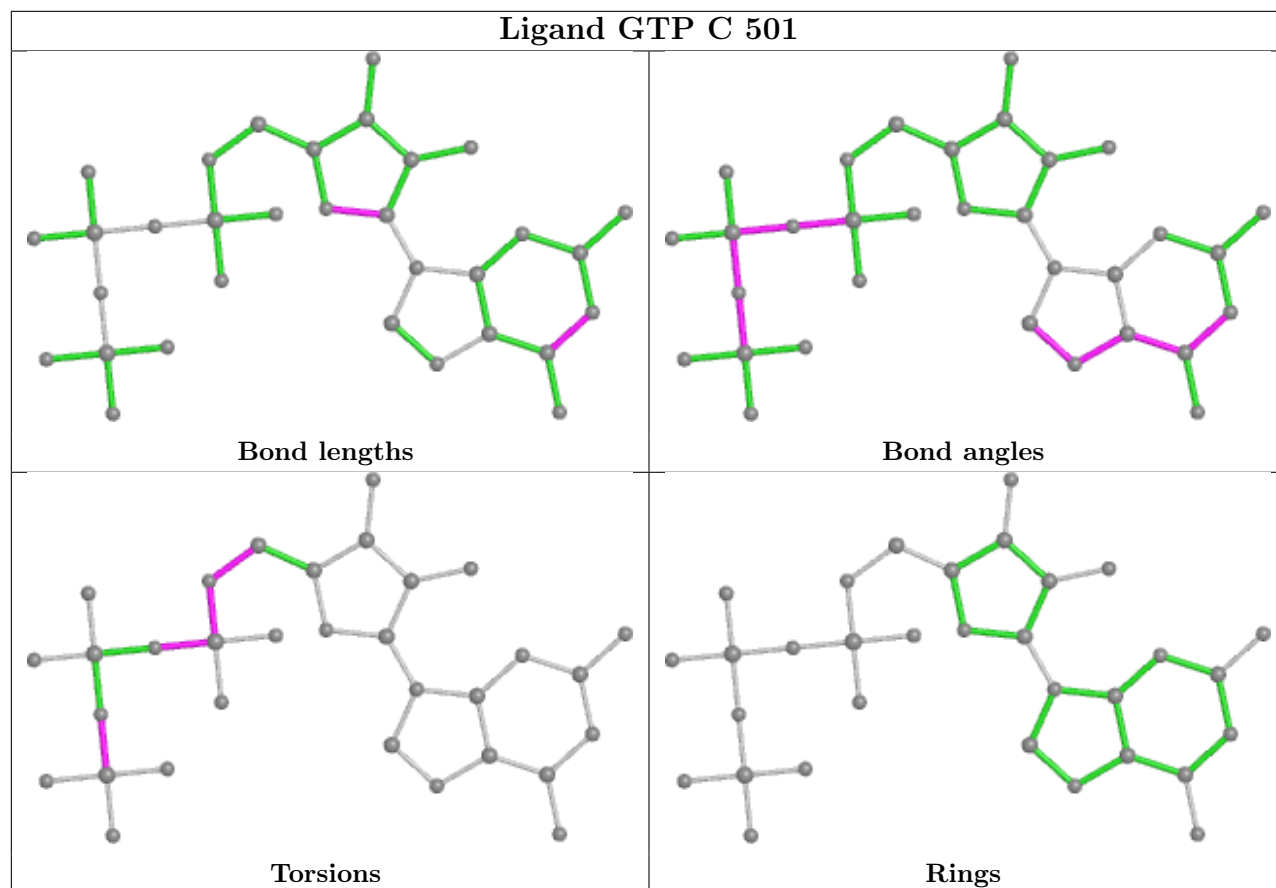












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

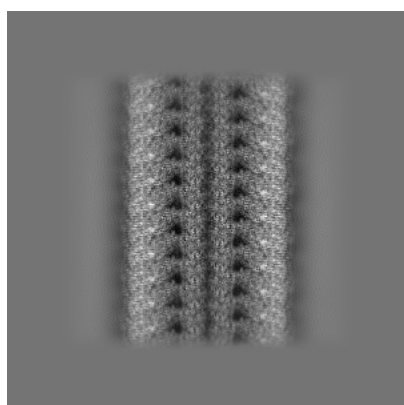
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7101. These allow visual inspection of the internal detail of the map and identification of artifacts.

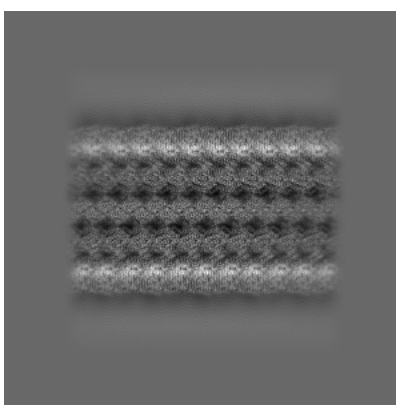
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

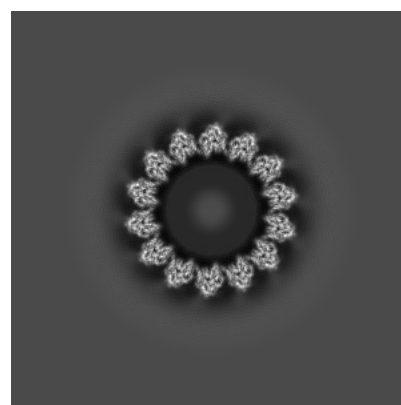
#### 6.1.1 Primary map



X



Y

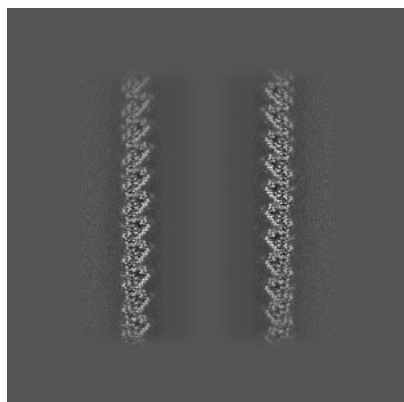


Z

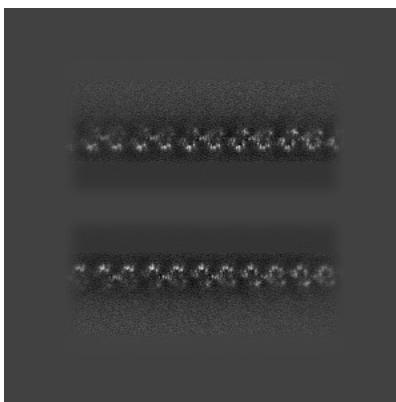
The images above show the map projected in three orthogonal directions.

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

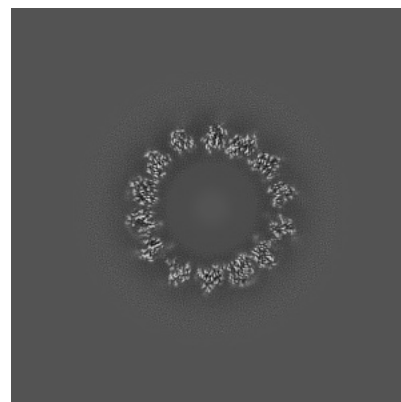
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

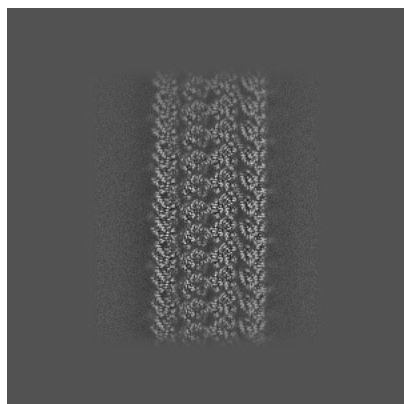


Z Index: 256

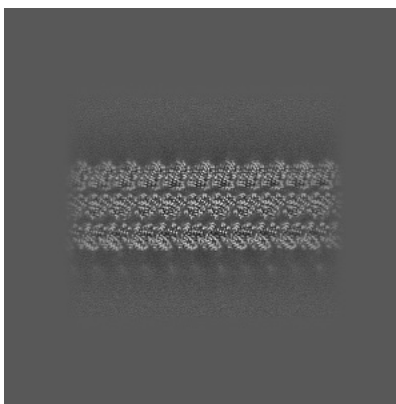
The images above show central slices of the map in three orthogonal directions.

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

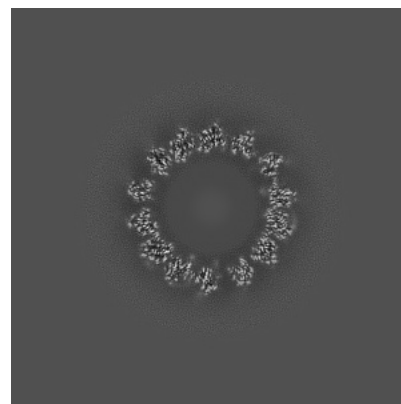
### 6.3.1 Primary map



X Index: 177



Y Index: 339

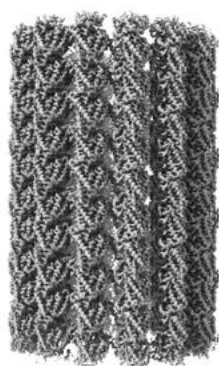


Z Index: 243

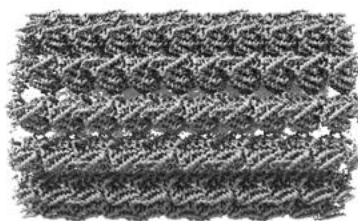
The images above show the largest variance slices of the map in three orthogonal directions.

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

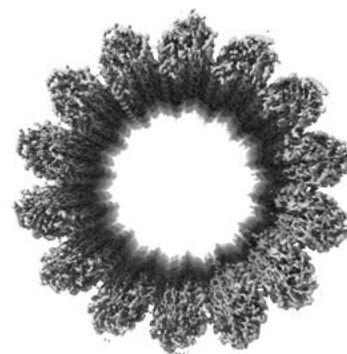
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

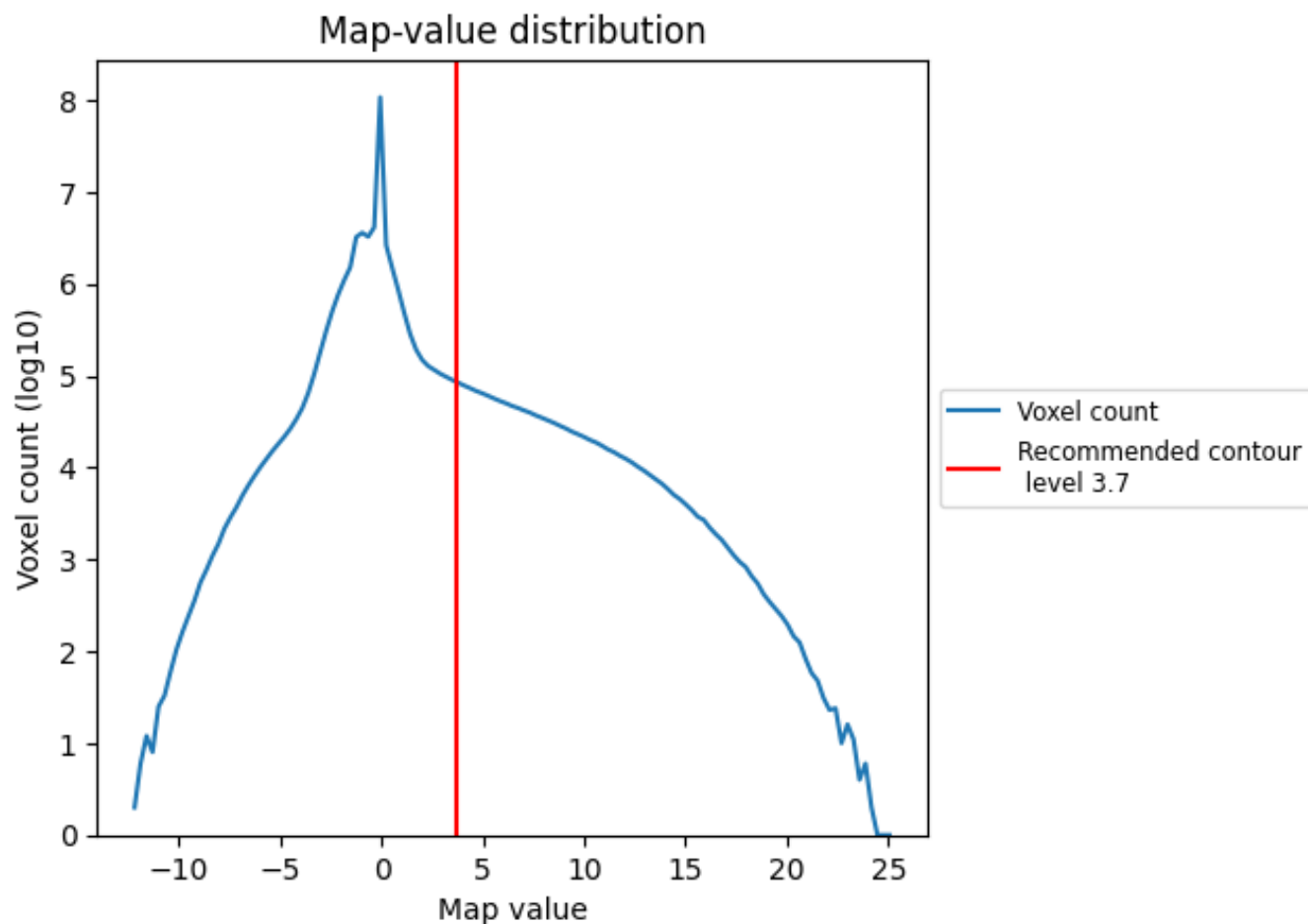
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

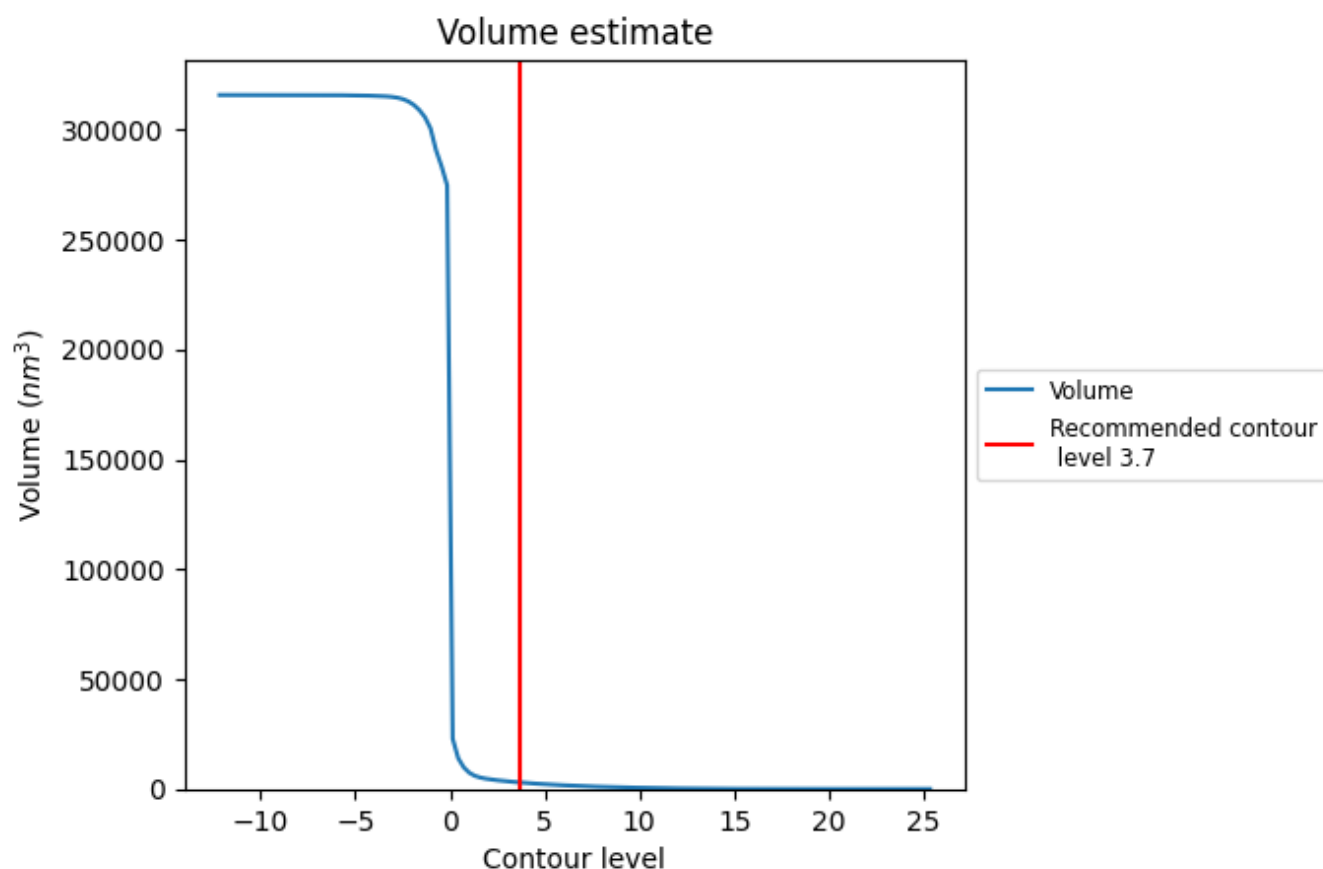
This section contains the results of statistical analysis of the map.

### 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](#)

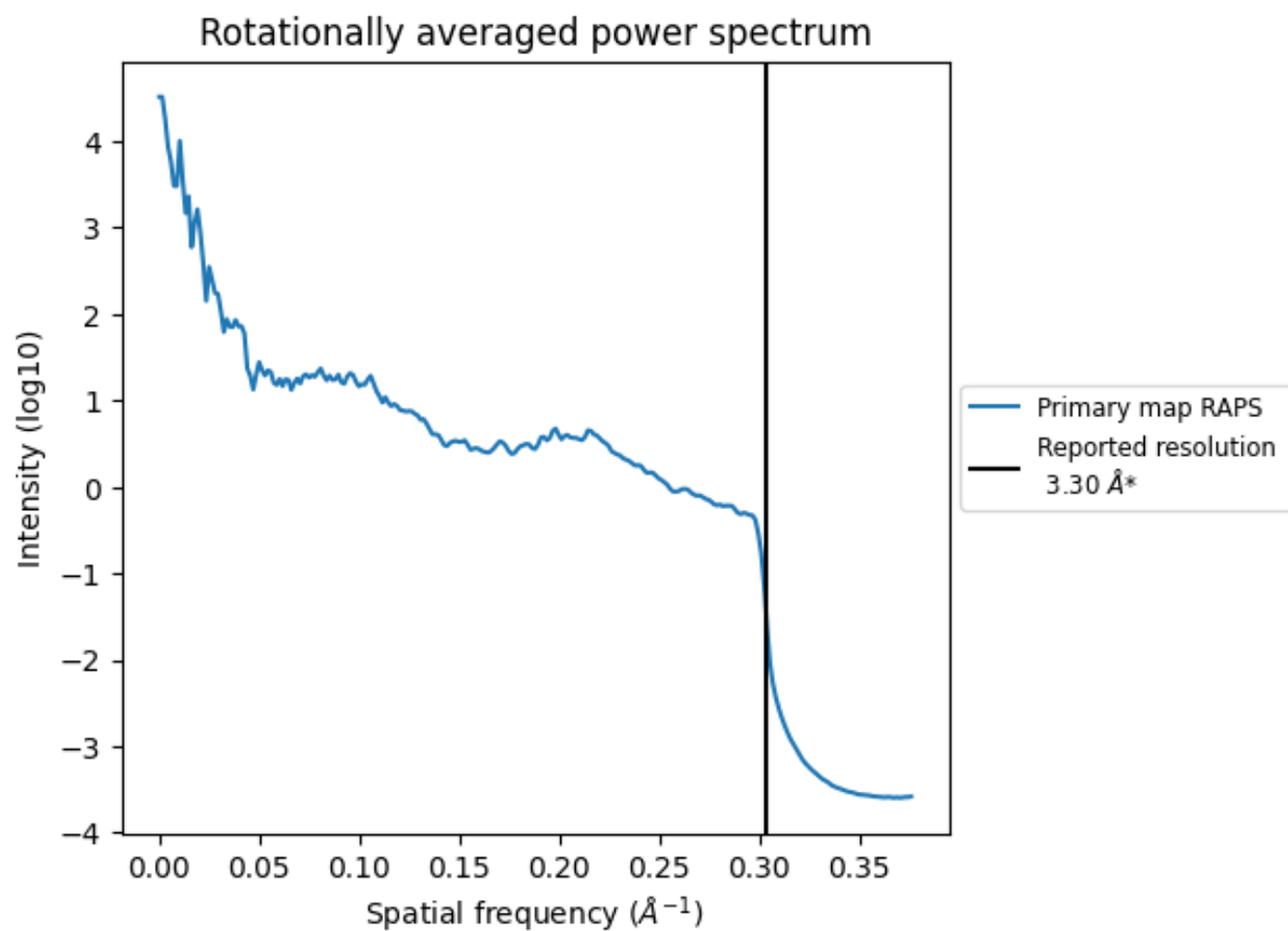


The volume at the recommended contour level is 2949 nm<sup>3</sup>; this corresponds to an approximate mass of 2664 kDa.

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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

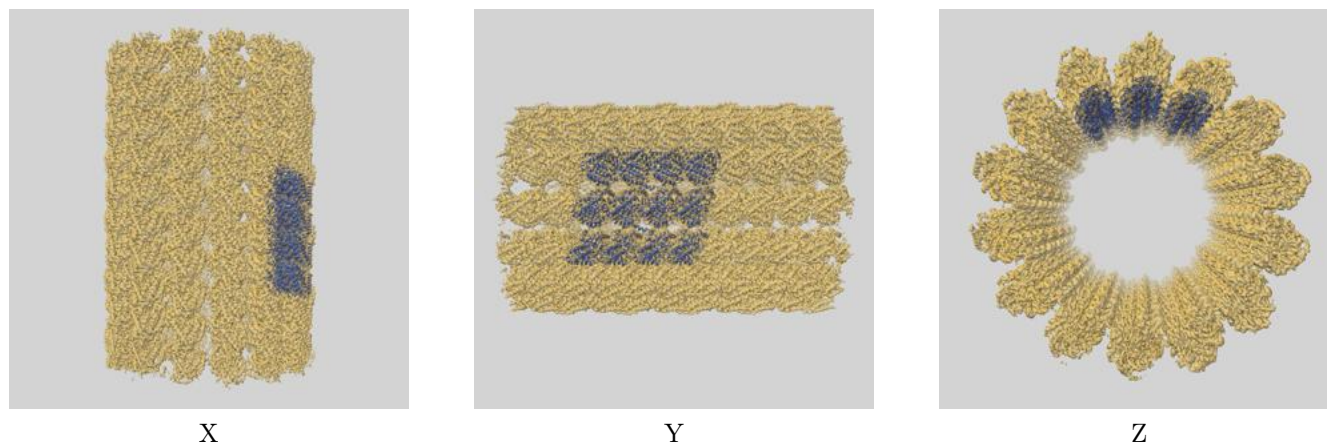
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

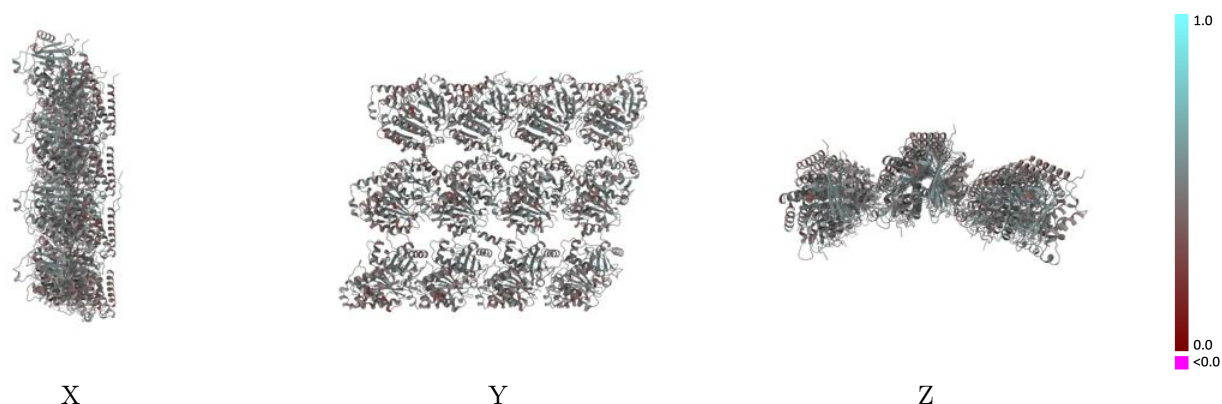
This section contains information regarding the fit between EMDB map EMD-7101 and PDB model 6BJC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

### 9.1 Map-model overlay [i](#)



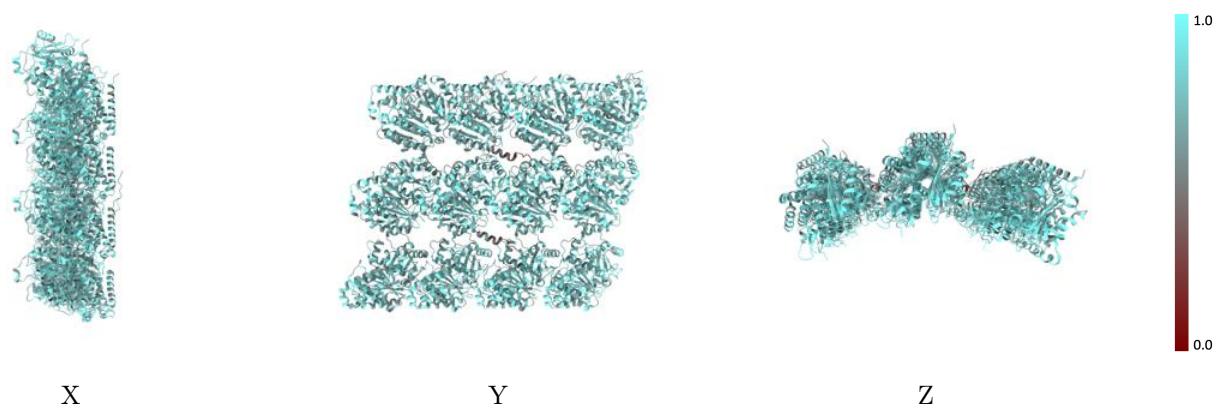
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



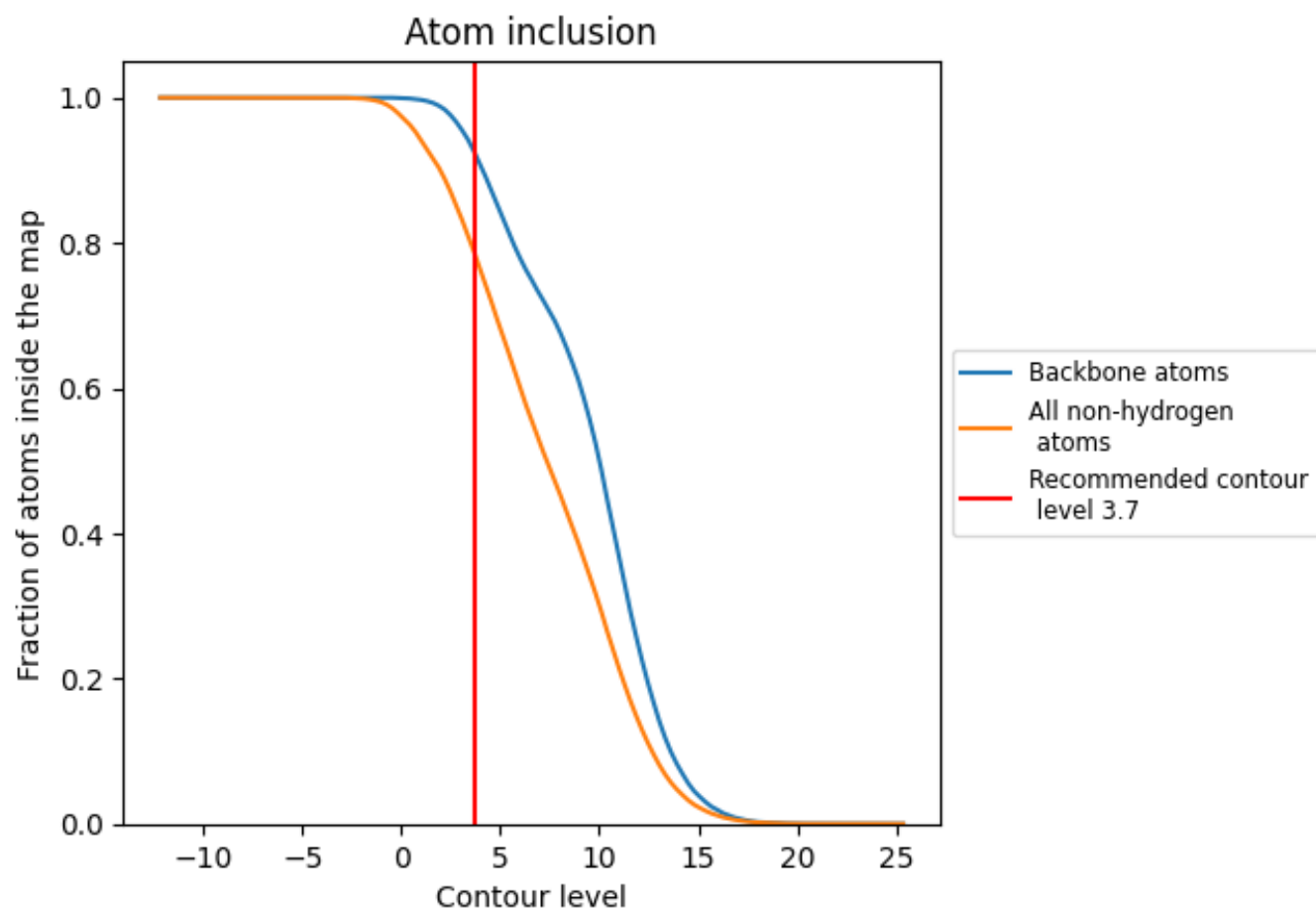
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.7).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7859	 0.4740
A	 0.7973	 0.4790
B	 0.8023	 0.4790
C	 0.7907	 0.4770
D	 0.7963	 0.4730
E	 0.7946	 0.4780
F	 0.7948	 0.4740
G	 0.7566	 0.4620
H	 0.7599	 0.4650
I	 0.7551	 0.4620
J	 0.8063	 0.4760
K	 0.8129	 0.4810
L	 0.8054	 0.4780
P	 0.4750	 0.4800
T	 0.5125	 0.4940

