



## wwPDB EM Validation Summary Report ⓘ

Mar 15, 2025 – 06:33 am GMT

PDB ID : 9I8G  
EMDB ID : EMD-52718  
Title : Inwards conformation' of the human gamma-TuRC from purified centrosomes obtained by rigid body docking  
Authors : Hofer, F.W.; Pfeffer, S.  
Deposited on : 2025-02-04  
Resolution : 22.40 Å(reported)  
Based on initial model : 6V6S

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>.

---

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) : 2.41

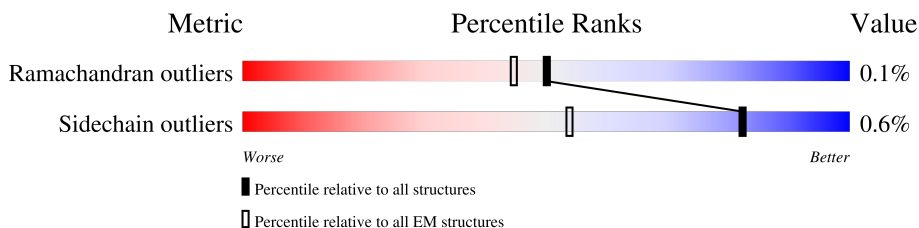
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 22.40 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.



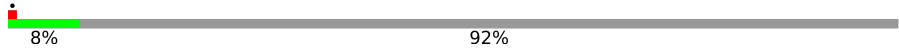


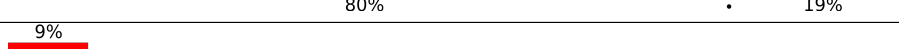

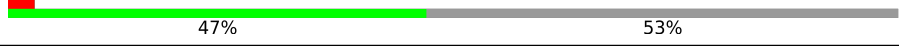

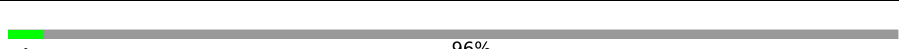

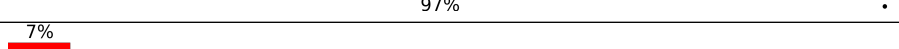



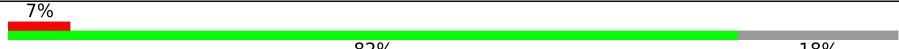

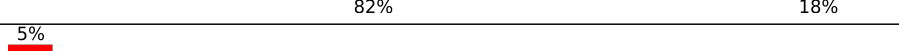



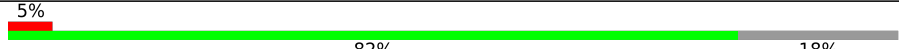

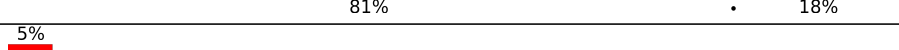

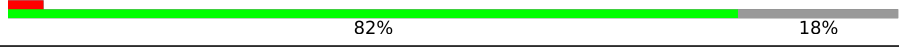
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\leq 5\%$ . 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	902	
1	C	902	
1	E	902	
1	G	902	
1	M	902	
2	B	907	
2	D	907	
2	F	907	
2	H	907	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	R	907	
2	T	907	
3	I	667	
3	K	667	
4	J	1024	
5	L	1819	
5	P	1819	
6	U	376	
7	Q	82	
7	S	82	
8	a	451	
8	b	451	
8	c	451	
8	d	451	
8	e	451	
8	f	451	
8	g	451	
8	h	451	
8	i	451	
8	j	451	
8	k	451	
8	l	451	
8	m	451	
8	t	451	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 104073 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 Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	C	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	E	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	G	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	M	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		

- Molecule 2 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	D	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	F	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	H	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	T	572	Total	C	N	O		0	0
			2840	1696	572	572			
2	R	76	Total	C	N	O		0	0
			379	227	76	76			

- Molecule 3 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	543	Total	C	N	O	S	2	0
			4376	2844	734	780	18		
3	K	543	Total	C	N	O	S	2	0
			4376	2844	734	780	18		

- Molecule 4 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	484	Total	C	N	O	S	0	0
			3977	2603	656	695	23		

- Molecule 5 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	497	Total	C	N	O	S	0	0
			4007	2630	667	690	20		
5	P	77	Total	C	N	O		0	0
			382	228	77	77			

- Molecule 6 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	U	364	Total	C	N	O	0	0
			1795	1067	364	364		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	CYS	-	insertion	UNP P60709
U	3	GLU	ASP	conflict	UNP P60709
U	4	GLU	ASP	conflict	UNP P60709
U	5	VAL	ILE	conflict	UNP P60709
U	153	LEU	MET	conflict	UNP P60709
U	160	SER	THR	conflict	UNP P60709
U	204	GLU	ALA	conflict	UNP P60709
U	243	LYS	PRO	conflict	UNP P60709
U	271	ALA	SER	conflict	UNP P60709
U	279	TYR	PHE	conflict	UNP P60709

- Molecule 7 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	44	Total	C	N	O	0	0
			220	132	44	44		
7	S	57	Total	C	N	O	0	0
			284	170	57	57		

- Molecule 8 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	b	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	c	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	d	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	e	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	f	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	g	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	h	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	i	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	j	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	k	370	Total	C	N	O	S	0	0
			2954	1874	518	548	14		
8	l	370	Total	C	N	O	S	0	0
			2954	1874	518	548	14		
8	m	369	Total	C	N	O	S	0	0
			2950	1872	517	547	14		
8	t	370	Total	C	N	O		0	0
			1829	1089	370	370			

There are 14 discrepancies between the modelled and reference sequences:

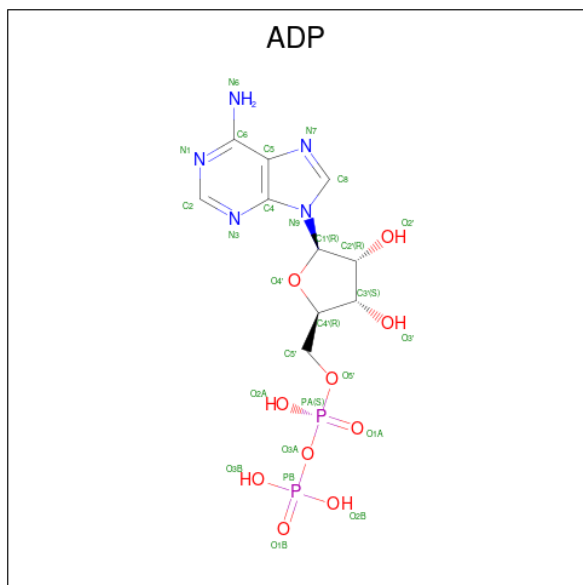
Chain	Residue	Modelled	Actual	Comment	Reference
a	202	LEU	VAL	conflict	UNP P23258
b	202	LEU	VAL	conflict	UNP P23258
c	202	LEU	VAL	conflict	UNP P23258
d	202	LEU	VAL	conflict	UNP P23258
e	202	LEU	VAL	conflict	UNP P23258
f	202	LEU	VAL	conflict	UNP P23258
g	202	LEU	VAL	conflict	UNP P23258
h	202	LEU	VAL	conflict	UNP P23258
i	202	LEU	VAL	conflict	UNP P23258
j	202	LEU	VAL	conflict	UNP P23258
k	202	LEU	VAL	conflict	UNP P23258
l	202	LEU	VAL	conflict	UNP P23258

*Continued on next page...*

*Continued from previous page...*

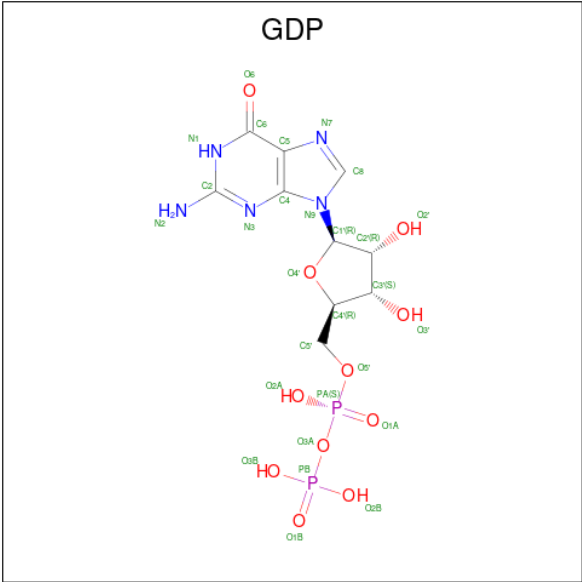
Chain	Residue	Modelled	Actual	Comment	Reference
m	202	LEU	VAL	conflict	UNP P23258
t	202	LEU	VAL	conflict	UNP P23258

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
9	U	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



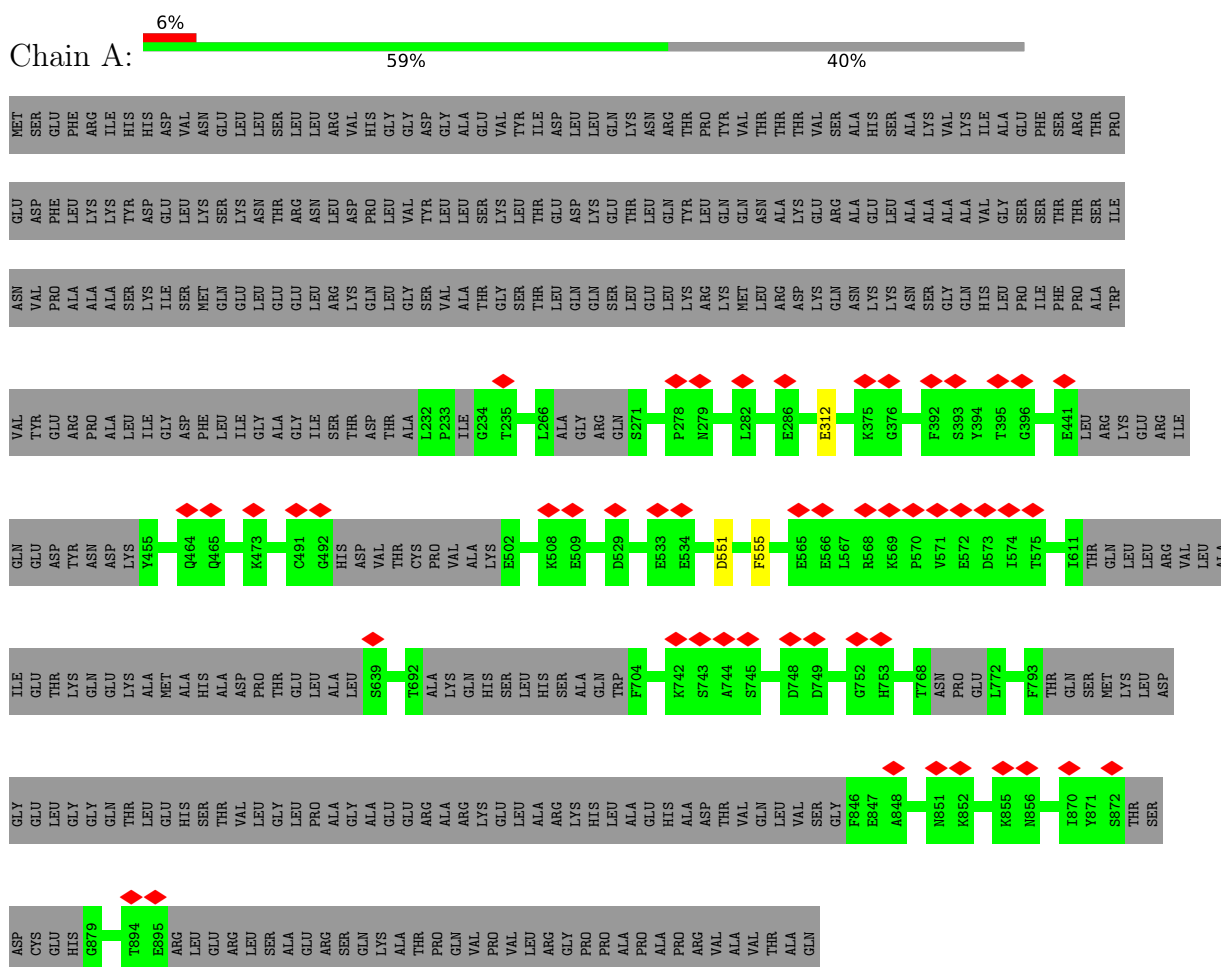
Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	c	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	d	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	e	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	f	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	g	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	h	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	j	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	k	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	l	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	m	1	Total	C	N	O	P	0
			28	10	5	11	2	
10	t	1	Total	C	N	O	P	0
			28	10	5	11	2	



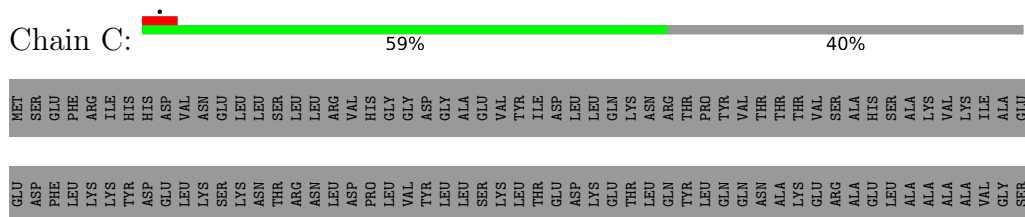
### 3 Residue-property plots

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 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.

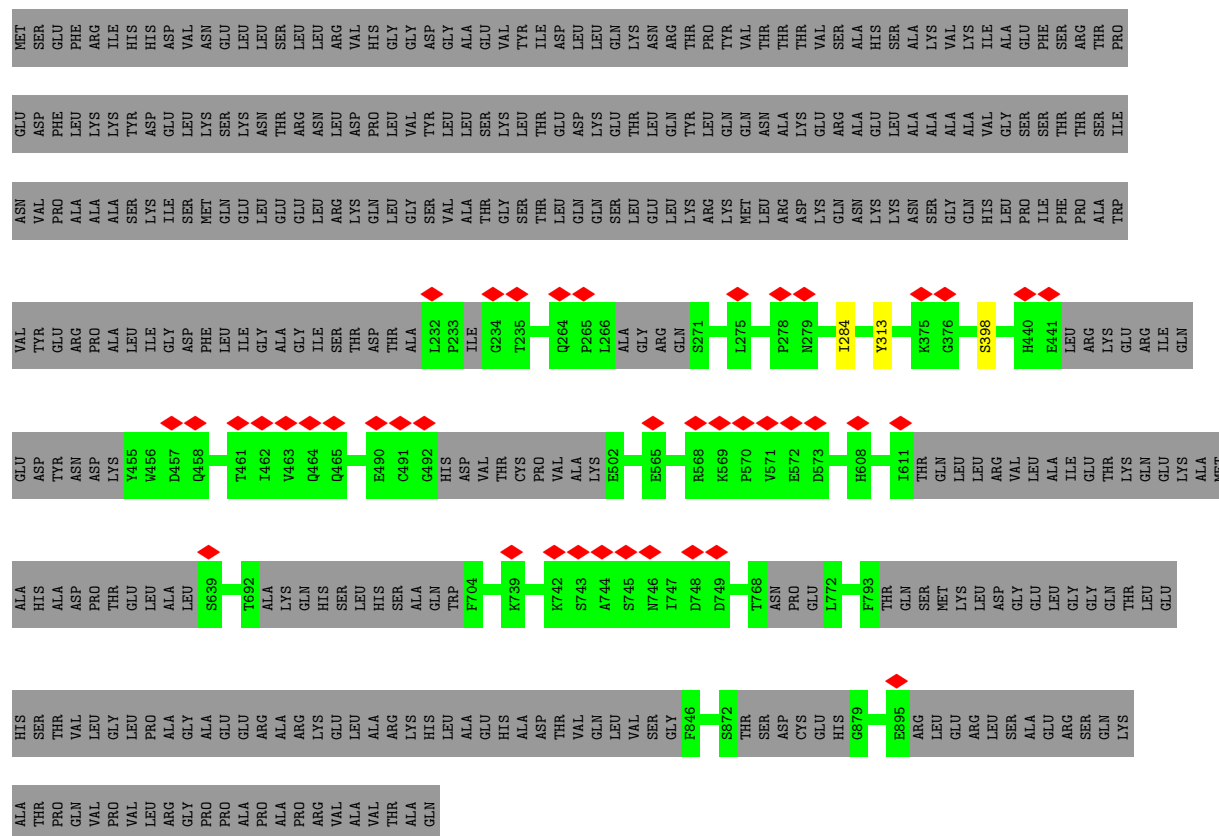
#### • Molecule 1: Gamma-tubulin complex component 2



#### • Molecule 1: Gamma-tubulin complex component 2

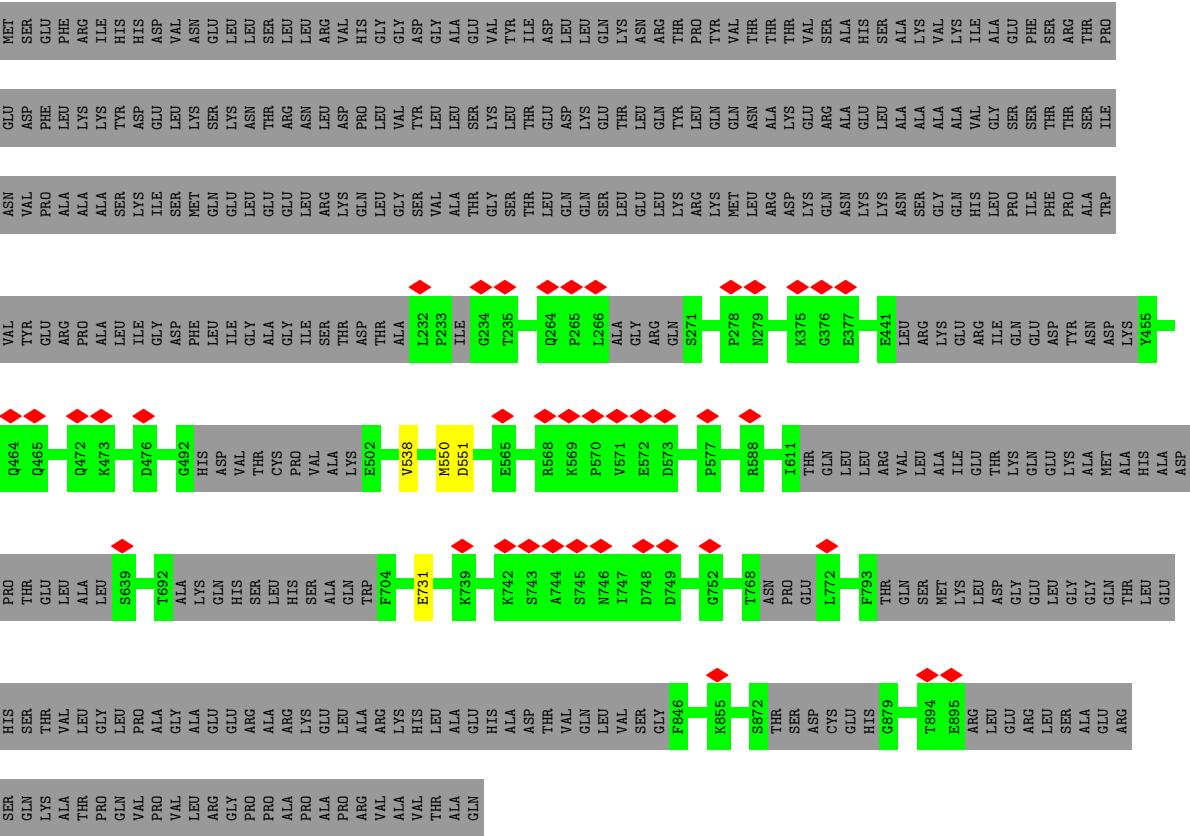


- Molecule 1: Gamma-tubulin complex component 2

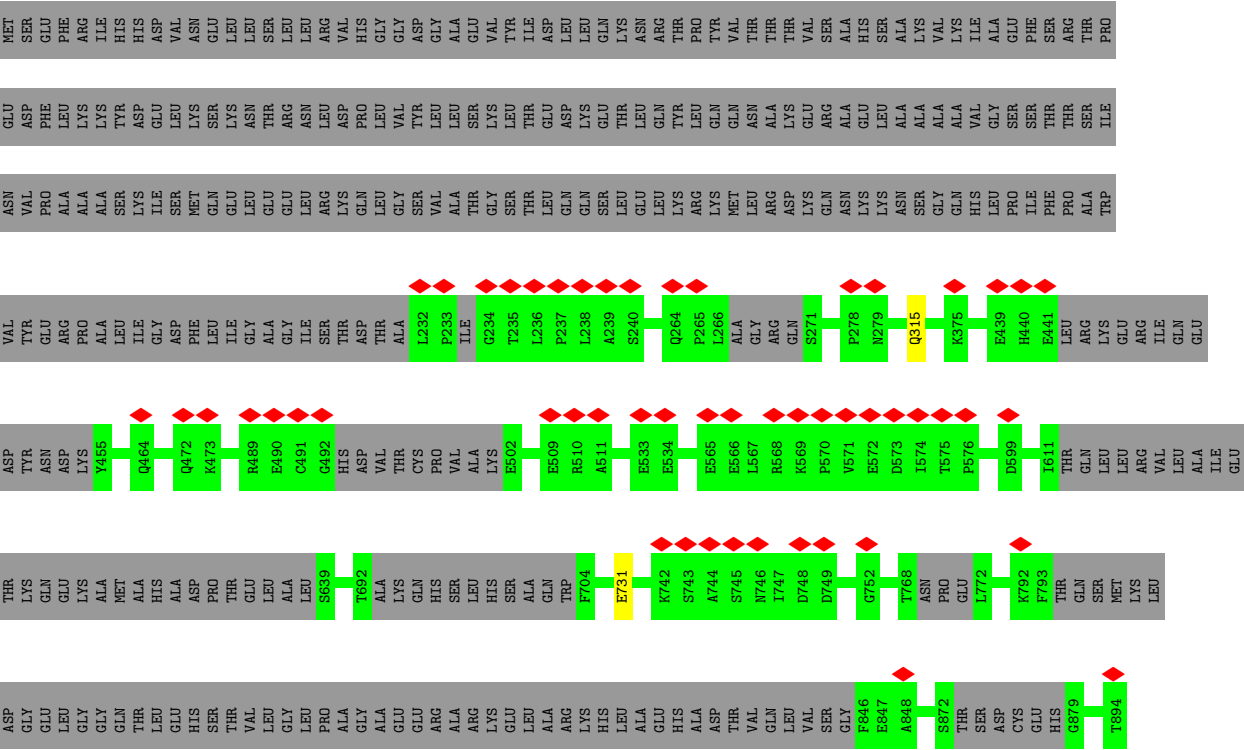


- Molecule 1: Gamma-tubulin complex component 2





• Molecule 1: Gamma-tubulin complex component 2







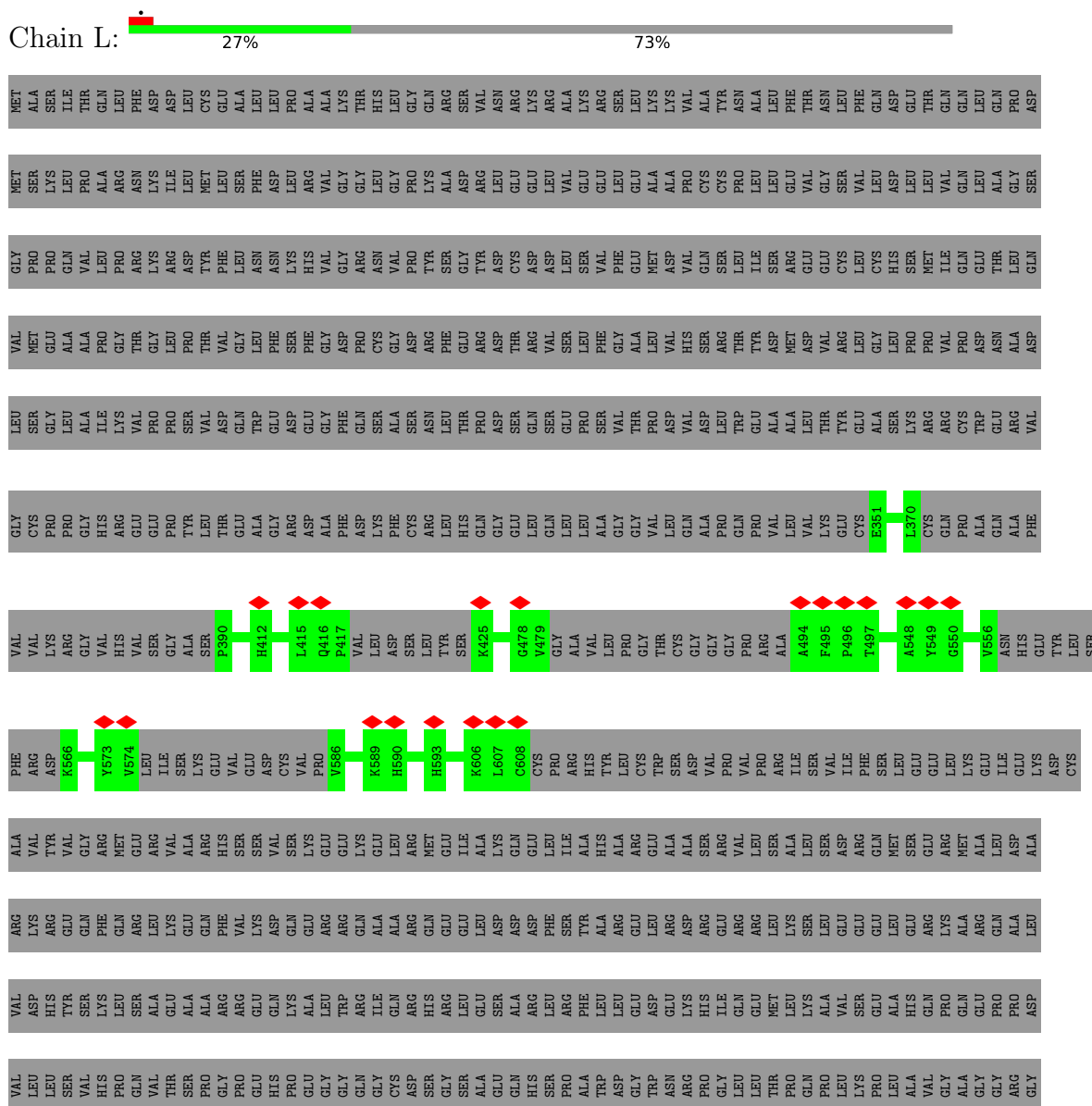








- Molecule 5: Gamma-tubulin complex component 6

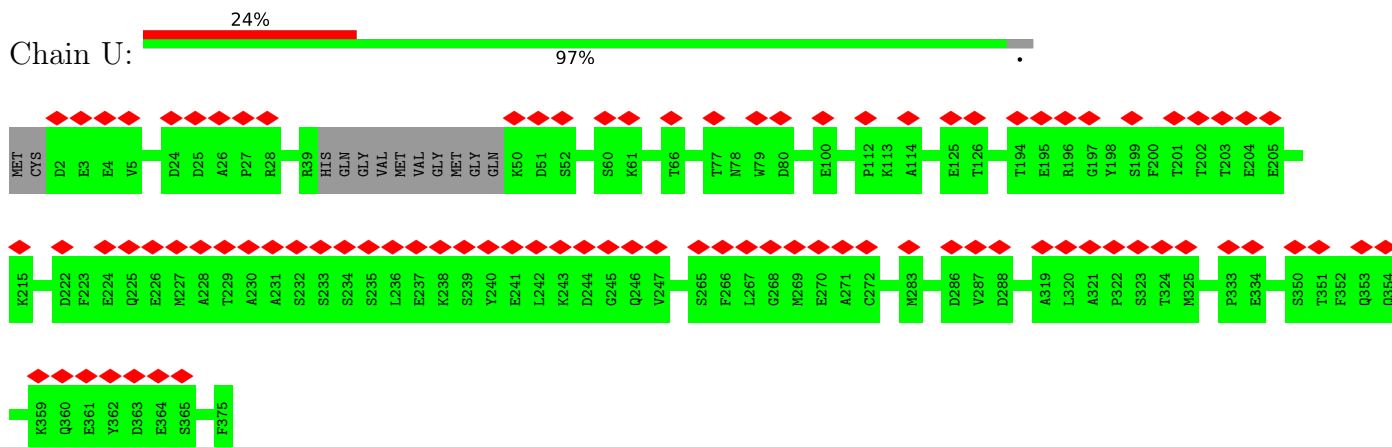




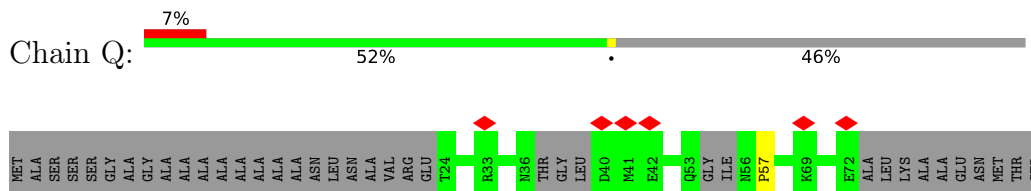


[illegible]

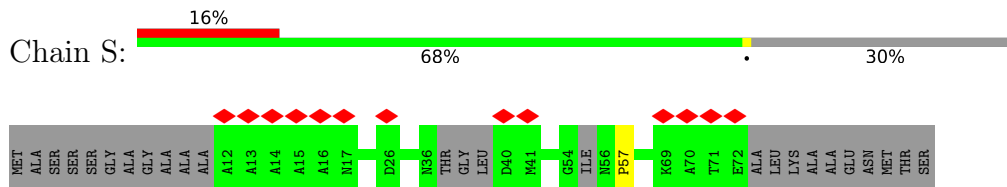
- Molecule 6: Actin, cytoplasmic 1



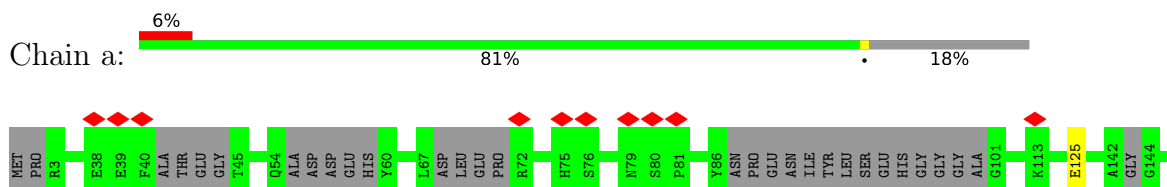
- Molecule 7: Mitotic-spindle organizing protein 1

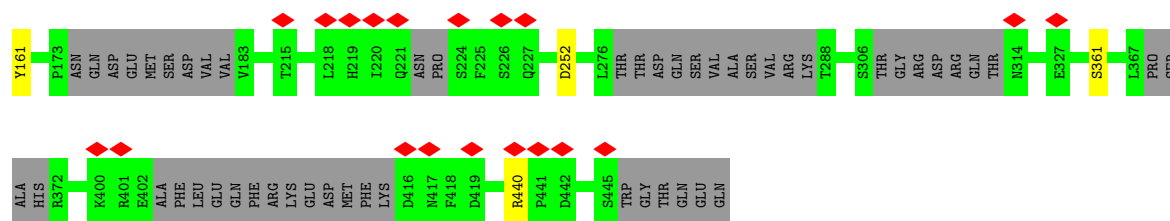


- Molecule 7: Mitotic-spindle organizing protein 1

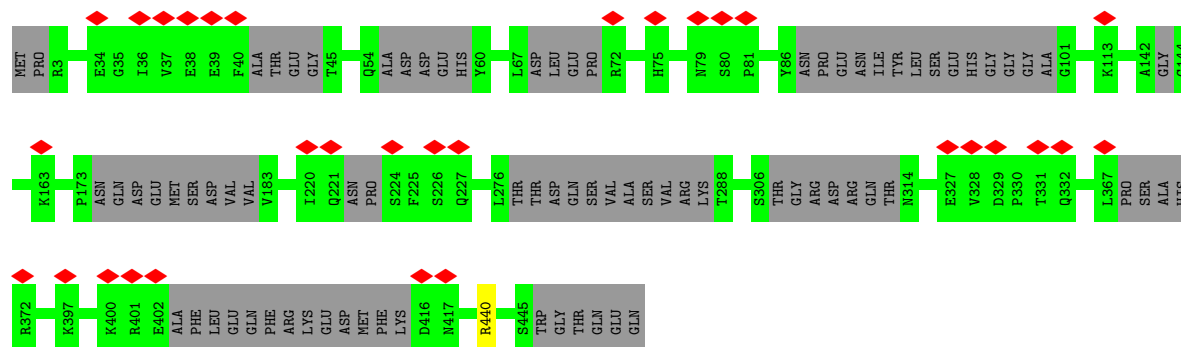
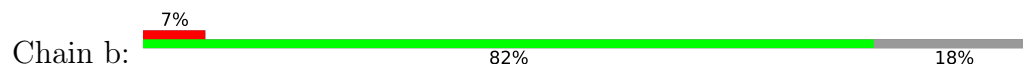


- Molecule 8: Tubulin gamma-1 chain

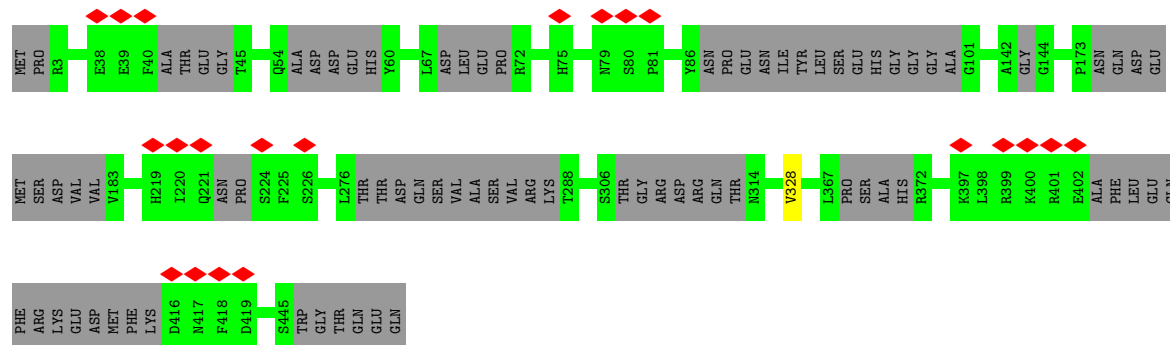
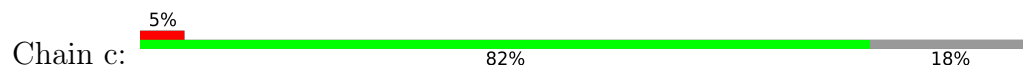




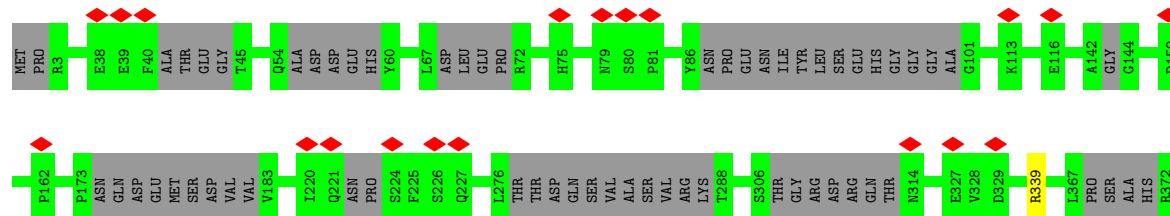
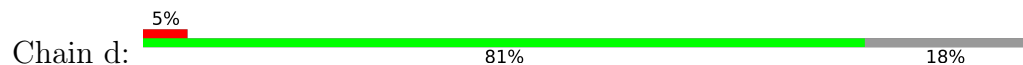
• Molecule 8: Tubulin gamma-1 chain

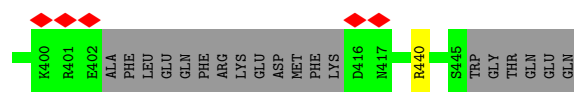


• Molecule 8: Tubulin gamma-1 chain



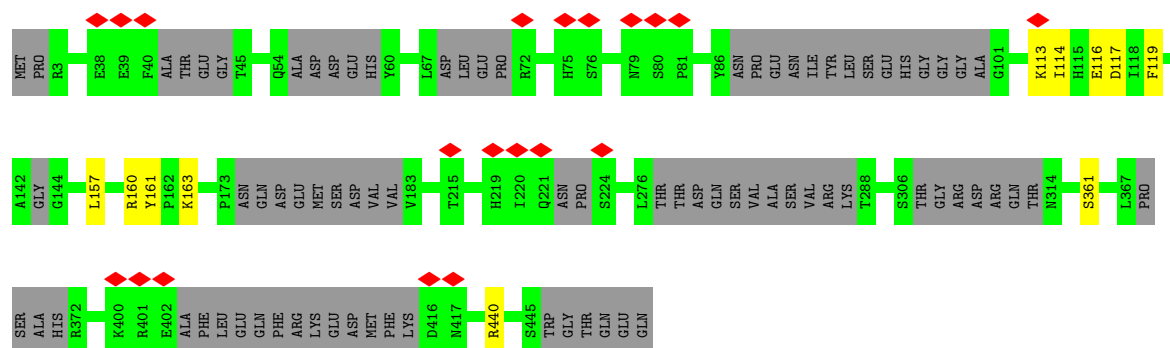
• Molecule 8: Tubulin gamma-1 chain





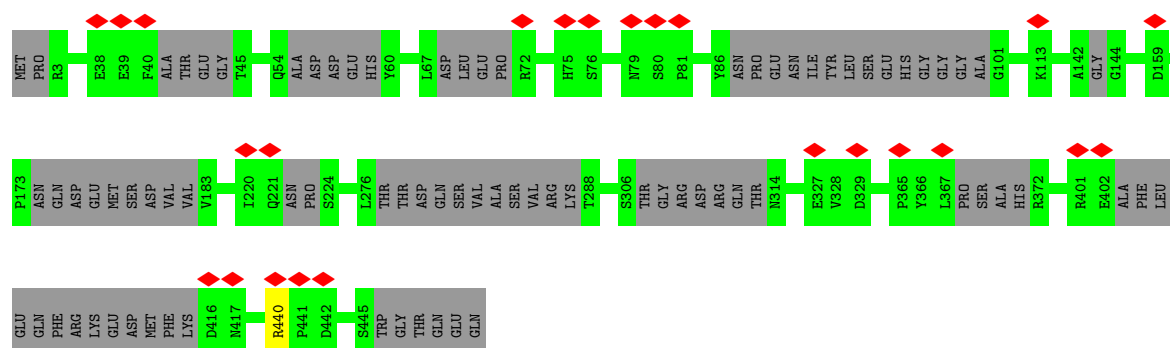
• Molecule 8: Tubulin gamma-1 chain

Chain e: 79% 18%



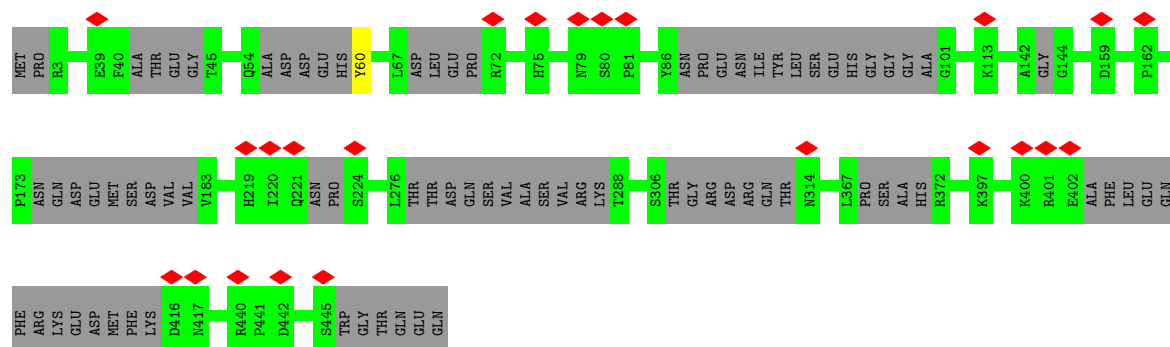
• Molecule 8: Tubulin gamma-1 chain

Chain f: 5% 82% 18%

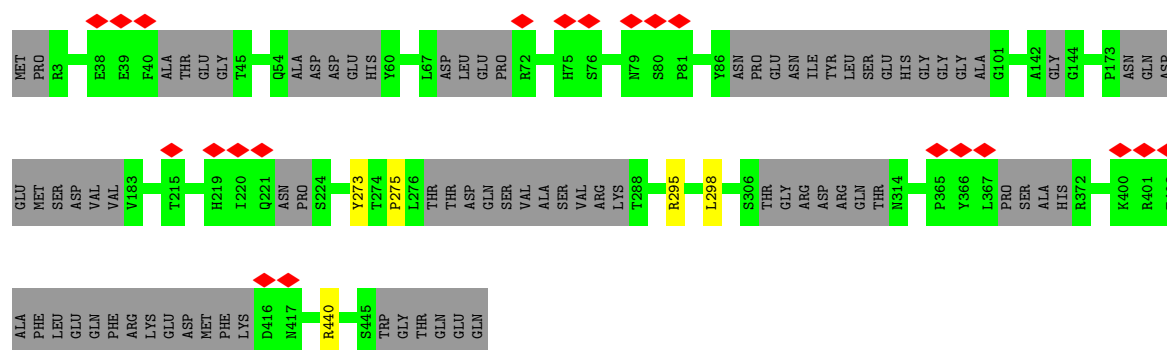
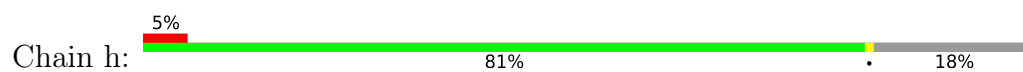


• Molecule 8: Tubulin gamma-1 chain

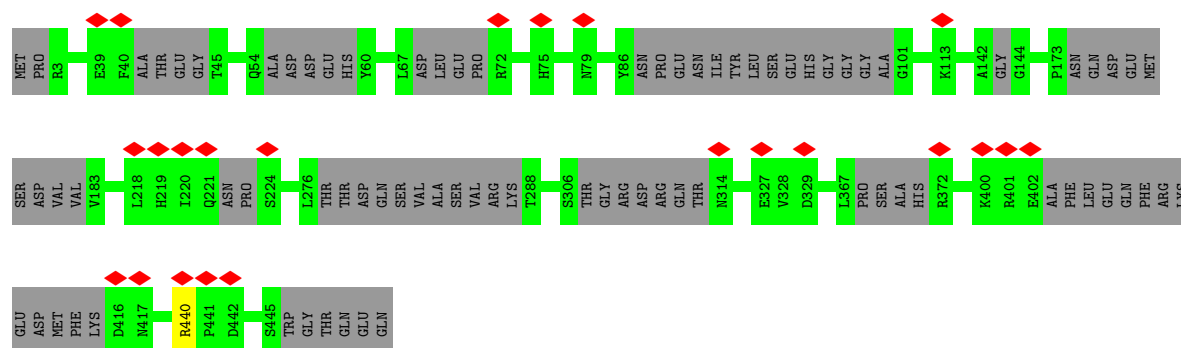
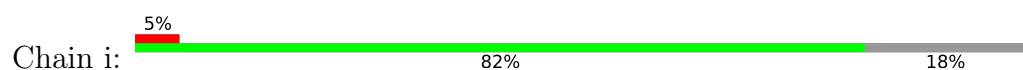
Chain g: 5% 82% 18%



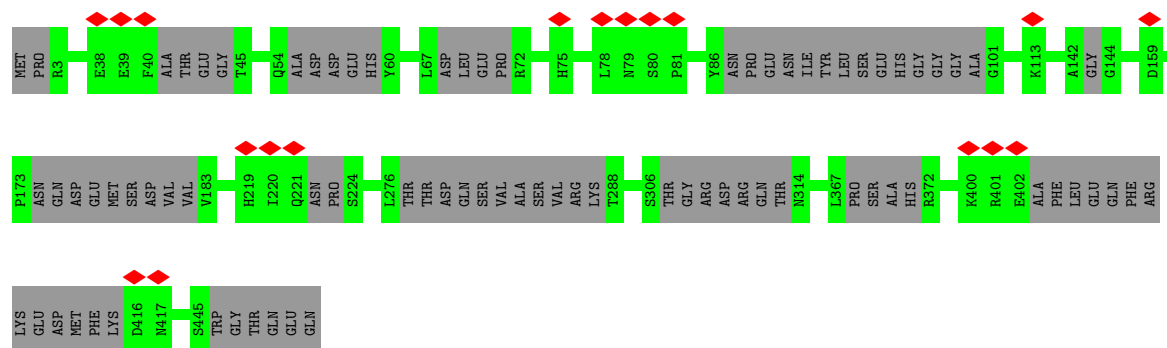
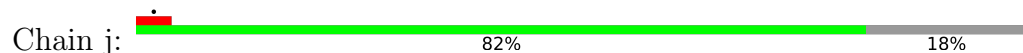
• Molecule 8: Tubulin gamma-1 chain



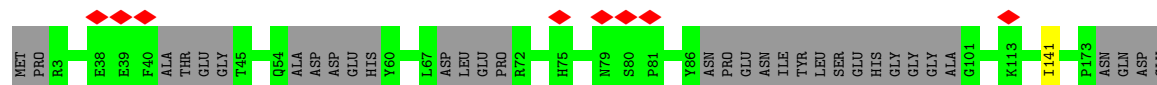
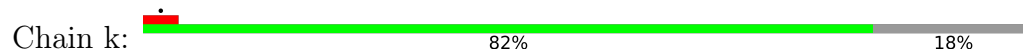
• Molecule 8: Tubulin gamma-1 chain



• Molecule 8: Tubulin gamma-1 chain

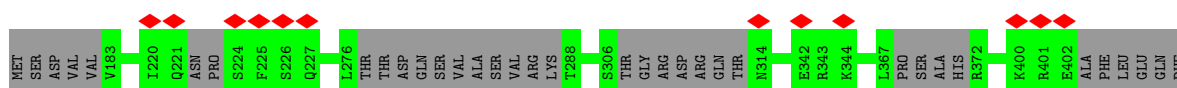
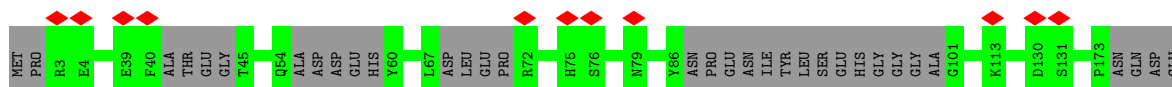
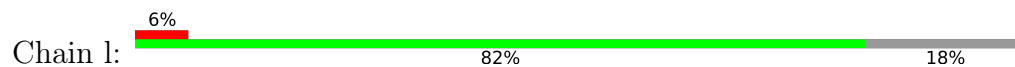


• Molecule 8: Tubulin gamma-1 chain

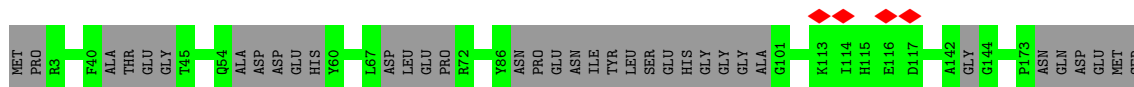
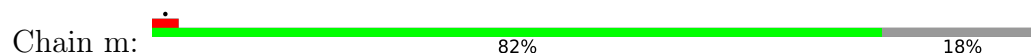




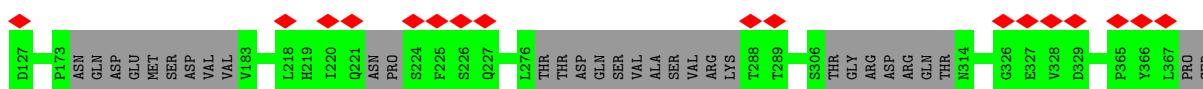
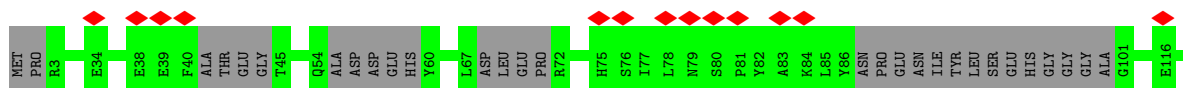
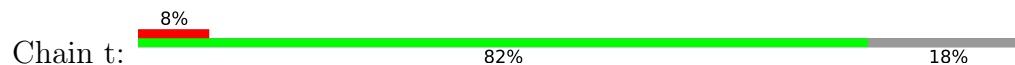
• Molecule 8: Tubulin gamma-1 chain



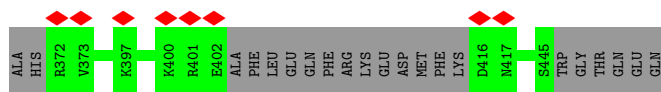
• Molecule 8: Tubulin gamma-1 chain



• Molecule 8: Tubulin gamma-1 chain







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	217.3	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.372	Depositor
Minimum map value	-0.500	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.686	Depositor
Map size (Å)	650.24, 650.24, 650.24	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	5.08, 5.08, 5.08	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: ADP, GDP

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	0.33	0/4460	0.43	0/6017
1	C	0.37	0/4460	0.44	0/6017
1	E	0.37	0/4460	0.45	0/6017
1	G	0.37	0/4460	0.45	0/6017
1	M	0.35	0/4460	0.44	0/6017
2	B	0.34	0/4838	0.43	0/6519
2	D	0.36	0/4838	0.44	0/6519
2	F	0.35	0/4838	0.43	0/6519
2	H	0.36	0/4838	0.44	0/6519
2	R	0.85	0/374	0.70	1/515 (0.2%)
2	T	0.27	0/2829	0.41	0/3931
3	I	0.33	0/4478	0.42	0/6070
3	K	0.27	0/4478	0.40	0/6070
4	J	0.31	0/4049	0.41	0/5463
5	L	0.28	0/4101	0.40	0/5542
5	P	0.85	0/377	0.74	1/518 (0.2%)
6	U	0.24	0/1793	0.59	0/2492
7	Q	0.85	0/217	0.72	1/299 (0.3%)
7	S	0.84	0/281	0.71	1/388 (0.3%)
8	a	0.33	0/3000	0.44	0/4050
8	b	0.29	0/3000	0.42	0/4050
8	c	0.28	0/3000	0.41	0/4050
8	d	0.30	0/3000	0.42	0/4050
8	e	0.35	0/3000	0.44	0/4050
8	f	0.29	0/3000	0.42	0/4050
8	g	0.32	0/3000	0.42	0/4050
8	h	0.34	0/3000	0.43	0/4050
8	i	0.30	0/3000	0.42	0/4050
8	j	0.25	0/3000	0.41	0/4050
8	k	0.30	0/3005	0.43	0/4058
8	l	0.28	0/3005	0.42	0/4058
8	m	0.28	0/3000	0.40	0/4050

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	t	0.27	0/1818	0.42	0/2515
All	All	0.33	0/105457	0.43	4/142630 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	84	PRO	N-CA-CB	5.15	109.48	103.30
2	R	9	PRO	N-CA-CB	5.14	109.47	103.30
7	S	57	PRO	N-CA-CB	5.06	109.38	103.30
7	Q	57	PRO	N-CA-CB	5.01	109.32	103.30

There are no chirality outliers.

There are no planarity outliers.

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	519/902 (58%)	479 (92%)	39 (8%)	1 (0%)	44	78
1	C	519/902 (58%)	486 (94%)	32 (6%)	1 (0%)	44	78
1	E	519/902 (58%)	480 (92%)	37 (7%)	2 (0%)	30	68
1	G	519/902 (58%)	486 (94%)	33 (6%)	0	100	100
1	M	519/902 (58%)	483 (93%)	35 (7%)	1 (0%)	44	78
2	B	550/907 (61%)	528 (96%)	22 (4%)	0	100	100
2	D	550/907 (61%)	530 (96%)	20 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	550/907 (61%)	528 (96%)	22 (4%)	0	100	100
2	H	550/907 (61%)	530 (96%)	20 (4%)	0	100	100
2	R	66/907 (7%)	66 (100%)	0	0	100	100
2	T	550/907 (61%)	529 (96%)	21 (4%)	0	100	100
3	I	529/667 (79%)	496 (94%)	31 (6%)	2 (0%)	30	68
3	K	529/667 (79%)	507 (96%)	22 (4%)	0	100	100
4	J	454/1024 (44%)	434 (96%)	19 (4%)	1 (0%)	44	78
5	L	469/1819 (26%)	436 (93%)	33 (7%)	0	100	100
5	P	67/1819 (4%)	67 (100%)	0	0	100	100
6	U	360/376 (96%)	352 (98%)	8 (2%)	0	100	100
7	Q	38/82 (46%)	38 (100%)	0	0	100	100
7	S	51/82 (62%)	51 (100%)	0	0	100	100
8	a	345/451 (76%)	328 (95%)	17 (5%)	0	100	100
8	b	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
8	c	345/451 (76%)	332 (96%)	13 (4%)	0	100	100
8	d	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
8	e	345/451 (76%)	326 (94%)	18 (5%)	1 (0%)	37	73
8	f	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
8	g	345/451 (76%)	330 (96%)	15 (4%)	0	100	100
8	h	345/451 (76%)	325 (94%)	19 (6%)	1 (0%)	37	73
8	i	345/451 (76%)	330 (96%)	15 (4%)	0	100	100
8	j	345/451 (76%)	329 (95%)	16 (5%)	0	100	100
8	k	348/451 (77%)	330 (95%)	18 (5%)	0	100	100
8	l	348/451 (77%)	329 (94%)	19 (6%)	0	100	100
8	m	345/451 (76%)	332 (96%)	13 (4%)	0	100	100
8	t	348/451 (77%)	332 (95%)	16 (5%)	0	100	100
All	All	12747/22802 (56%)	12110 (95%)	627 (5%)	10 (0%)	50	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	127	ASP
4	J	715	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	312	GLU
1	M	315	GLN
1	C	591	THR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/791 (61%)	479 (100%)	2 (0%)	89	91
1	C	481/791 (61%)	479 (100%)	2 (0%)	89	91
1	E	481/791 (61%)	480 (100%)	1 (0%)	92	94
1	G	481/791 (61%)	477 (99%)	4 (1%)	79	85
1	M	481/791 (61%)	480 (100%)	1 (0%)	92	94
2	B	519/798 (65%)	519 (100%)	0	100	100
2	D	519/798 (65%)	514 (99%)	5 (1%)	73	82
2	F	519/798 (65%)	516 (99%)	3 (1%)	84	88
2	H	519/798 (65%)	517 (100%)	2 (0%)	89	91
3	I	474/594 (80%)	464 (98%)	10 (2%)	48	66
3	K	474/594 (80%)	469 (99%)	5 (1%)	70	80
4	J	445/933 (48%)	445 (100%)	0	100	100
5	L	436/1546 (28%)	436 (100%)	0	100	100
8	a	328/400 (82%)	323 (98%)	5 (2%)	60	75
8	b	328/400 (82%)	327 (100%)	1 (0%)	91	92
8	c	328/400 (82%)	327 (100%)	1 (0%)	91	92
8	d	328/400 (82%)	326 (99%)	2 (1%)	84	88
8	e	328/400 (82%)	318 (97%)	10 (3%)	36	55
8	f	328/400 (82%)	327 (100%)	1 (0%)	91	92
8	g	328/400 (82%)	327 (100%)	1 (0%)	91	92
8	h	328/400 (82%)	324 (99%)	4 (1%)	67	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	328/400 (82%)	327 (100%)	1 (0%)	91	92
8	j	328/400 (82%)	328 (100%)	0	100	100
8	k	328/400 (82%)	327 (100%)	1 (0%)	91	92
8	l	328/400 (82%)	328 (100%)	0	100	100
8	m	328/400 (82%)	328 (100%)	0	100	100
All	All	10574/16014 (66%)	10512 (99%)	62 (1%)	82	88

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	472[B]	GLU
8	g	60	TYR
8	a	125	GLU
8	f	440	ARG
8	h	440	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 212 such sidechains are listed below:

Mol	Chain	Res	Type
5	L	1705	HIS
8	c	381	HIS
8	l	211	ASN
1	M	317	ASN
8	b	24	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

15 ligands are modelled in this entry.

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$
10	GDP	d	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
10	GDP	j	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
10	GDP	b	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
10	GDP	h	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
10	GDP	m	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.38	4 (13%)
10	GDP	e	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.39	4 (13%)
10	GDP	g	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.37	4 (13%)
10	GDP	t	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
10	GDP	k	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
10	GDP	i	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
10	GDP	c	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
9	ADP	U	800	-	24,29,29	0.68	0	29,45,45	0.84	2 (6%)
10	GDP	a	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
10	GDP	f	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
10	GDP	l	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)

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
10	GDP	d	501	-	-	2/12/32/32	0/3/3/3
10	GDP	j	501	-	-	1/12/32/32	0/3/3/3
10	GDP	b	501	-	-	2/12/32/32	0/3/3/3
10	GDP	h	501	-	-	2/12/32/32	0/3/3/3
10	GDP	m	501	-	-	1/12/32/32	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	e	501	-	-	0/12/32/32	0/3/3/3
10	GDP	g	501	-	-	1/12/32/32	0/3/3/3
10	GDP	t	501	-	-	2/12/32/32	0/3/3/3
10	GDP	k	501	-	-	1/12/32/32	0/3/3/3
10	GDP	i	501	-	-	1/12/32/32	0/3/3/3
10	GDP	c	501	-	-	1/12/32/32	0/3/3/3
9	ADP	U	800	-	-	0/12/32/32	0/3/3/3
10	GDP	a	501	-	-	1/12/32/32	0/3/3/3
10	GDP	f	501	-	-	2/12/32/32	0/3/3/3
10	GDP	l	501	-	-	1/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	e	501	GDP	C6-N1	-2.77	1.33	1.37
10	m	501	GDP	C6-N1	-2.67	1.33	1.37
10	a	501	GDP	C6-N1	-2.61	1.34	1.37
10	i	501	GDP	C6-N1	-2.60	1.34	1.37
10	g	501	GDP	C6-N1	-2.59	1.34	1.37

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	e	501	GDP	PA-O3A-PB	-4.23	118.33	132.83
10	a	501	GDP	PA-O3A-PB	-4.22	118.35	132.83
10	i	501	GDP	PA-O3A-PB	-4.05	118.94	132.83
10	j	501	GDP	PA-O3A-PB	-4.03	119.01	132.83
10	c	501	GDP	PA-O3A-PB	-4.01	119.07	132.83

There are no chirality outliers.

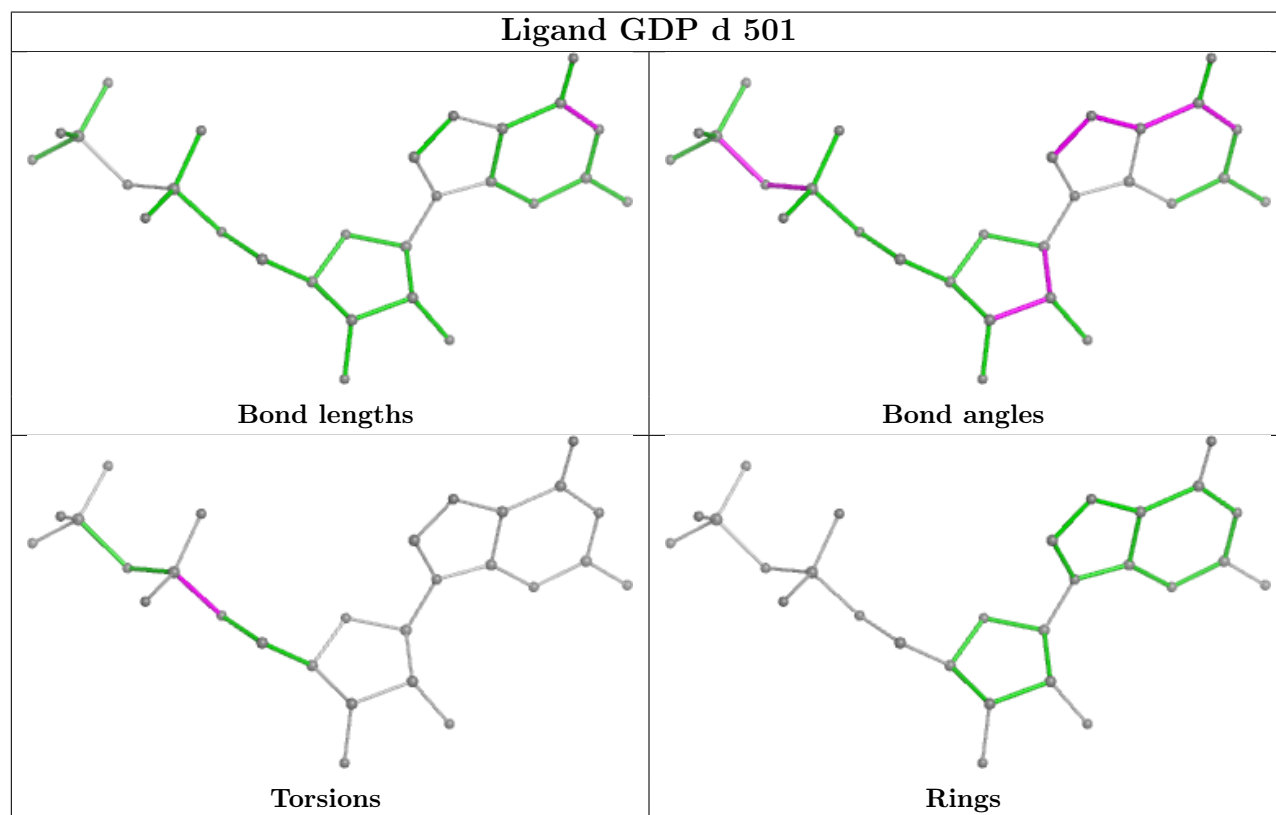
5 of 18 torsion outliers are listed below:

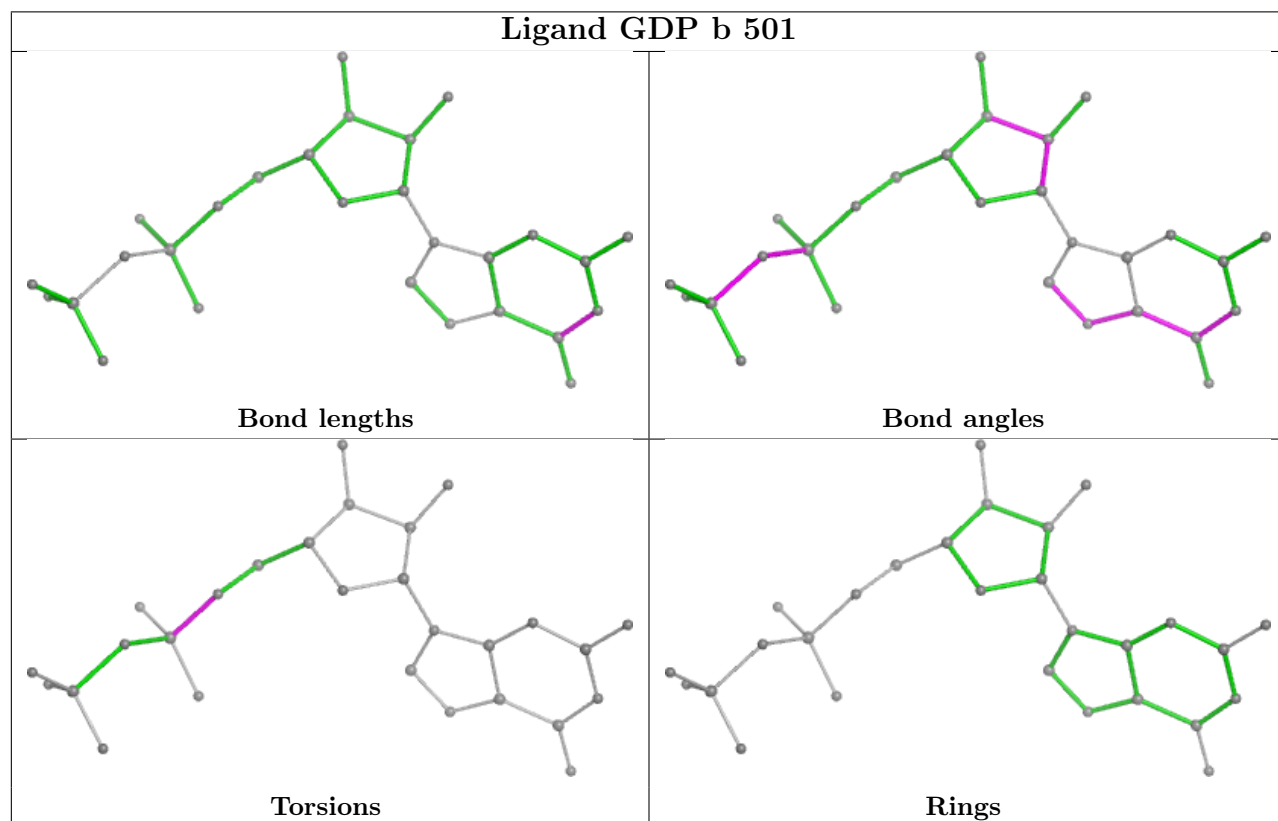
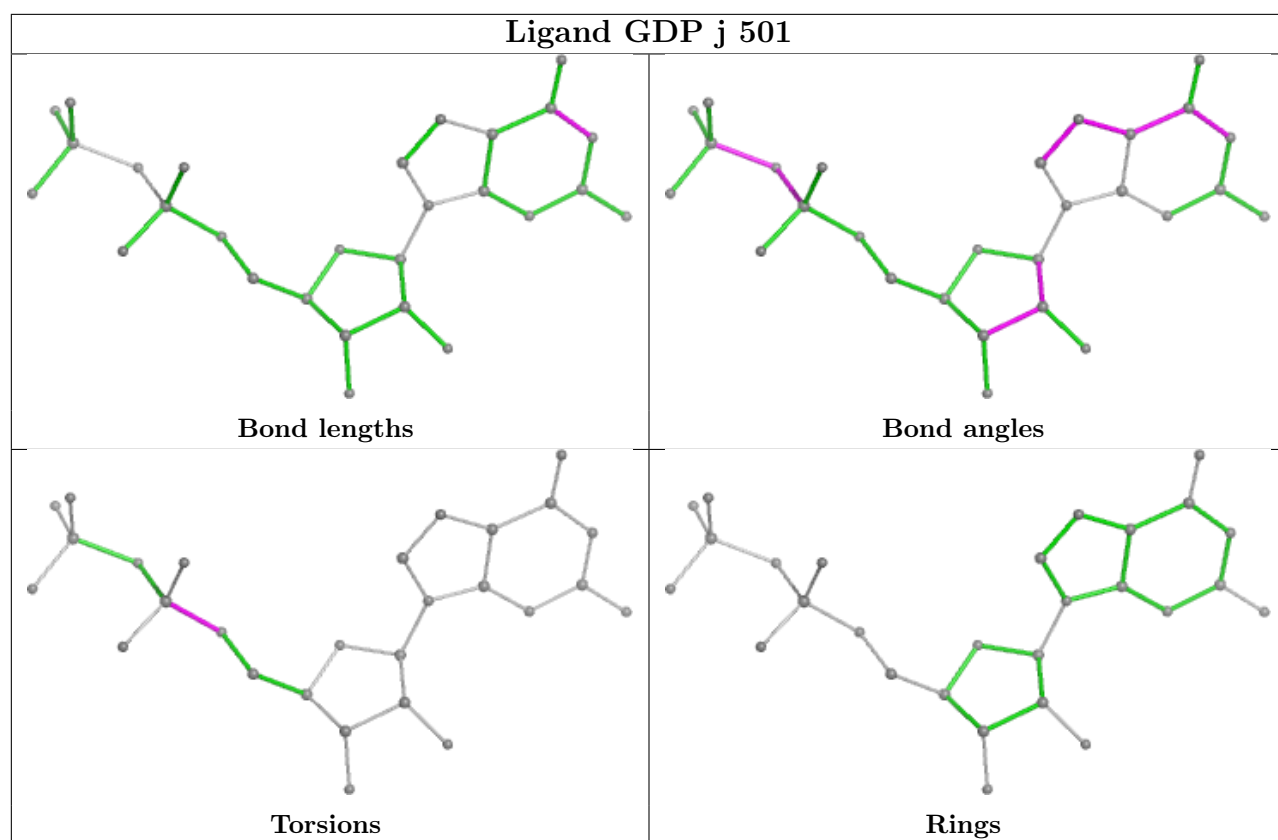
Mol	Chain	Res	Type	Atoms
10	b	501	GDP	C5'-O5'-PA-O1A
10	d	501	GDP	C5'-O5'-PA-O1A
10	f	501	GDP	C5'-O5'-PA-O1A
10	h	501	GDP	C5'-O5'-PA-O1A
10	k	501	GDP	C5'-O5'-PA-O1A

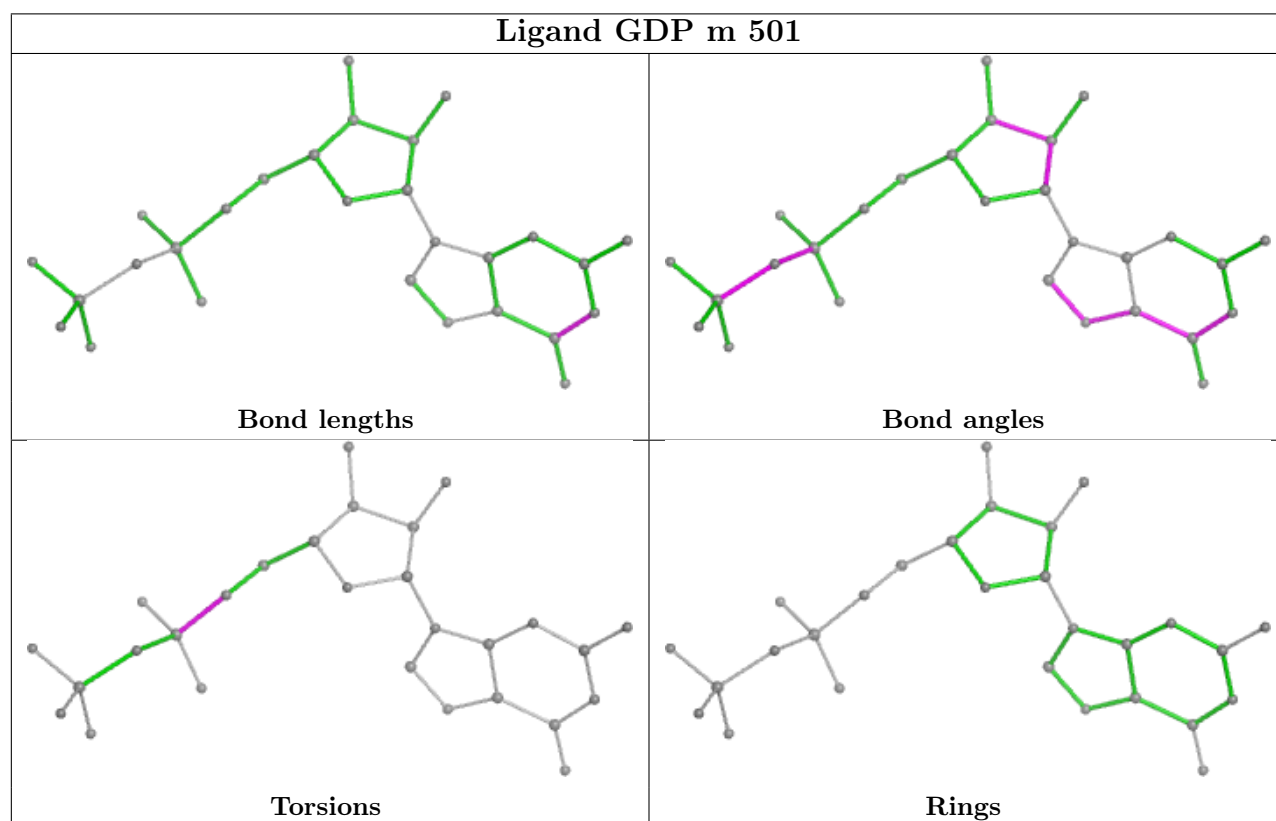
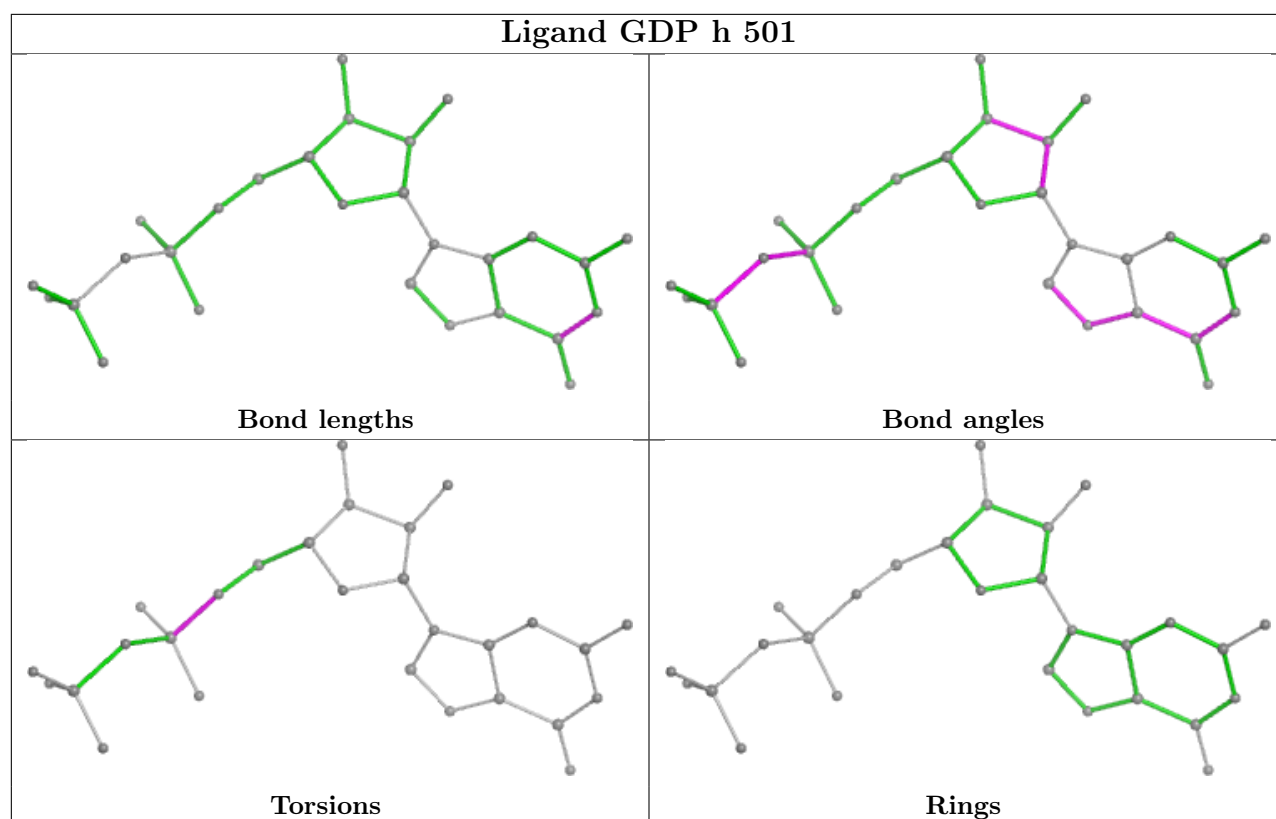
There are no ring outliers.

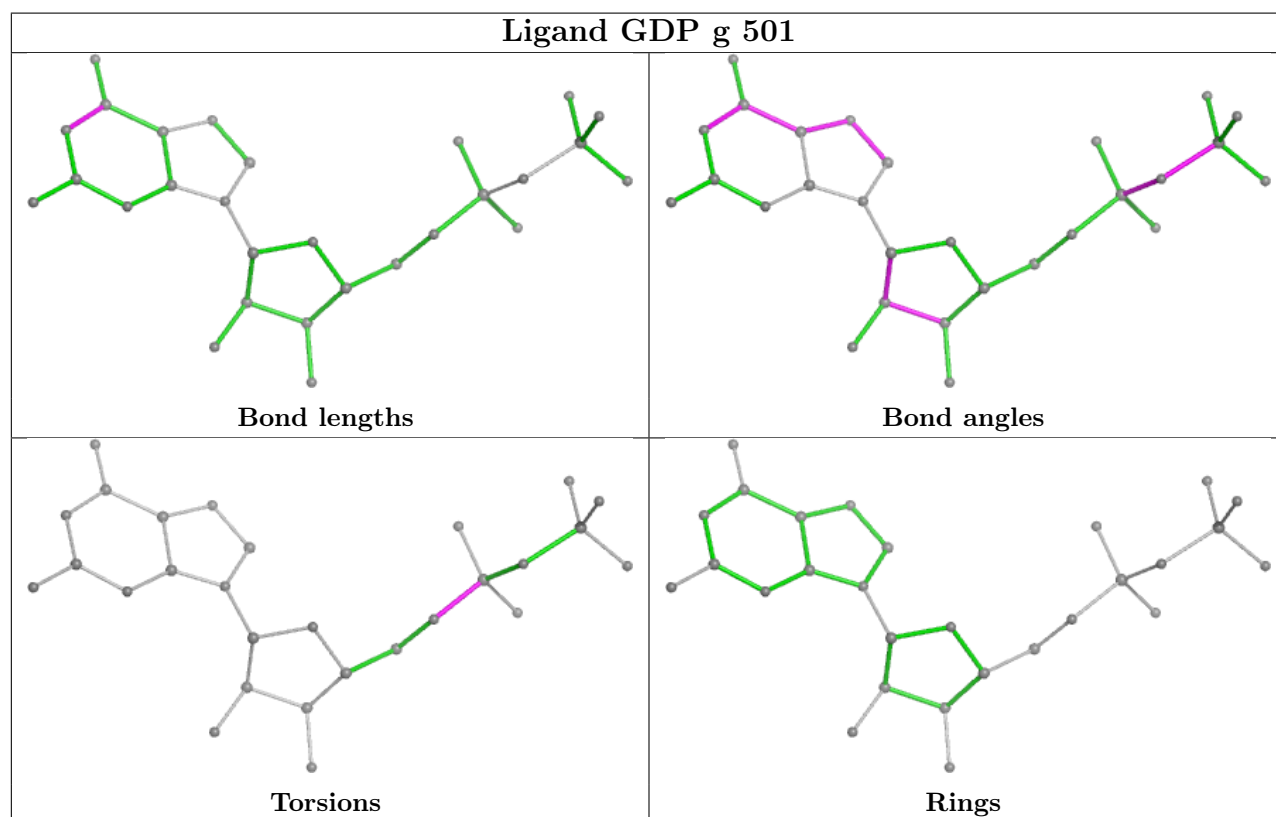
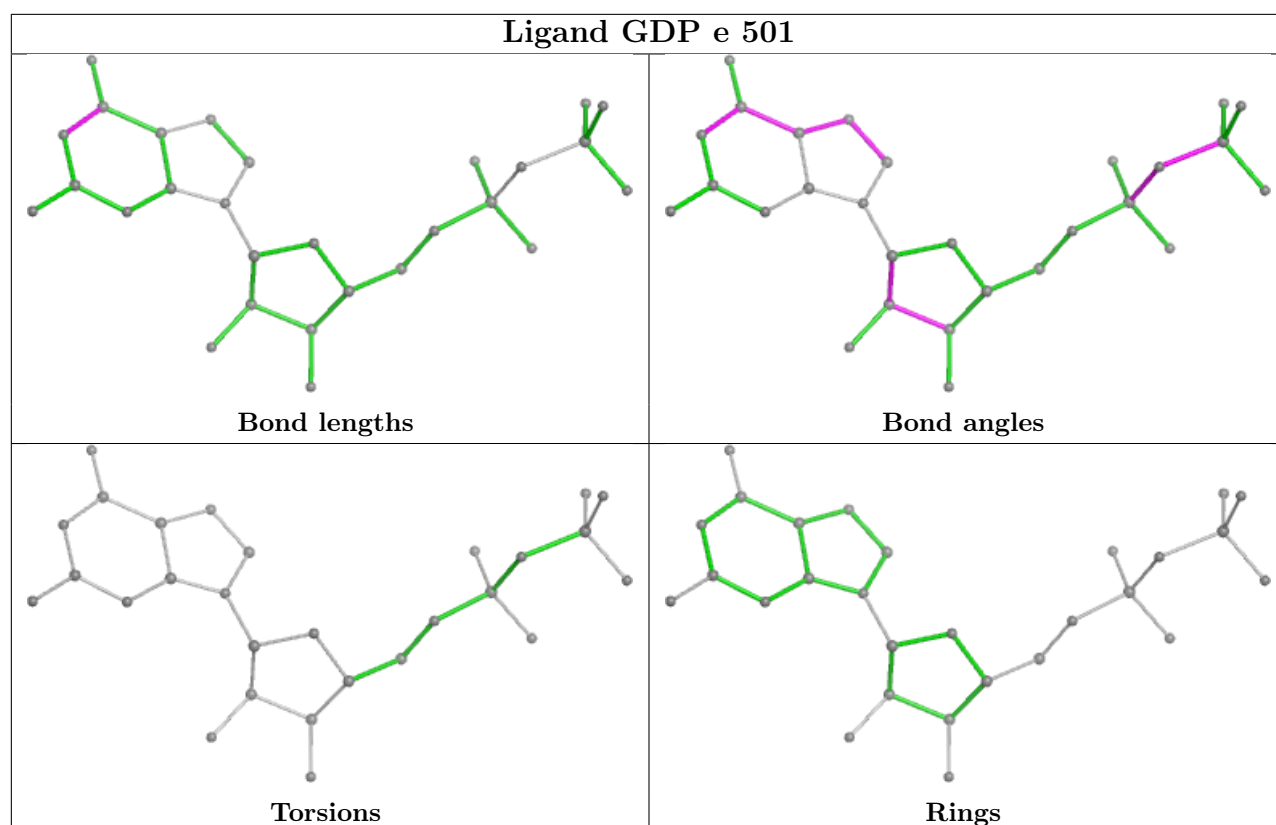
No monomer is involved in short contacts.

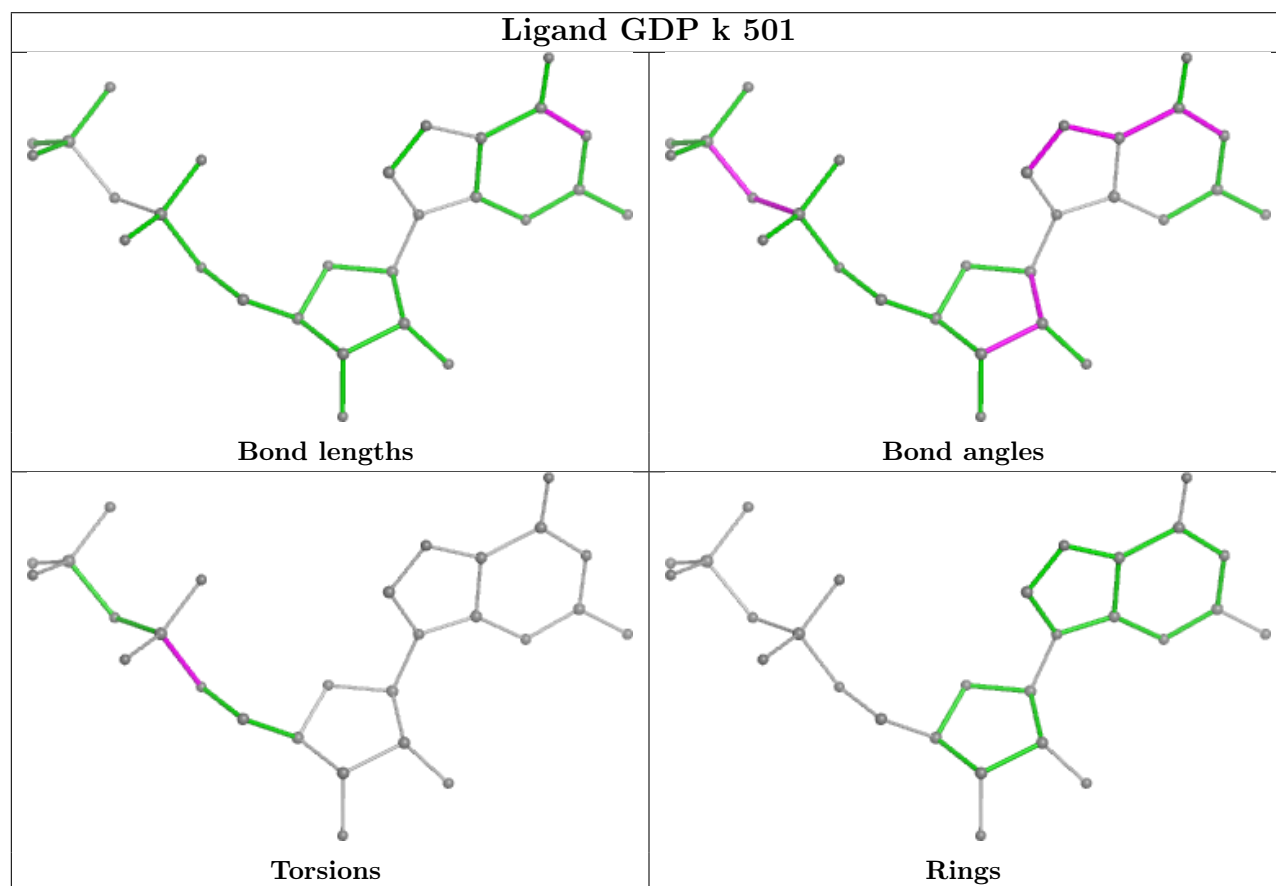
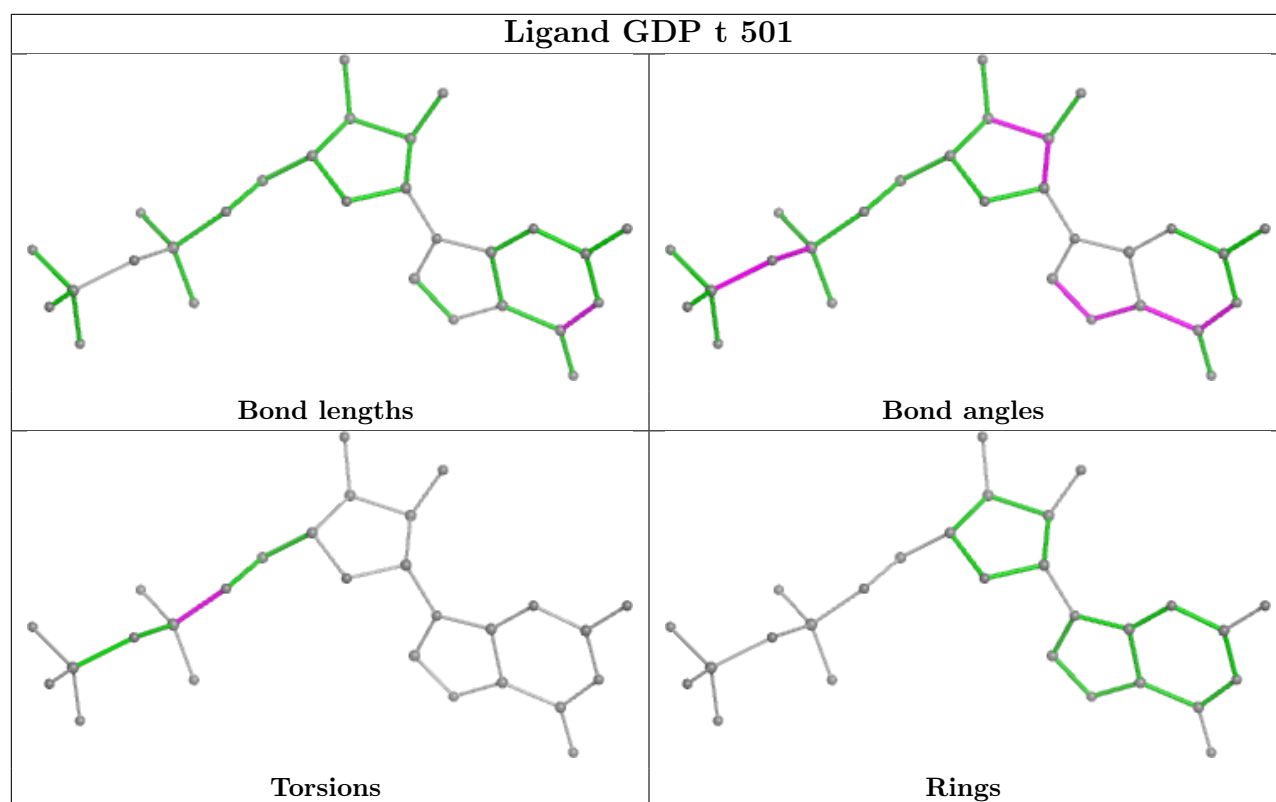
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



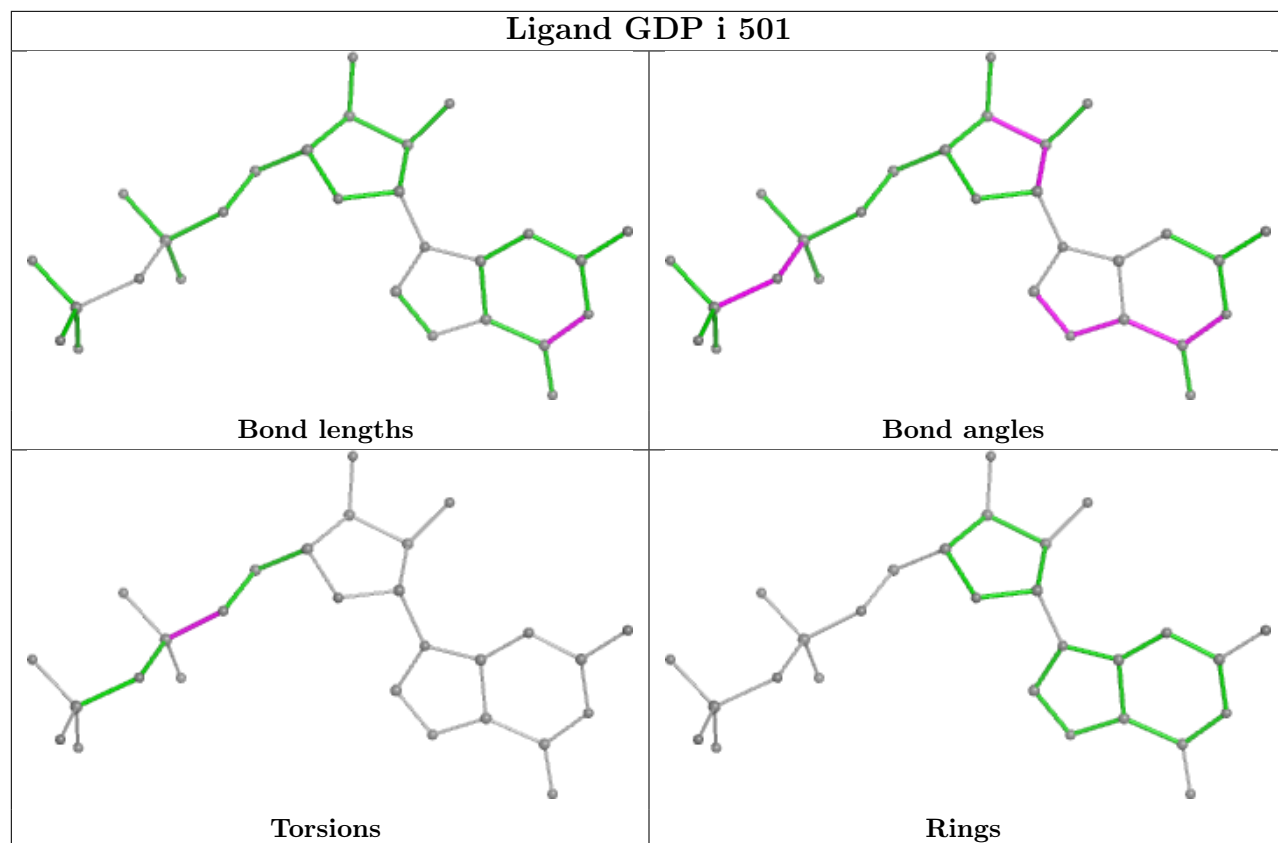




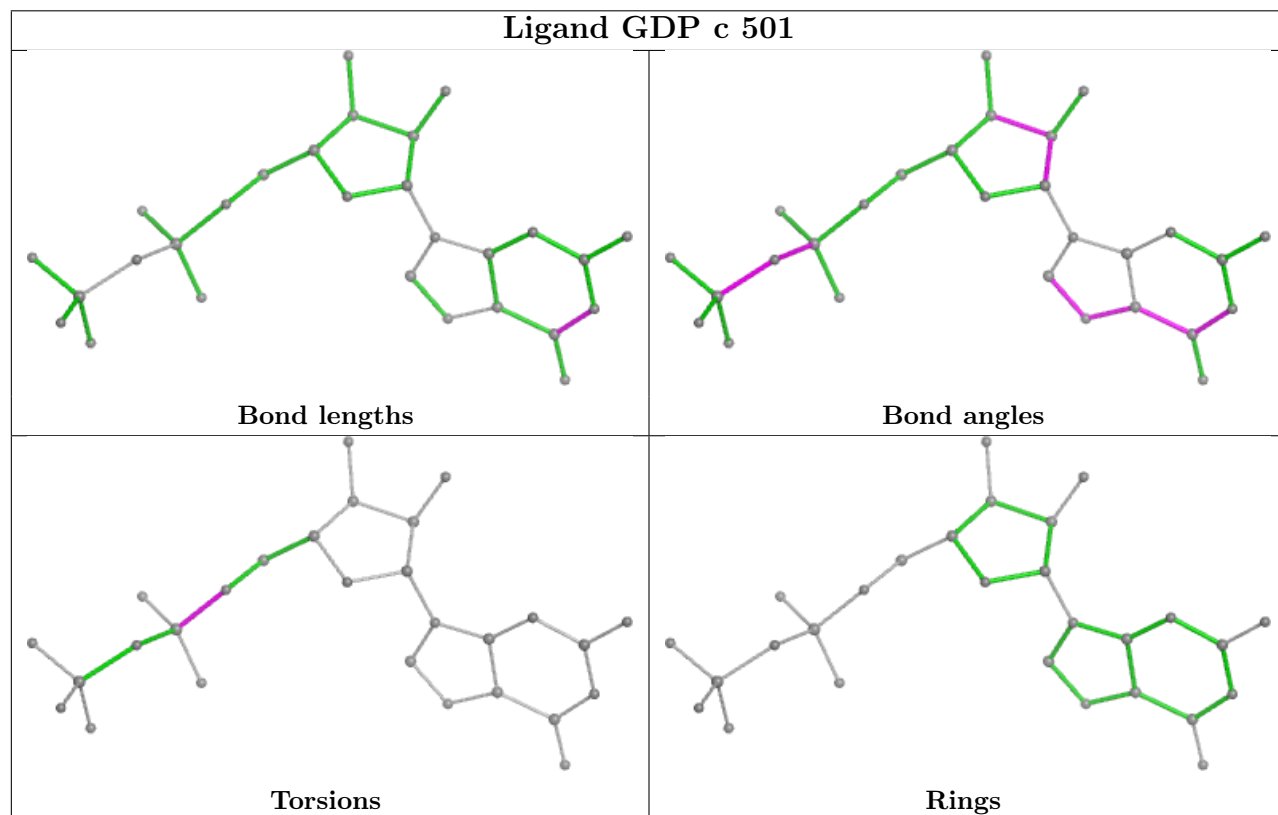


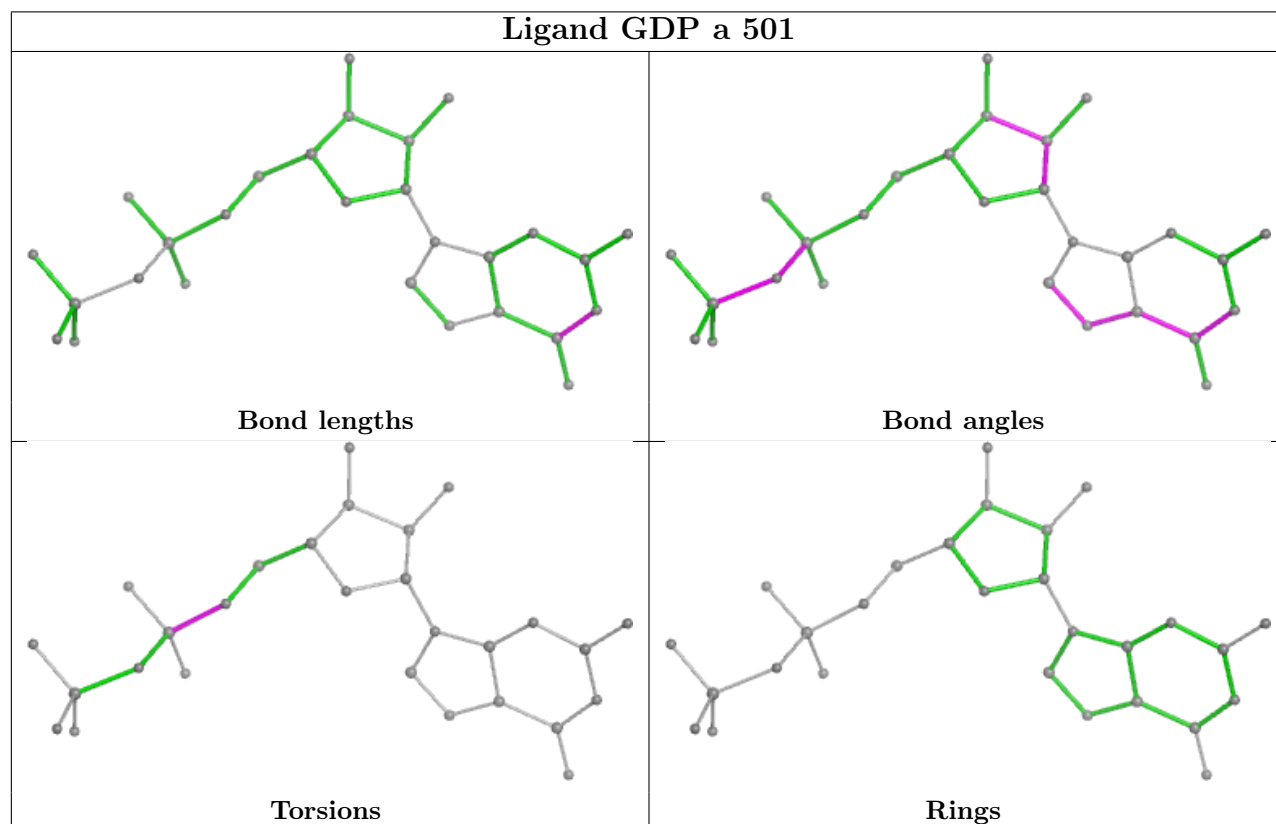
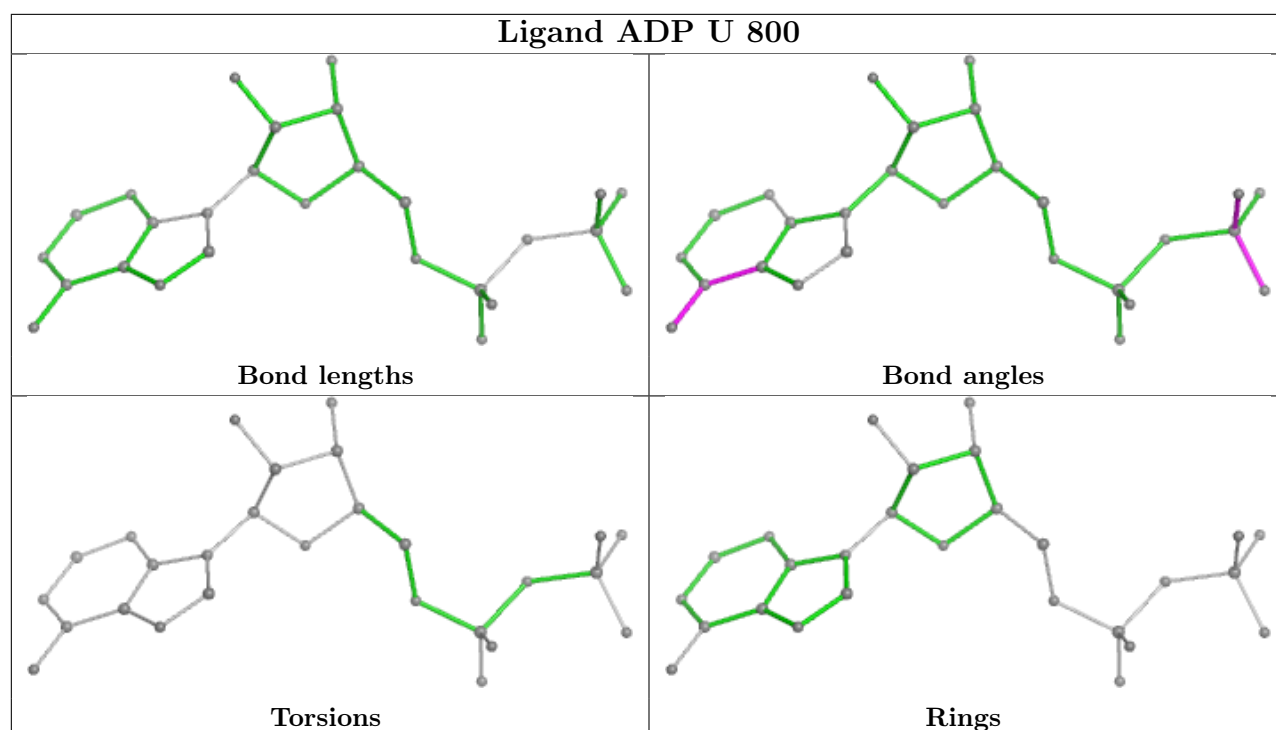


## Ligand GDP i 501

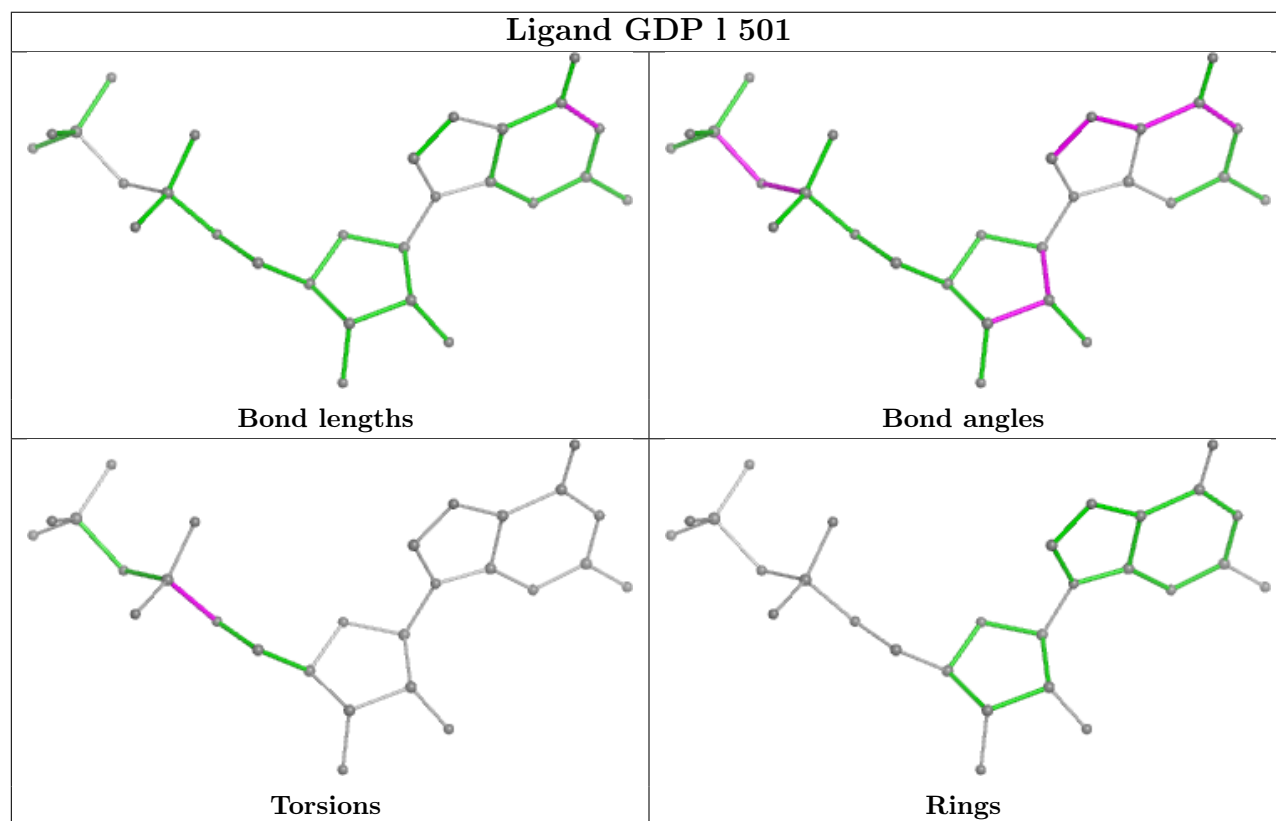
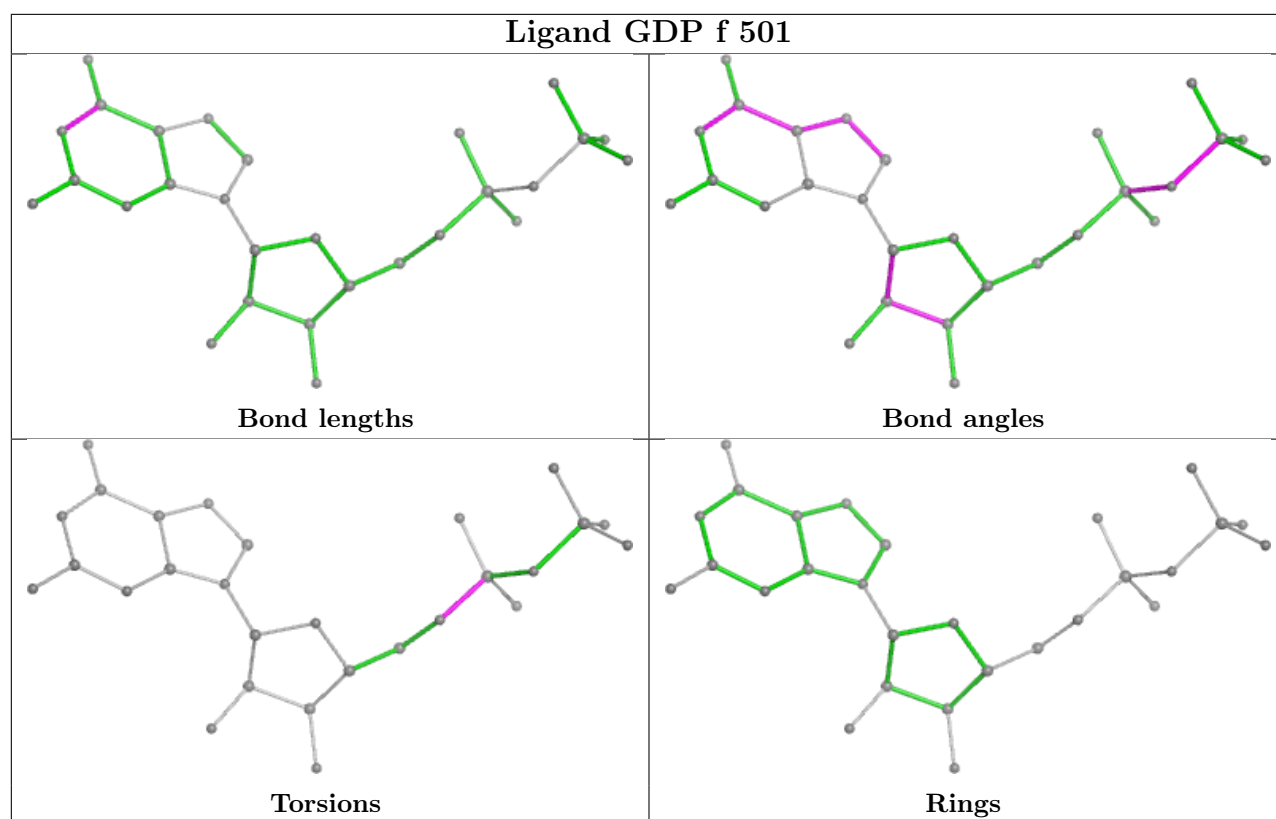


## Ligand GDP c 501









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	K	1
1	A	1
2	T	1
5	L	1
2	B	1
2	H	1
2	R	1
2	F	1
1	C	1
1	G	1
2	D	1
1	M	1
3	I	1
4	J	1
1	E	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	349:ASP	C	350:LEU	N	7.97
1	A	536:GLU	C	537:LEU	N	7.82
1	T	553:TYR	C	554:SER	N	7.28
1	L	1503:LEU	C	1504:HIS	N	7.03
1	B	553:TYR	C	554:SER	N	6.75

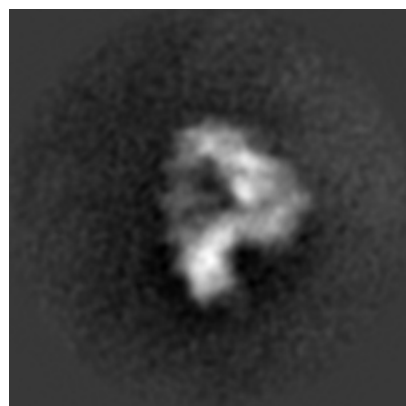
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52718. These allow visual inspection of the internal detail of the map and identification of artifacts.

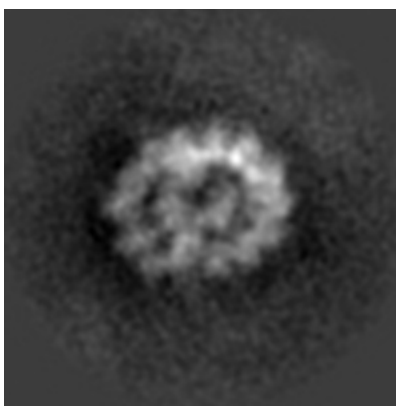
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

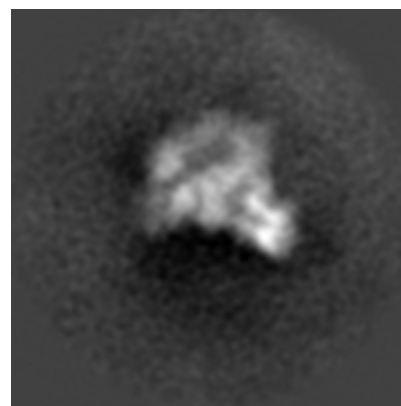
#### 6.1.1 Primary map



X

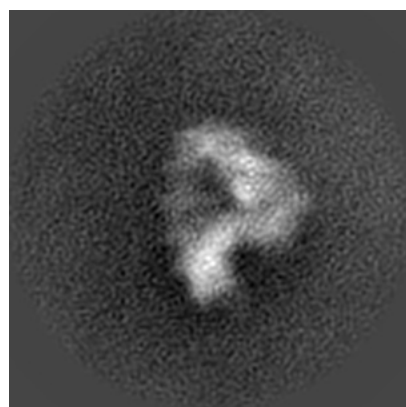


Y

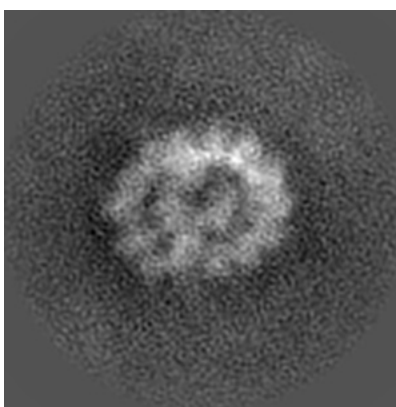


Z

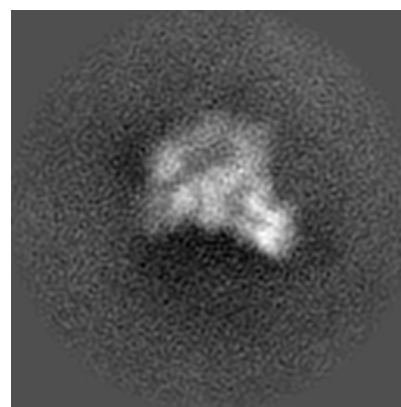
#### 6.1.2 Raw map



X



Y

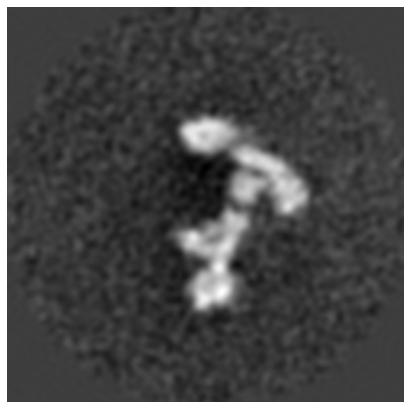


Z

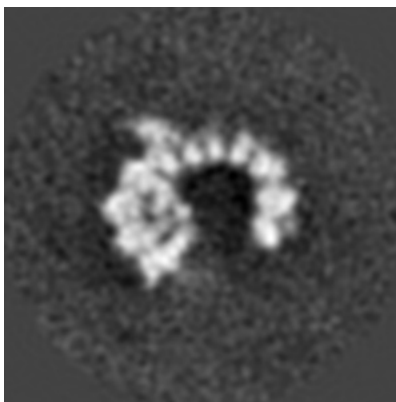
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

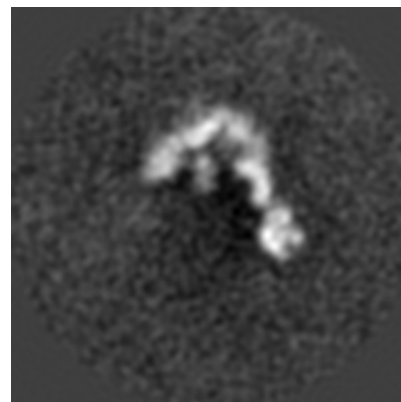
### 6.2.1 Primary map



X Index: 64

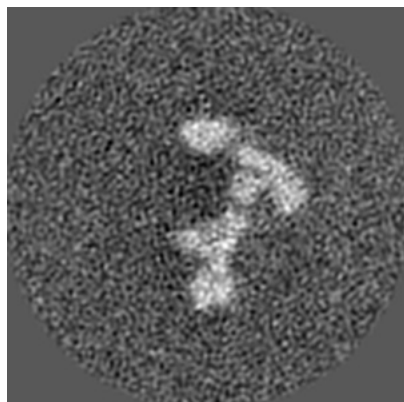


Y Index: 64

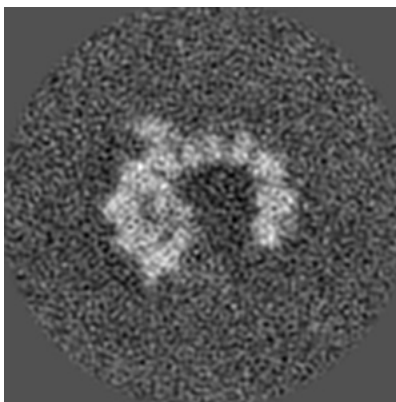


Z Index: 64

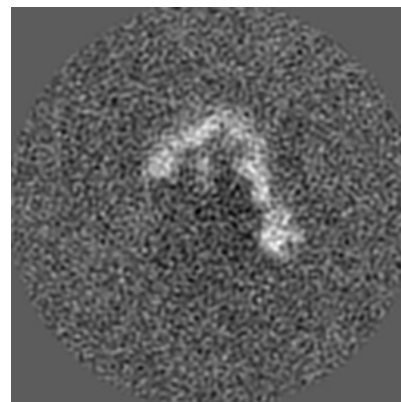
### 6.2.2 Raw map



X Index: 64



Y Index: 64

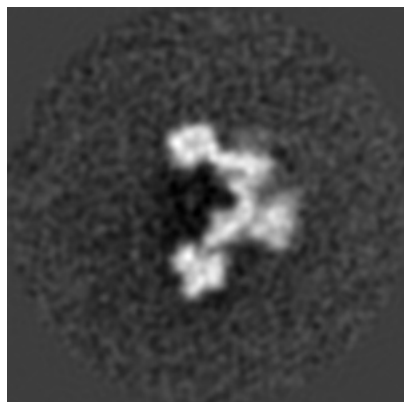


Z Index: 64

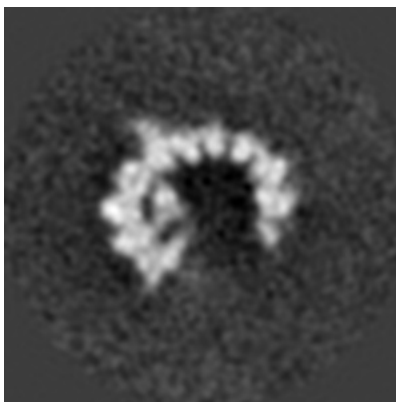
The images above show central slices of the map in three orthogonal directions.

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

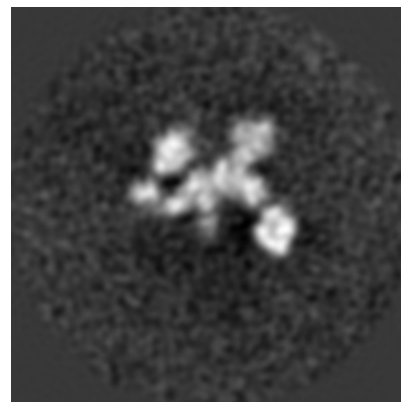
### 6.3.1 Primary map



X Index: 75

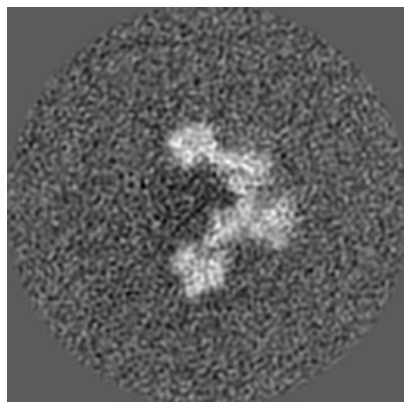


Y Index: 62

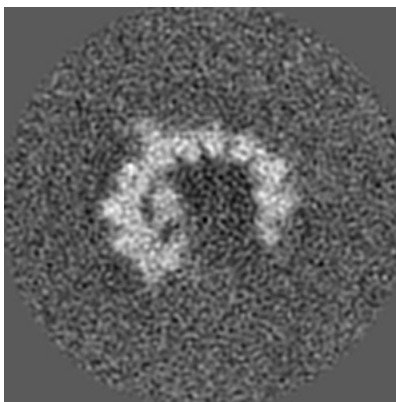


Z Index: 56

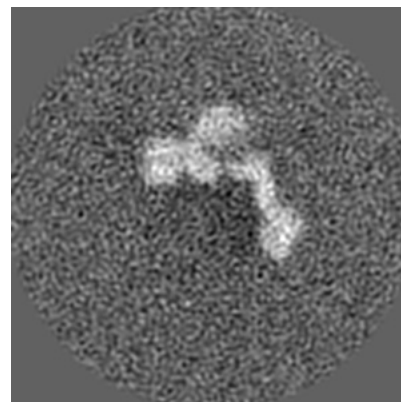
### 6.3.2 Raw map



X Index: 75



Y Index: 62

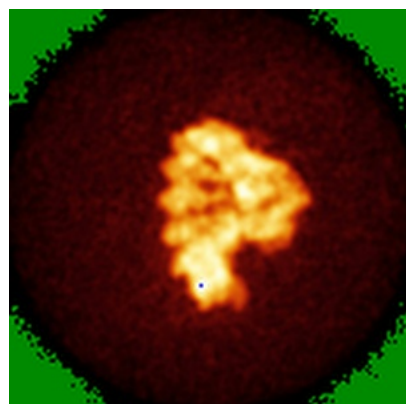


Z Index: 68

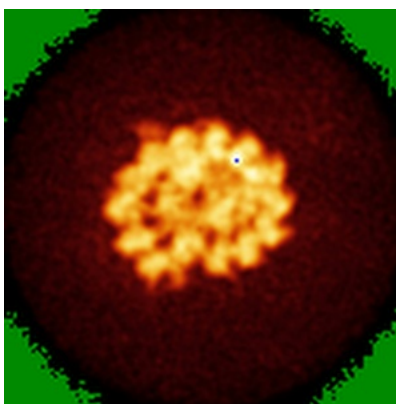
The images above show the largest variance slices of the map in three orthogonal directions.

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

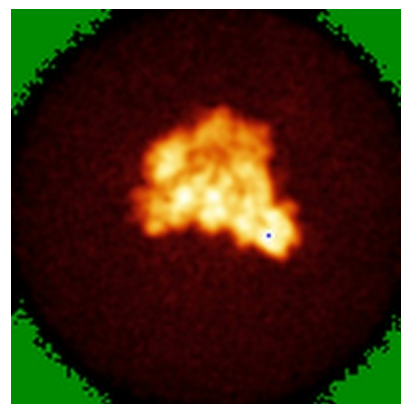
### 6.4.1 Primary map



X

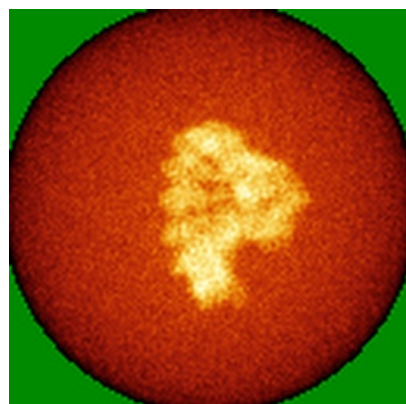


Y

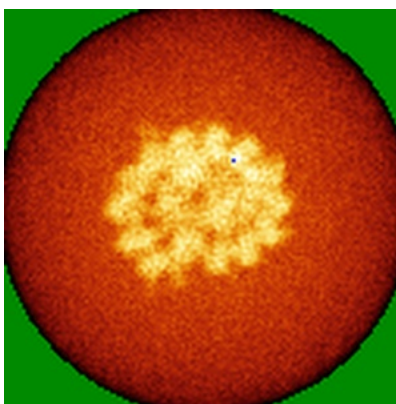


Z

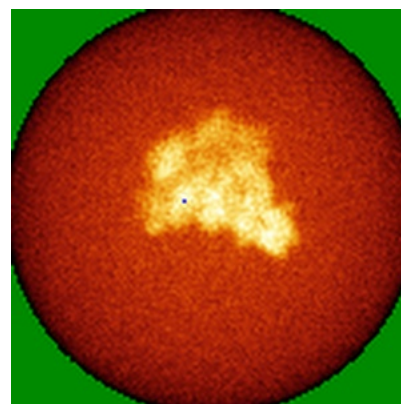
### 6.4.2 Raw map



X



Y



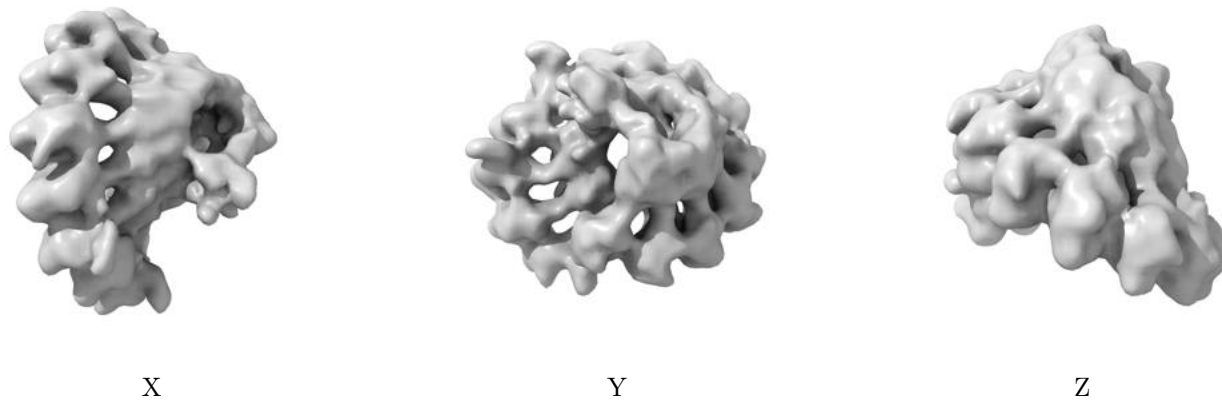
Z

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.



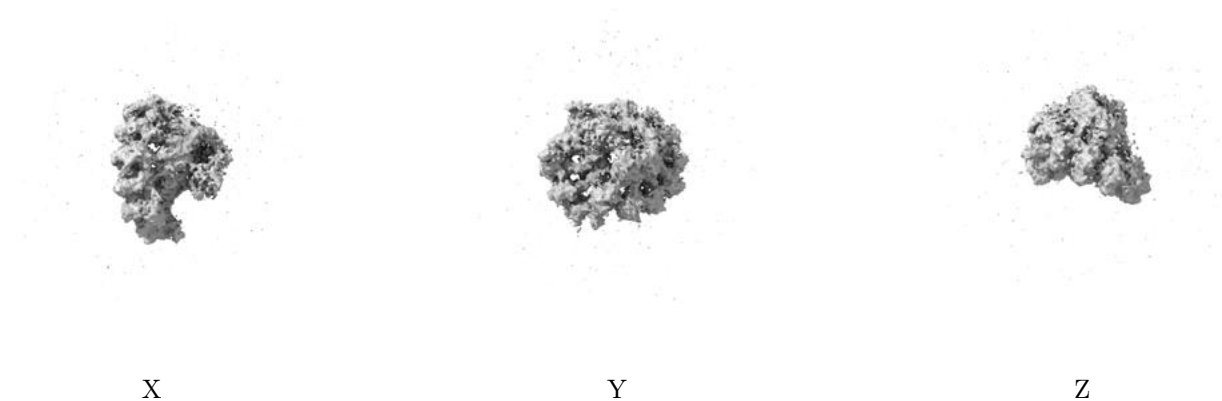
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.686. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

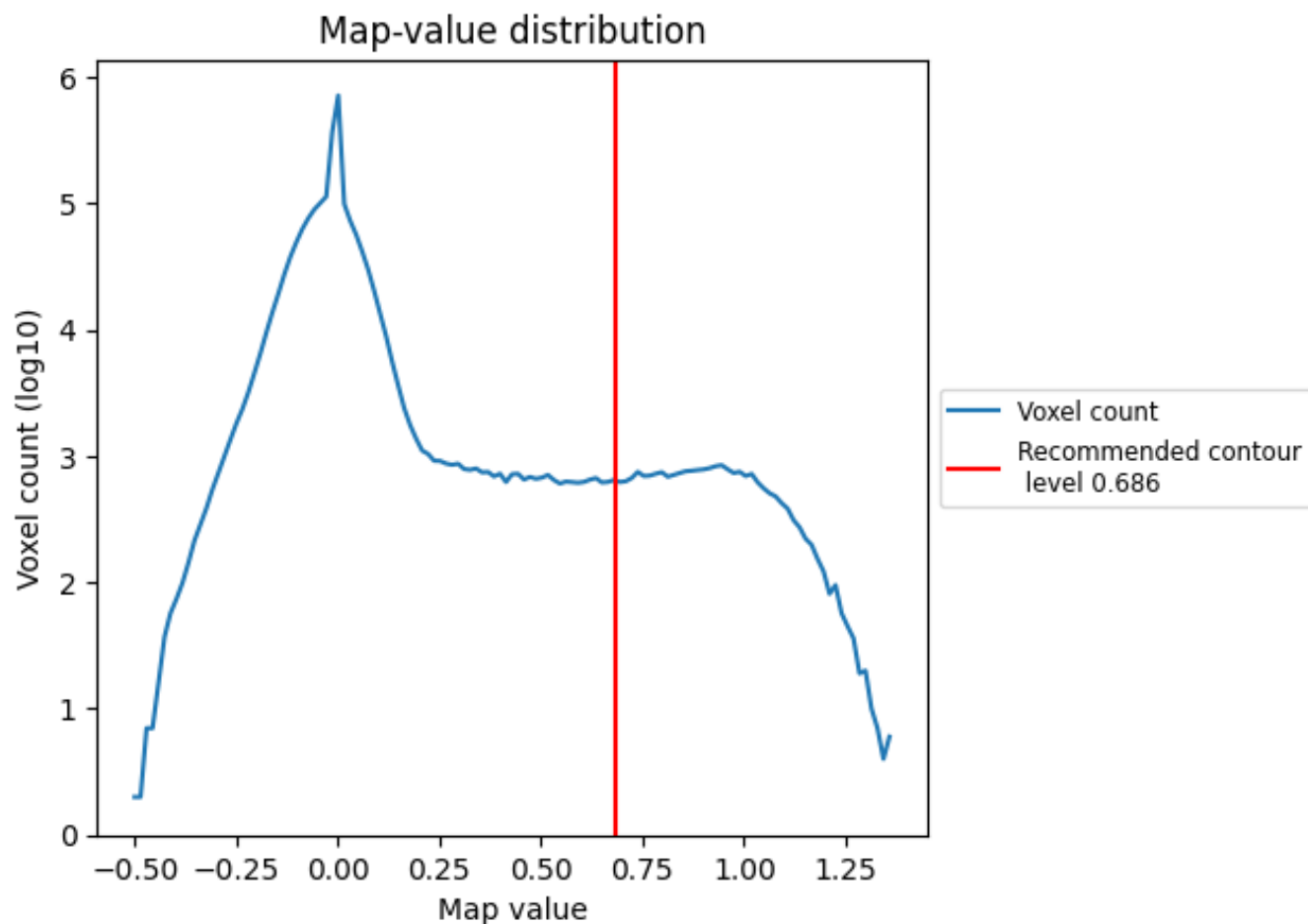
## 6.6 Mask visualisation [i](#)

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.

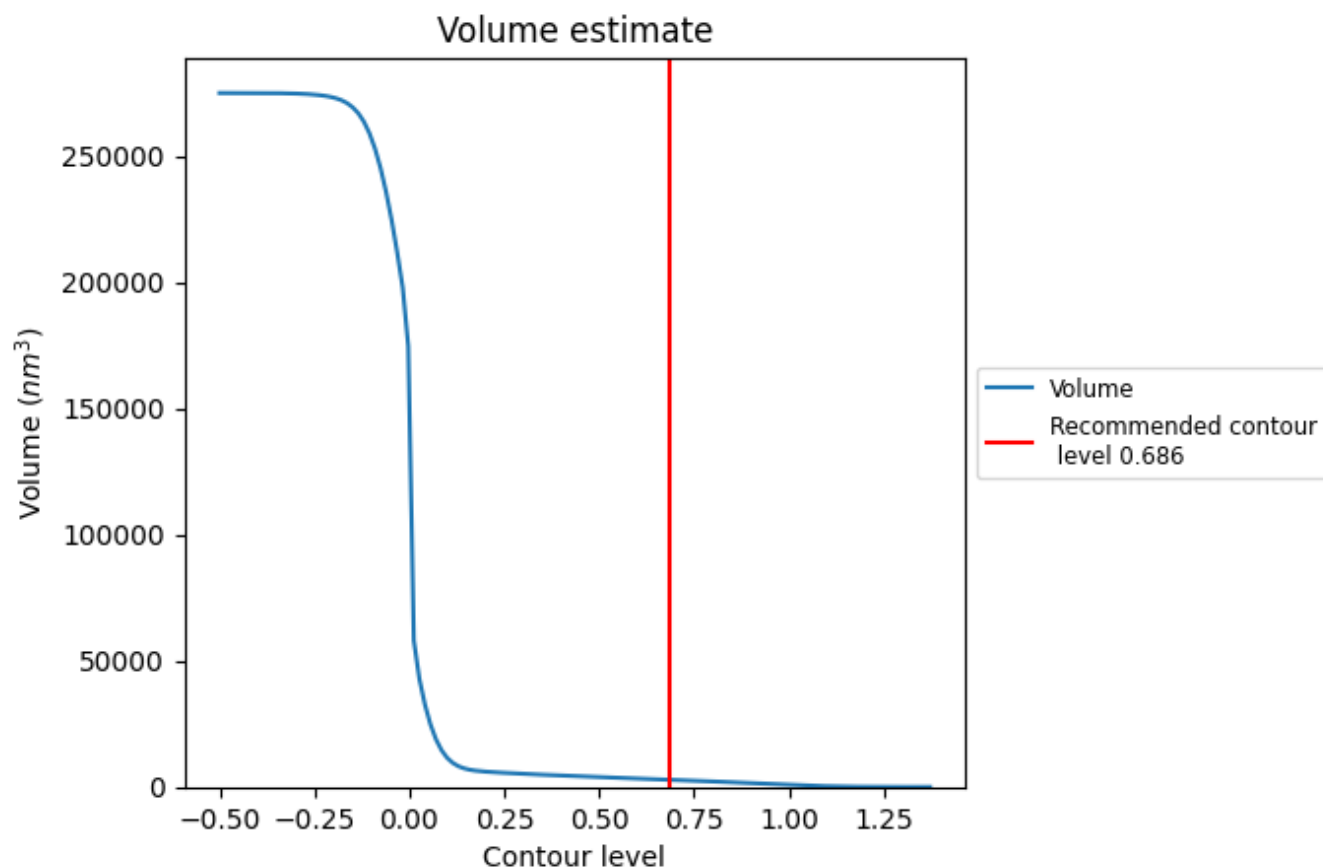
### 7.1 Map-value distribution [i](#)



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.



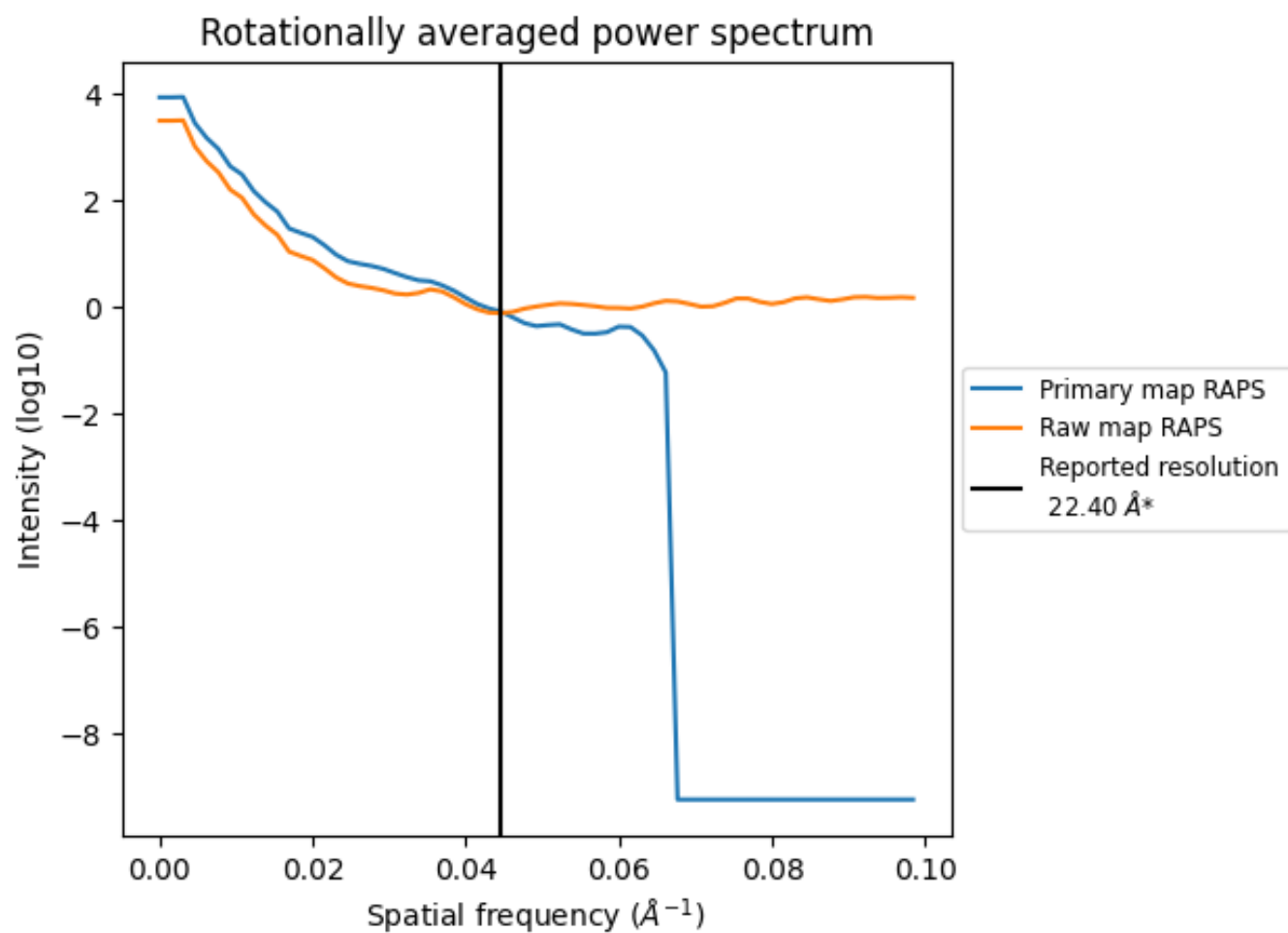
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2863 nm<sup>3</sup>; this corresponds to an approximate mass of 2586 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 ⓘ

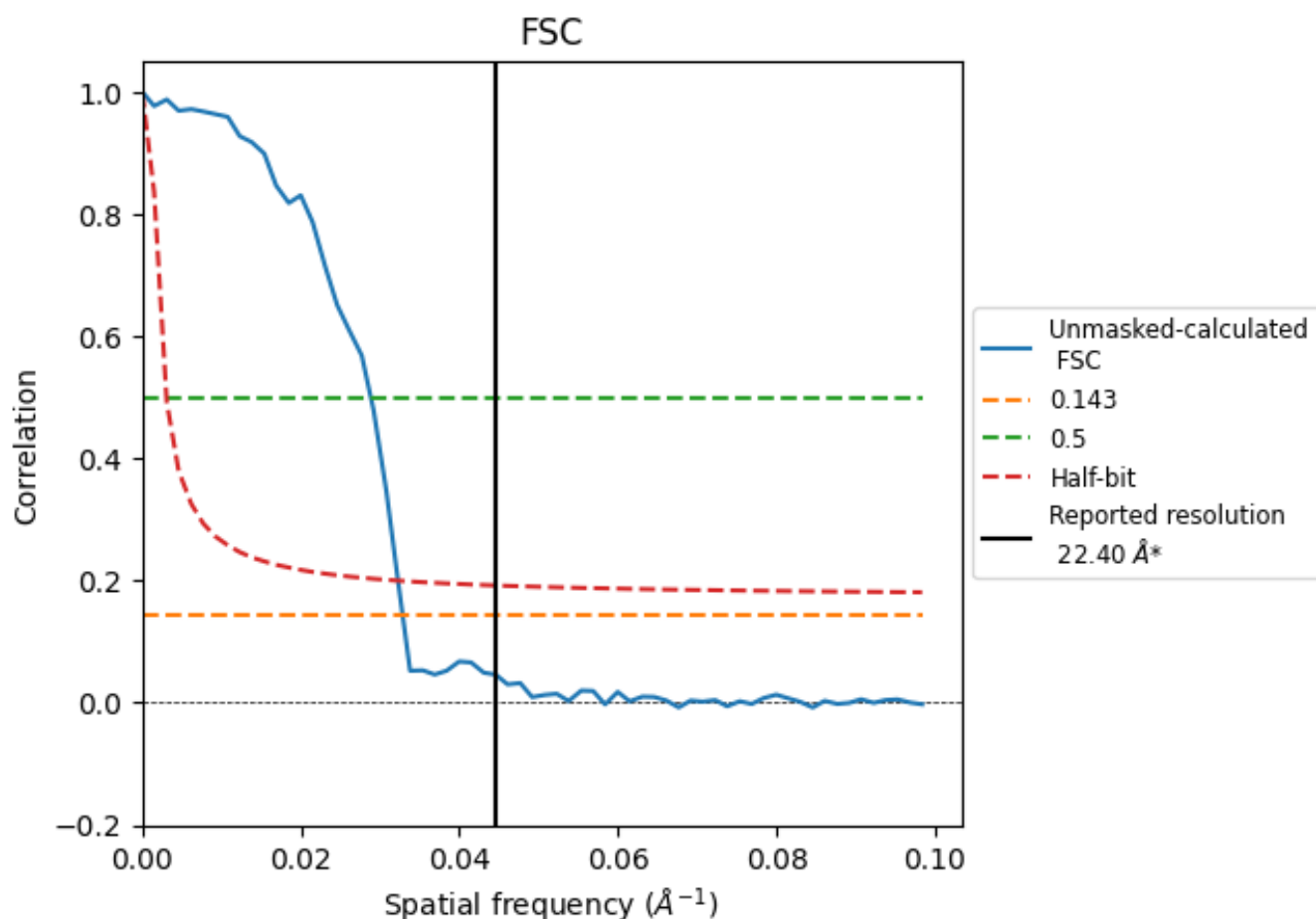


\*Reported resolution corresponds to spatial frequency of 0.045  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.045 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

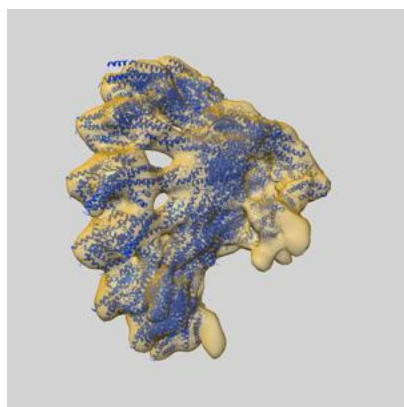
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	22.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	30.40	34.72	30.96

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 30.40 differs from the reported value 22.4 by more than 10 %

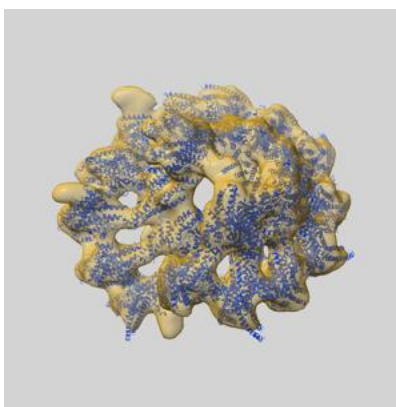
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52718 and PDB model 9I8G. Per-residue inclusion information can be found in section 3 on page 9.

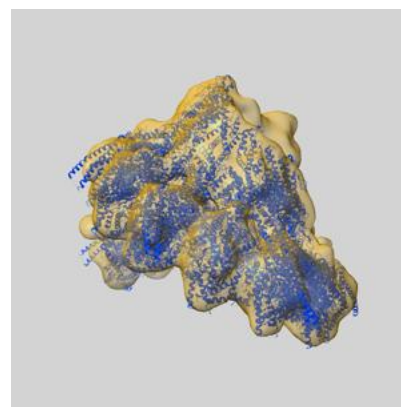
### 9.1 Map-model overlay [i](#)



X



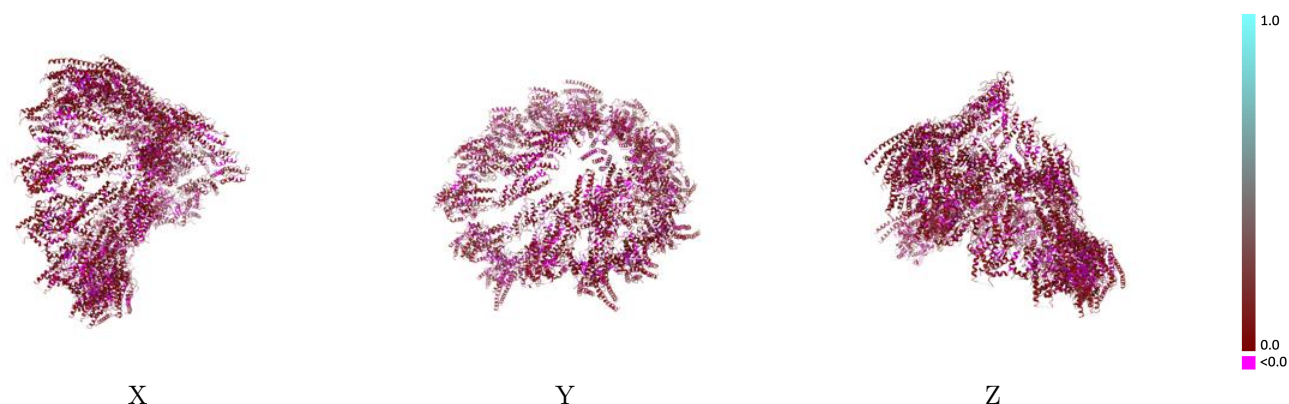
Y



Z

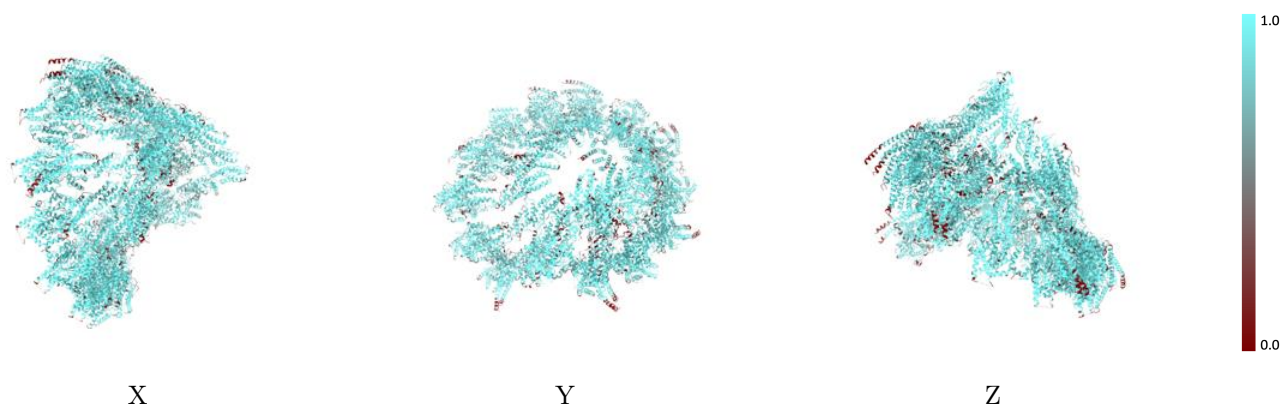
The images above show the 3D surface view of the map at the recommended contour level 0.686 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



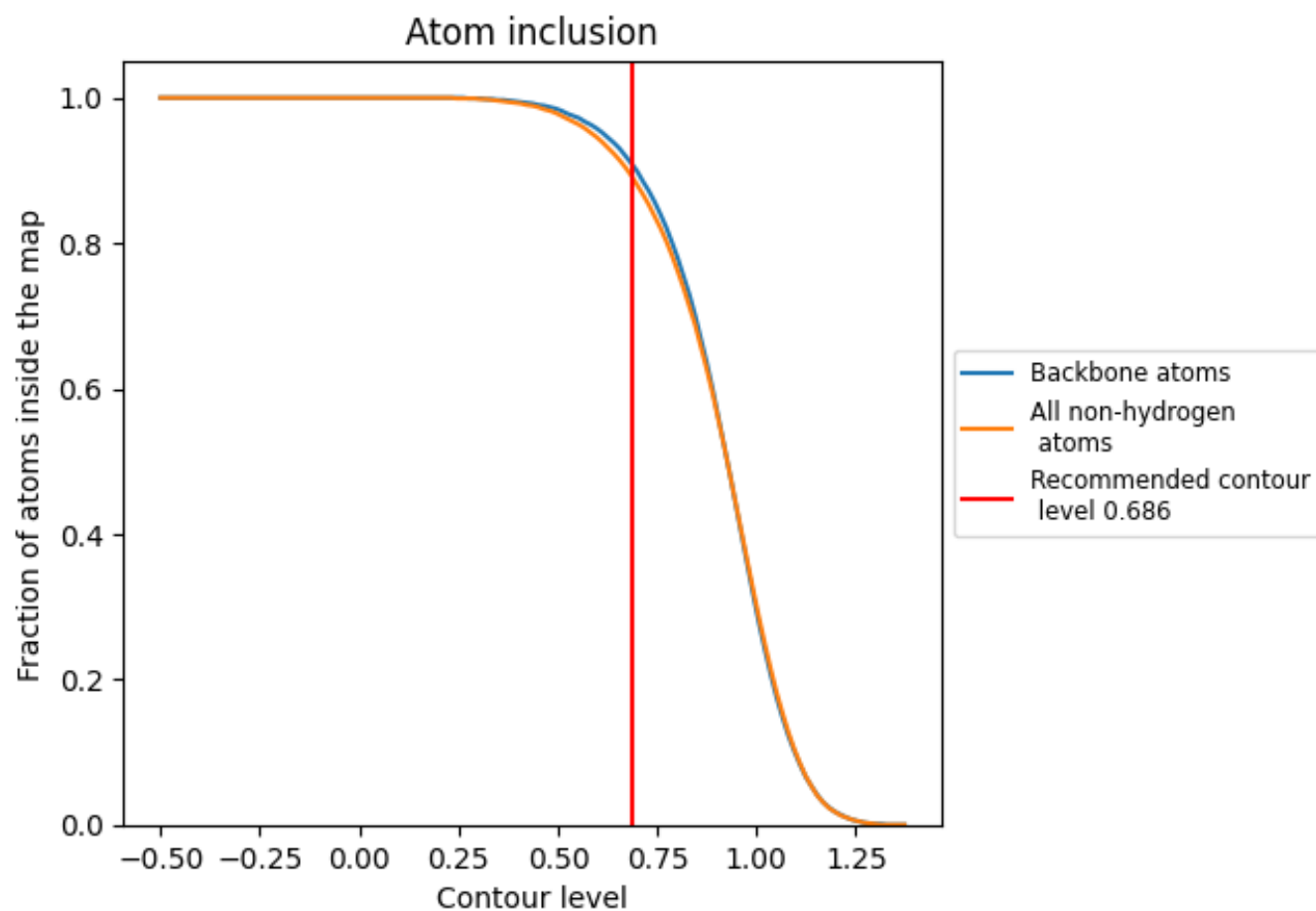
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.686).





































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.686) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.0550
A	 0.8930	 0.0670
B	 0.8320	 0.0610
C	 0.8920	 0.0600
D	 0.8440	 0.0620
E	 0.9030	 0.0630
F	 0.8450	 0.0620
G	 0.9060	 0.0620
H	 0.8850	 0.0570
I	 0.8820	 0.0580
J	 0.9230	 0.0510
K	 0.8750	 0.0540
L	 0.8960	 0.0610
M	 0.8870	 0.0550
P	 0.8930	 0.0860
Q	 0.8410	 0.0730
R	 0.9420	 0.0650
S	 0.7610	 0.0400
T	 0.8140	 0.0620
U	 0.7510	 0.0660
a	 0.8980	 0.0470
b	 0.8930	 0.0420
c	 0.9250	 0.0490
d	 0.9190	 0.0450
e	 0.9280	 0.0470
f	 0.9180	 0.0480
g	 0.9230	 0.0490
h	 0.9380	 0.0470
i	 0.9230	 0.0510
j	 0.9350	 0.0570
k	 0.9300	 0.0490
l	 0.9130	 0.0450
m	 0.9400	 0.0470
t	 0.8890	 0.0410

