



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 09:36 PM EST

PDB ID : 6V6S
EMDB ID : EMD-21073
Title : Structure of the native human gamma-tubulin ring complex
Authors : Wieczorek, M.; Urnavicius, L.; Ti, S.; Molloy, K.R.; Chait, B.T.; Kapoor, T.M.
Deposited on : 2019-12-05
Resolution : 4.30 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

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:

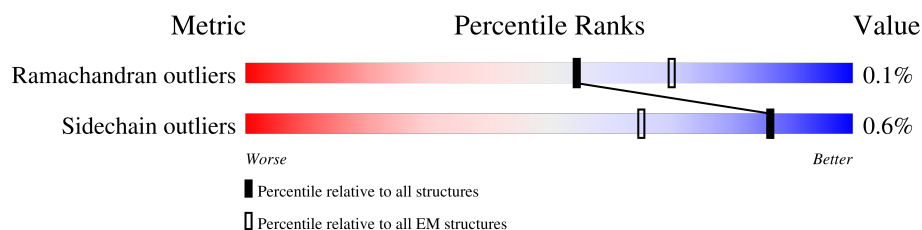
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.30 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)
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 ≥ 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	930	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	C	930	<div> <div>58%</div> <div>42%</div> </div>
1	E	930	<div> <div>58%</div> <div>42%</div> </div>
1	G	930	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
1	M	930	<div> <div>45%</div> <div>58%</div> <div>42%</div> </div>
2	B	907	<div> <div>63%</div> <div>37%</div> </div>
2	D	907	<div> <div>63%</div> <div>37%</div> </div>
2	F	907	<div> <div>63%</div> <div>37%</div> </div>
2	H	907	<div> <div>63%</div> <div>37%</div> </div>

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Mol	Chain	Length	Quality of chain
2	T	907	
3	I	667	
3	K	667	
4	J	1024	
5	L	1819	
6	N	50	
6	O	50	
6	Q	50	
6	R	50	
6	S	50	
7	U	374	
8	V	66	
8	Y	66	
9	W	165	
10	X	263	
11	a	451	
11	b	451	
11	c	451	
11	d	451	
11	e	451	
11	f	451	
11	g	451	
11	h	451	
11	i	451	
11	j	451	

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Mol	Chain	Length	Quality of chain		
11	k	451	<div><div></div><div></div><div></div></div>	23%	82% 18%
11	l	451	<div><div></div><div></div><div></div></div>	40%	82% 18%
11	m	451	<div><div></div><div></div><div></div></div>	78%	82% 18%
11	t	451	<div><div></div><div></div><div></div></div>	82%	82% 18%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 106422 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			

- 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		

- Molecule 6 is a protein called Unassigned poly-alanine chain ("staple").

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	35	Total	C	N	O	0	0
			175	105	35	35		
6	O	40	Total	C	N	O	0	0
			200	120	40	40		
6	Q	38	Total	C	N	O	0	0
			190	114	38	38		
6	R	39	Total	C	N	O	0	0
			195	117	39	39		
6	S	40	Total	C	N	O	0	0
			200	120	40	40		

- Molecule 7 is a protein called beta actin.

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

- Molecule 8 is a protein called Unassigned poly-alanine model ("CC").

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	62	Total	C	N	O	0	0
			310	186	62	62		
8	Y	57	Total	C	N	O	0	0
			285	171	57	57		

- Molecule 9 is a protein called Unassigned poly-alanine model ("HB").

Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	155	Total	C	N	O	0	0
			775	465	155	155		

- Molecule 10 is a protein called Unassigned poly-alanine model ("Lumenal bridge helical bundles").

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	254	Total	C	N	O	0	0
			1270	762	254	254		

- Molecule 11 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	b	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	c	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	d	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	e	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	f	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	g	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	h	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	i	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	j	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	k	370	Total	C	N	O	S	0	0
			2955	1875	518	548	14		
11	l	370	Total	C	N	O	S	0	0
			2955	1875	518	548	14		
11	m	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	t	370	Total	C	N	O		0	0
			1830	1090	370	370			

There are 28 discrepancies between the modelled and reference sequences:

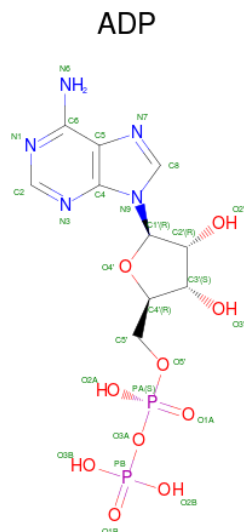
Chain	Residue	Modelled	Actual	Comment	Reference
a	35	ALA	GLY	conflict	UNP P23258
a	202	LEU	VAL	conflict	UNP P23258
b	35	ALA	GLY	conflict	UNP P23258

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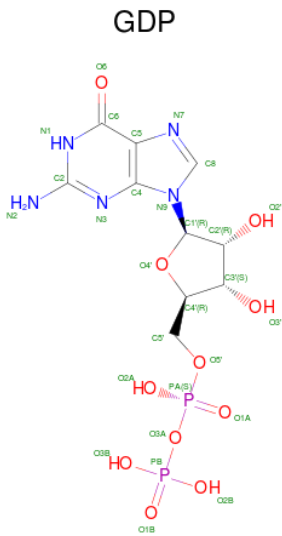
Chain	Residue	Modelled	Actual	Comment	Reference
b	202	LEU	VAL	conflict	UNP P23258
c	35	ALA	GLY	conflict	UNP P23258
c	202	LEU	VAL	conflict	UNP P23258
d	35	ALA	GLY	conflict	UNP P23258
d	202	LEU	VAL	conflict	UNP P23258
e	35	ALA	GLY	conflict	UNP P23258
e	202	LEU	VAL	conflict	UNP P23258
f	35	ALA	GLY	conflict	UNP P23258
f	202	LEU	VAL	conflict	UNP P23258
g	35	ALA	GLY	conflict	UNP P23258
g	202	LEU	VAL	conflict	UNP P23258
h	35	ALA	GLY	conflict	UNP P23258
h	202	LEU	VAL	conflict	UNP P23258
i	35	ALA	GLY	conflict	UNP P23258
i	202	LEU	VAL	conflict	UNP P23258
j	35	ALA	GLY	conflict	UNP P23258
j	202	LEU	VAL	conflict	UNP P23258
k	35	ALA	GLY	conflict	UNP P23258
k	202	LEU	VAL	conflict	UNP P23258
l	35	ALA	GLY	conflict	UNP P23258
l	202	LEU	VAL	conflict	UNP P23258
m	35	ALA	GLY	conflict	UNP P23258
m	202	LEU	VAL	conflict	UNP P23258
t	35	ALA	GLY	conflict	UNP P23258
t	202	LEU	VAL	conflict	UNP P23258

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 13 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 28	C 10	N 5	O 11	P 2	0
13	b	1	Total 28	C 10	N 5	O 11	P 2	0

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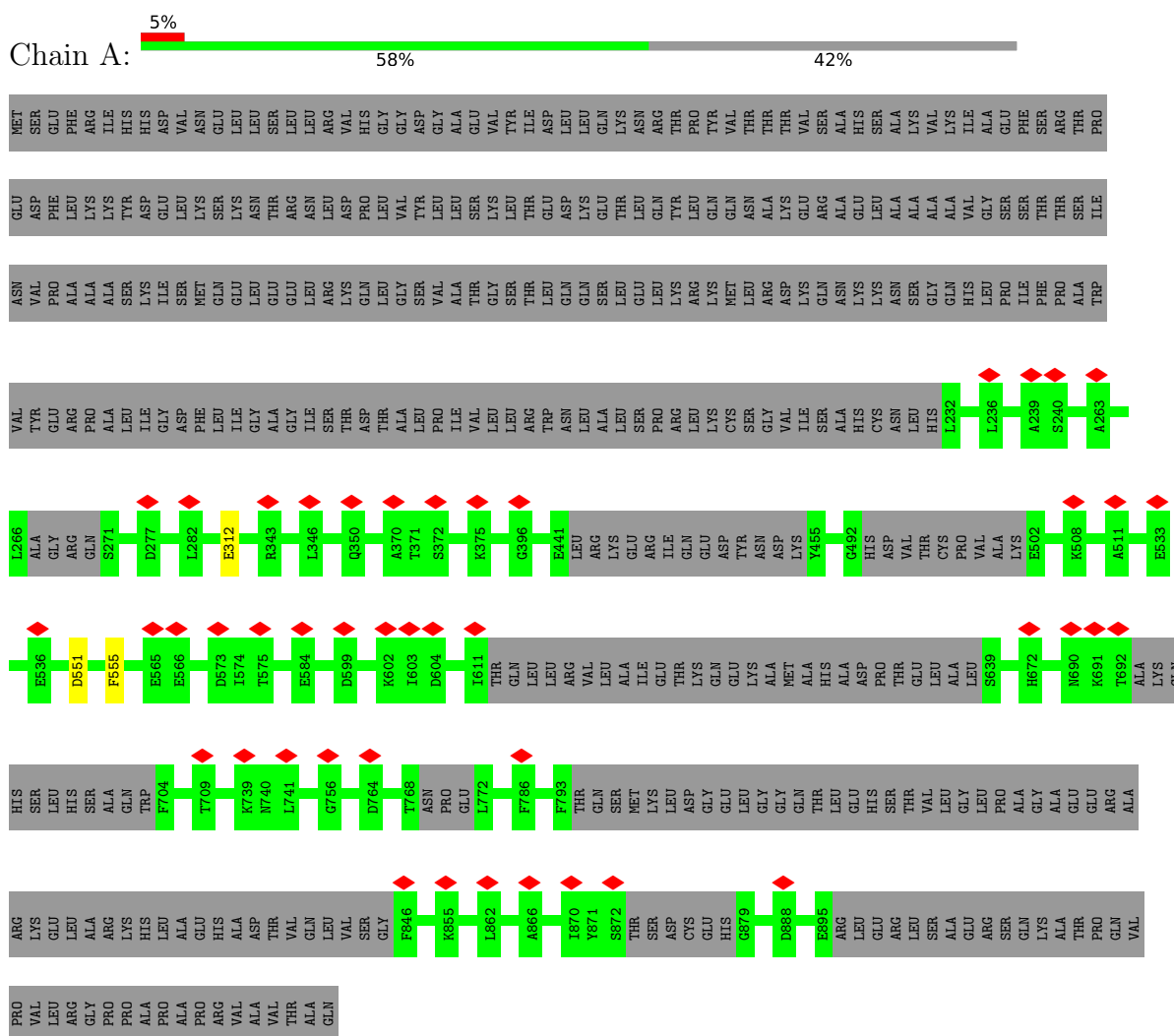
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Mol	Chain	Residues	Atoms					AltConf
13	c	1	Total 28	C 10	N 5	O 11	P 2	0
13	d	1	Total 28	C 10	N 5	O 11	P 2	0
13	e	1	Total 28	C 10	N 5	O 11	P 2	0
13	f	1	Total 28	C 10	N 5	O 11	P 2	0
13	g	1	Total 28	C 10	N 5	O 11	P 2	0
13	h	1	Total 28	C 10	N 5	O 11	P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

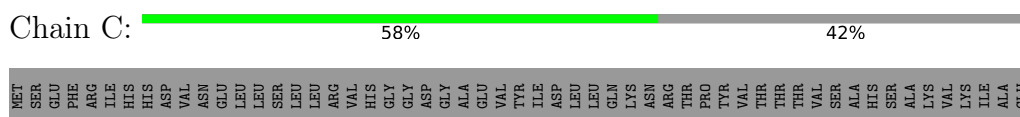
3 Residue-property plots

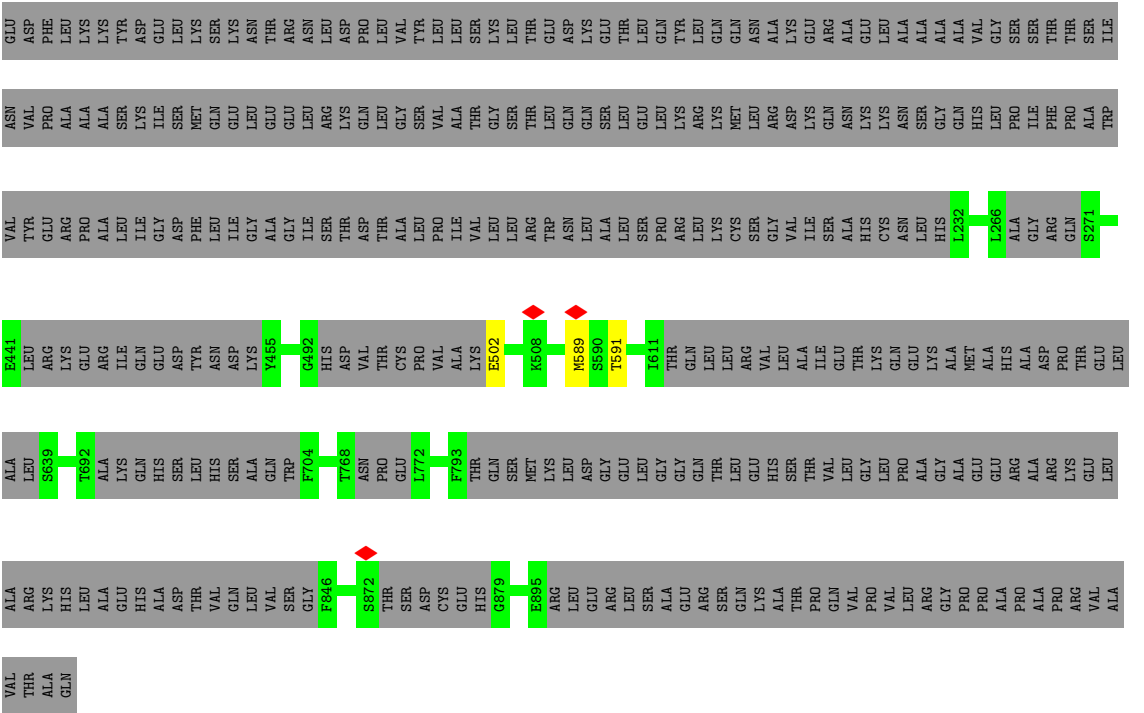
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

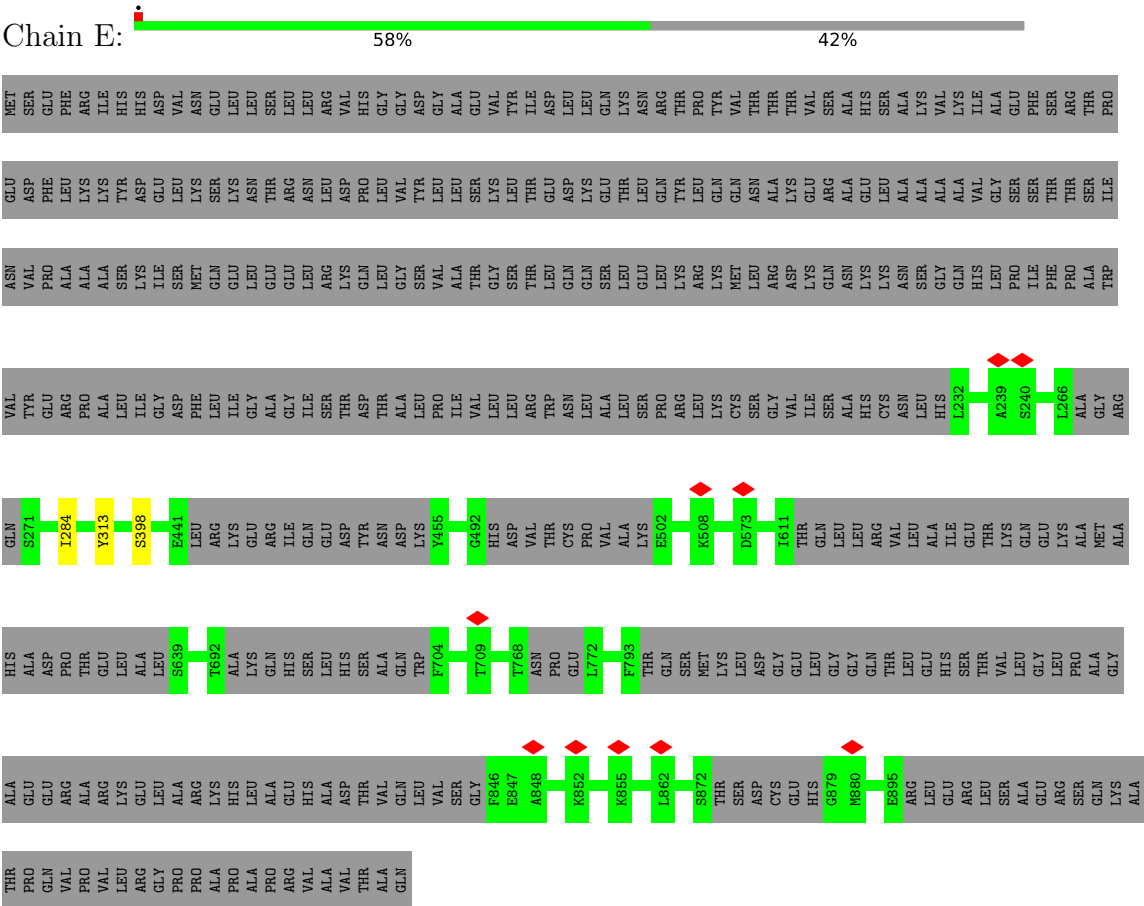


- Molecule 1: Gamma-tubulin complex component 2

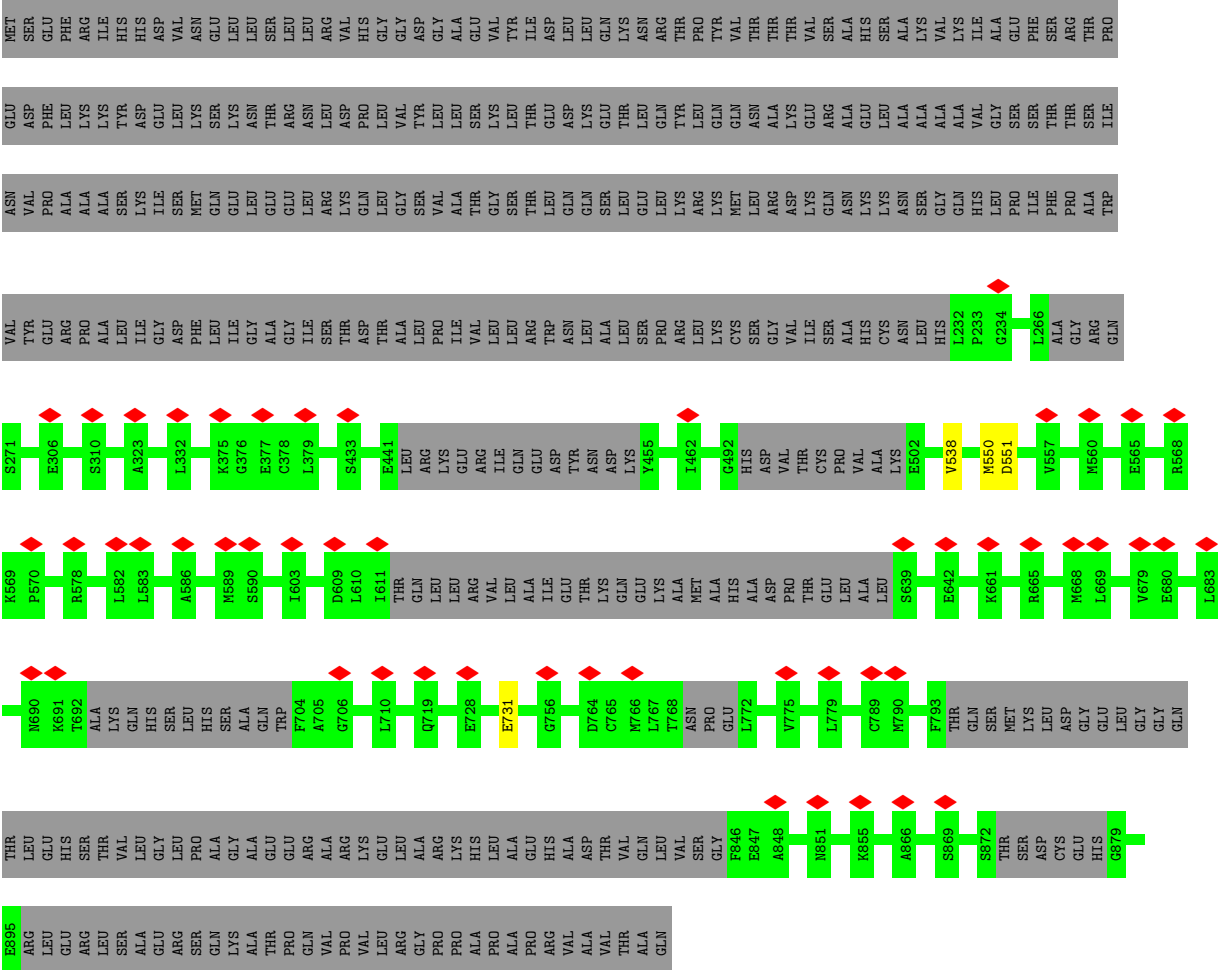




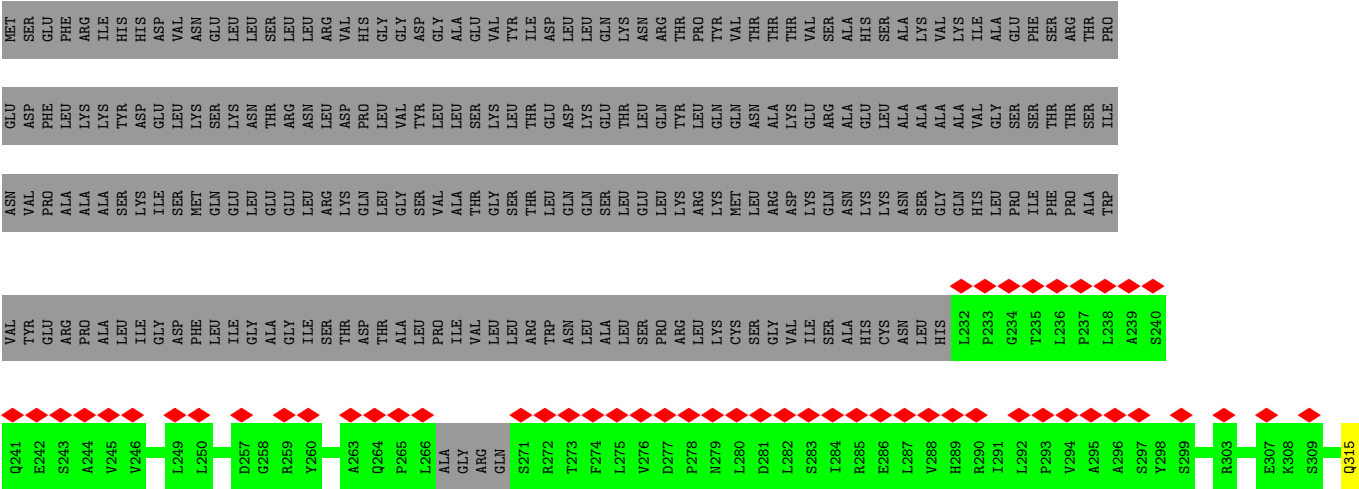
● Molecule 1: Gamma-tubulin complex component 2

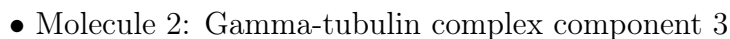


● Molecule 1: Gamma-tubulin complex component 2



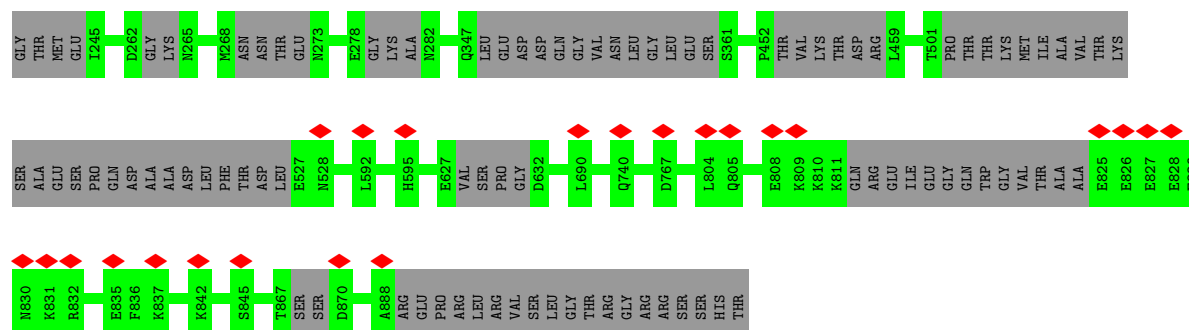
● Molecule 1: Gamma-tubulin complex component 2





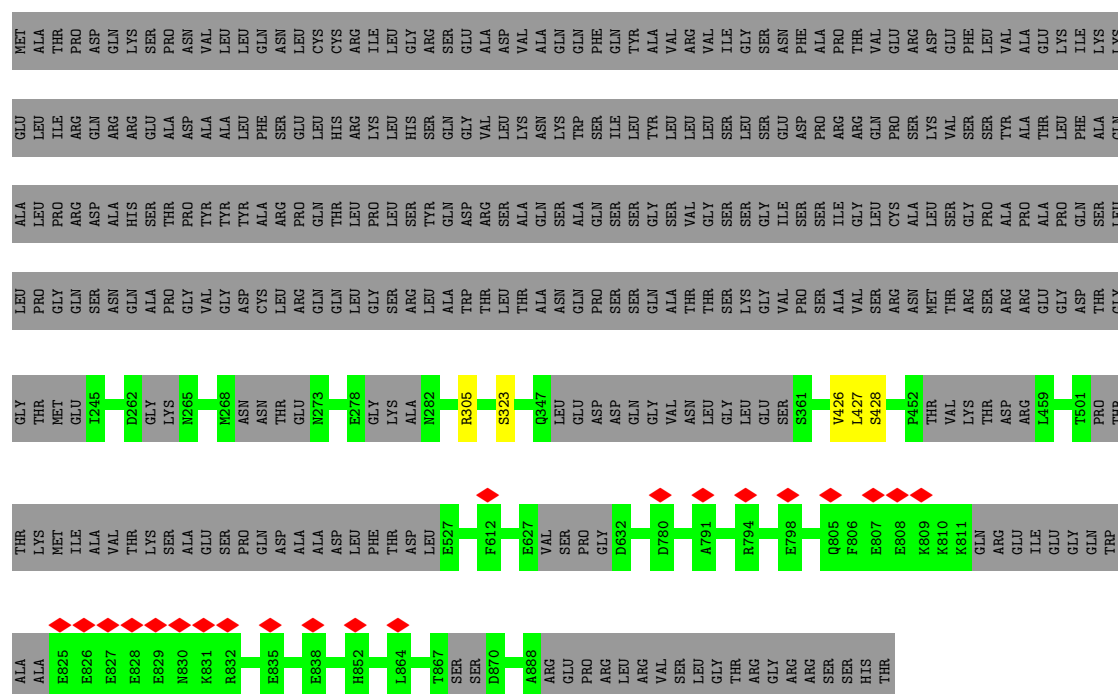
Frequency	Percentage
Often	63%
Sometimes	37%

[illegible]



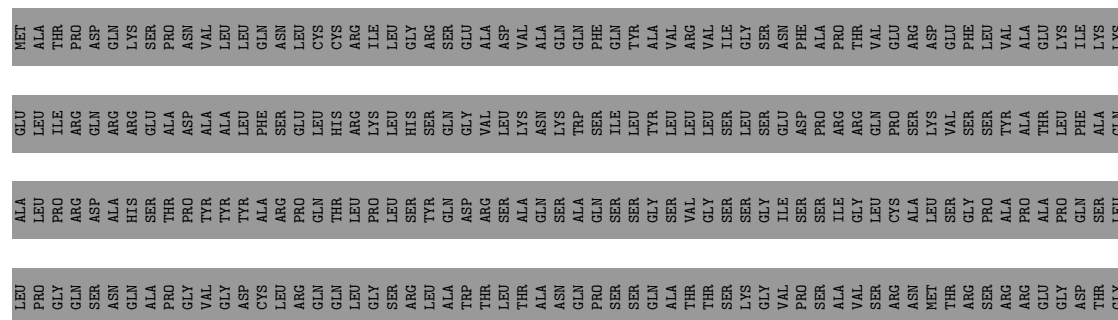
• Molecule 2: Gamma-tubulin complex component 3

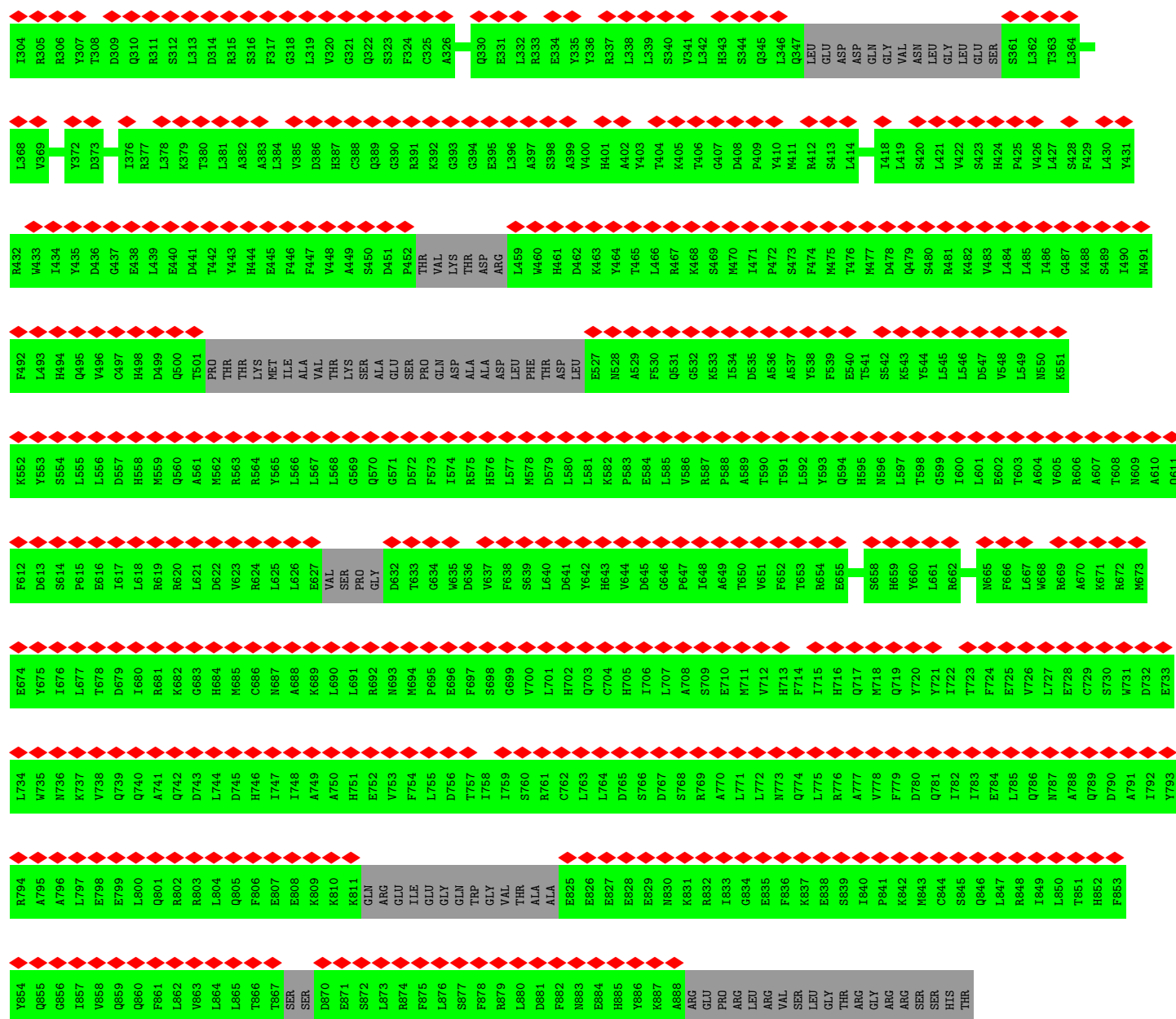
Chain D: 63% 37%



• Molecule 2: Gamma-tubulin complex component 3

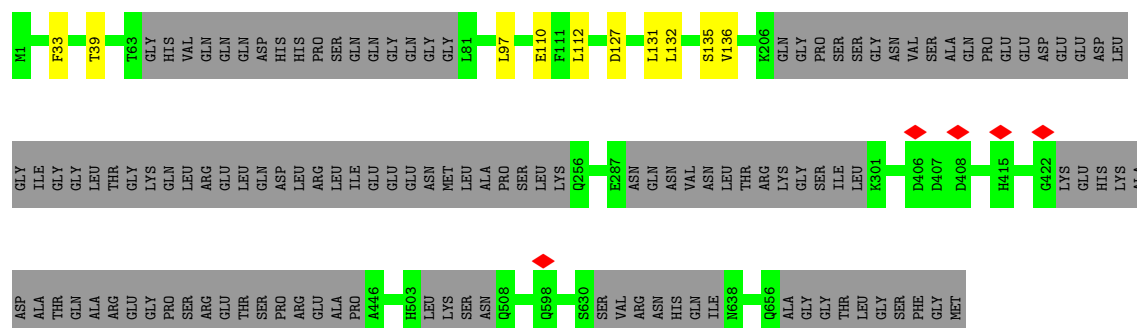
Chain F: 63% 37%





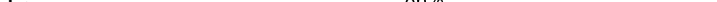
• Molecule 3: Gamma-tubulin complex component 4

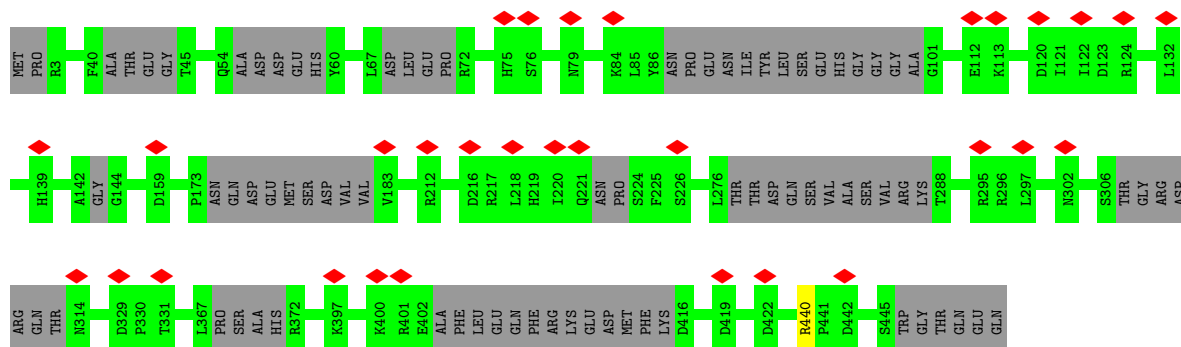
Chain I: 80% 19%



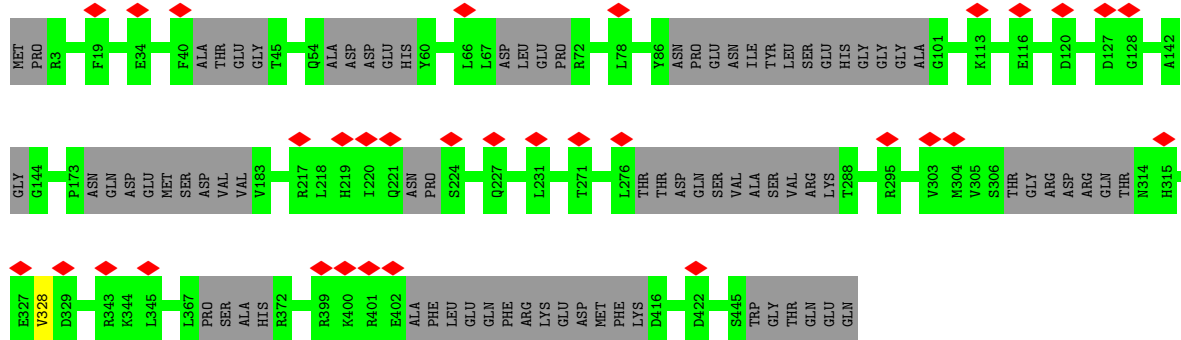
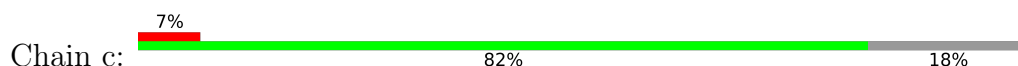
Chain K:



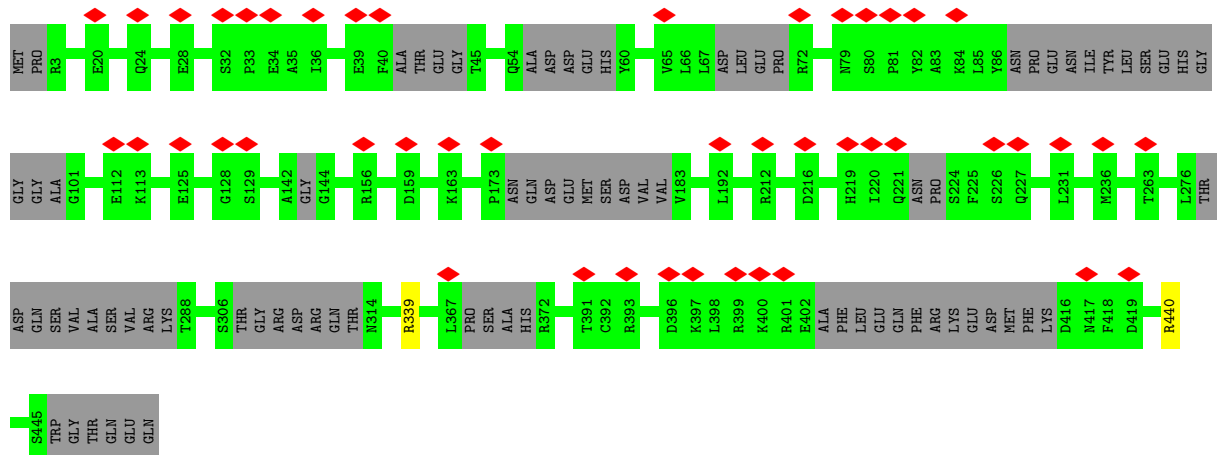
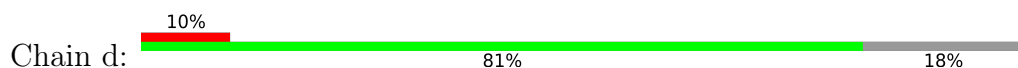
- Chain Y:  86% 14%



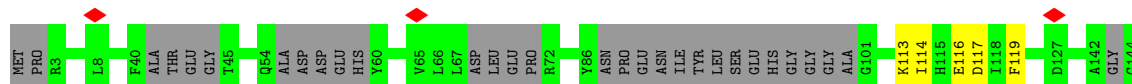
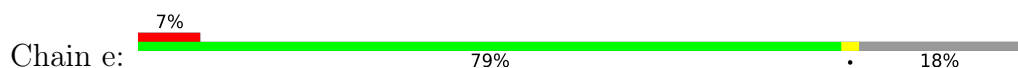
• Molecule 11: Tubulin gamma-1 chain

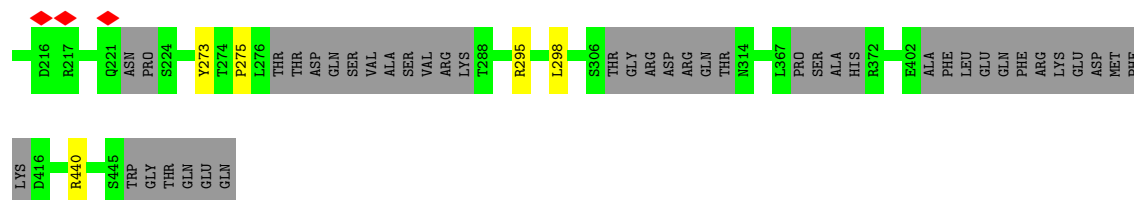


• Molecule 11: Tubulin gamma-1 chain



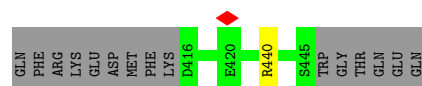
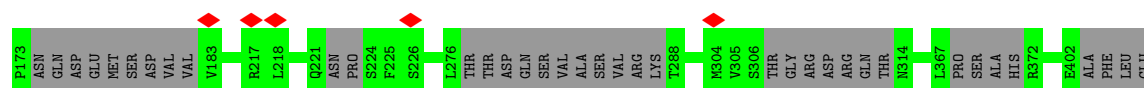
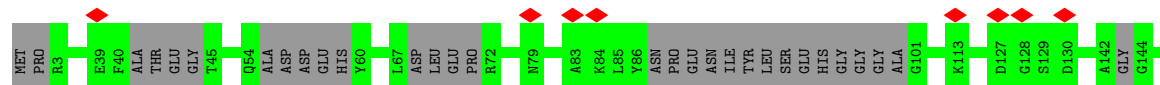
• Molecule 11: Tubulin gamma-1 chain





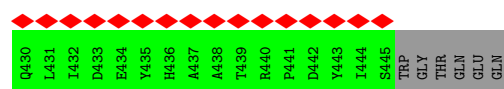
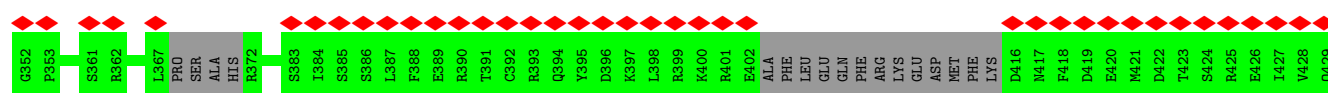
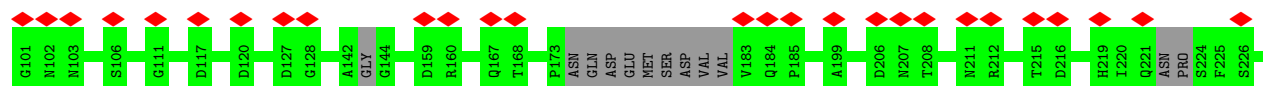
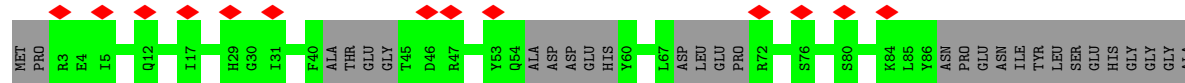
• Molecule 11: Tubulin gamma-1 chain

Chain i: 82% 18%



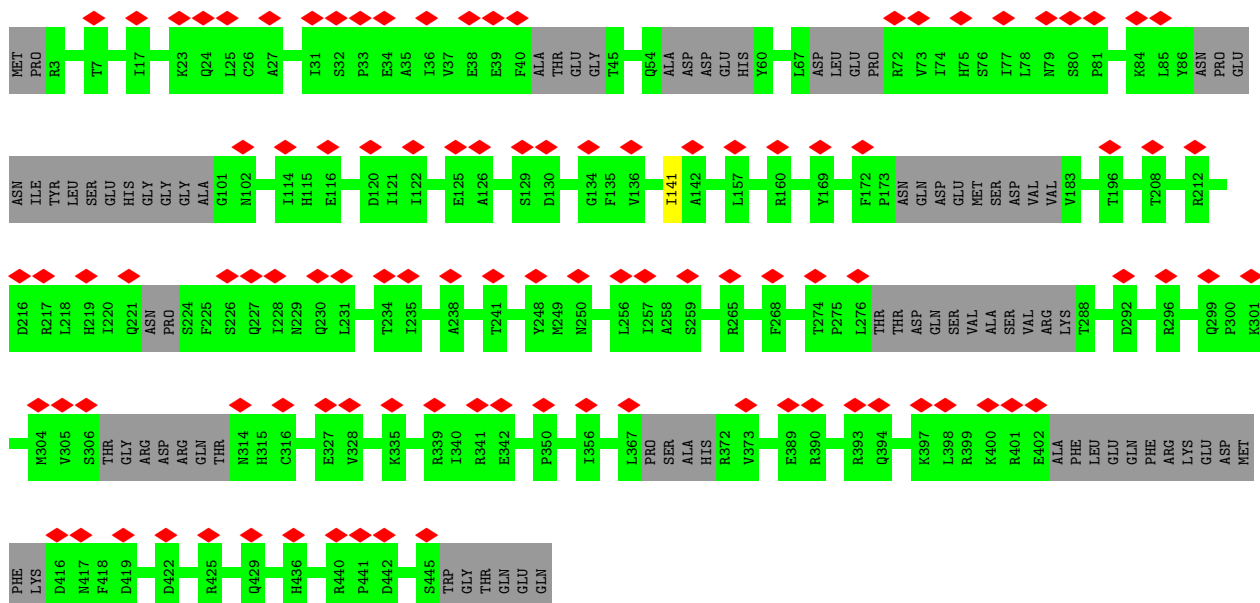
• Molecule 11: Tubulin gamma-1 chain

Chain j: 27% 82% 18%

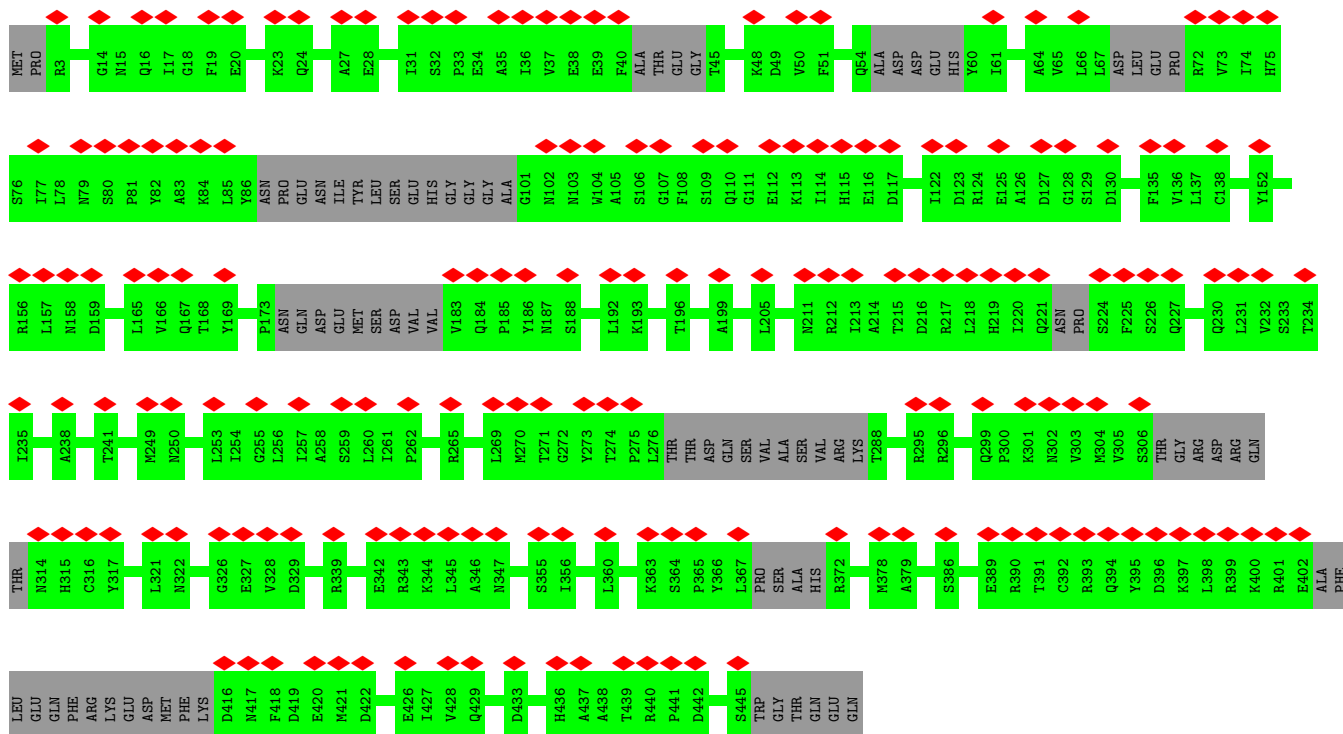
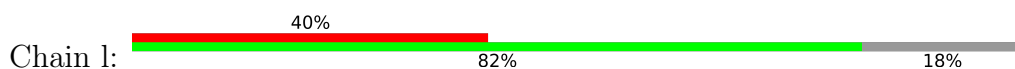


• Molecule 11: Tubulin gamma-1 chain

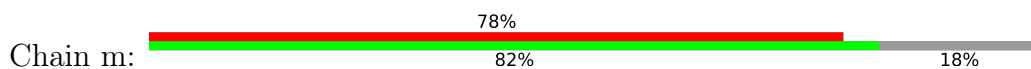
Chain k: 23% 82% 18%



• Molecule 11: Tubulin gamma-1 chain



• Molecule 11: Tubulin gamma-1 chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103172	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 ($e^-/\text{\AA}^2$)	45	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	0.135	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	491.28003, 491.28003, 491.28003	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.335, 1.335, 1.335	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, ADP

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	0/4461	0.43	0/6020
1	C	0.37	0/4461	0.44	0/6020
1	E	0.37	0/4461	0.45	0/6020
1	G	0.37	0/4461	0.45	0/6020
1	M	0.35	0/4461	0.44	0/6020
2	B	0.33	0/4839	0.43	0/6522
2	D	0.36	0/4839	0.43	0/6522
2	F	0.35	0/4839	0.43	0/6522
2	H	0.36	0/4839	0.44	0/6522
2	T	0.27	0/2830	0.41	0/3934
3	I	0.32	0/4479	0.42	0/6073
3	K	0.27	0/4479	0.40	0/6073
4	J	0.31	0/4050	0.41	0/5466
5	L	0.28	0/4102	0.40	0/5545
7	U	0.24	0/1793	0.59	0/2492
11	a	0.33	0/3001	0.44	0/4052
11	b	0.29	0/3001	0.42	0/4052
11	c	0.28	0/3001	0.40	0/4052
11	d	0.30	0/3001	0.42	0/4052
11	e	0.35	0/3001	0.44	0/4052
11	f	0.29	0/3001	0.42	0/4052
11	g	0.32	0/3001	0.42	0/4052
11	h	0.33	0/3001	0.43	0/4052
11	i	0.29	0/3001	0.42	0/4052
11	j	0.25	0/3001	0.40	0/4052
11	k	0.30	0/3006	0.43	0/4060
11	l	0.27	0/3006	0.42	0/4060
11	m	0.27	0/3001	0.40	0/4052
11	t	0.26	0/1819	0.42	0/2517
All	All	0.32	0/104236	0.43	0/140980

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](#)

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	521/930 (56%)	483 (93%)	37 (7%)	1 (0%)	47	81
1	C	521/930 (56%)	488 (94%)	32 (6%)	1 (0%)	47	81
1	E	521/930 (56%)	483 (93%)	36 (7%)	2 (0%)	34	72
1	G	521/930 (56%)	487 (94%)	34 (6%)	0	100	100
1	M	521/930 (56%)	485 (93%)	35 (7%)	1 (0%)	47	81
2	B	552/907 (61%)	530 (96%)	22 (4%)	0	100	100
2	D	552/907 (61%)	532 (96%)	20 (4%)	0	100	100
2	F	552/907 (61%)	531 (96%)	21 (4%)	0	100	100
2	H	552/907 (61%)	532 (96%)	20 (4%)	0	100	100
2	T	552/907 (61%)	531 (96%)	21 (4%)	0	100	100
3	I	531/667 (80%)	497 (94%)	32 (6%)	2 (0%)	34	72
3	K	531/667 (80%)	508 (96%)	22 (4%)	1 (0%)	47	81
4	J	456/1024 (44%)	435 (95%)	20 (4%)	1 (0%)	47	81
5	L	471/1819 (26%)	438 (93%)	33 (7%)	0	100	100
7	U	360/374 (96%)	352 (98%)	8 (2%)	0	100	100
11	a	345/451 (76%)	328 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	b	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
11	c	345/451 (76%)	332 (96%)	13 (4%)	0	100	100
11	d	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
11	e	345/451 (76%)	326 (94%)	18 (5%)	1 (0%)	41	76
11	f	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
11	g	345/451 (76%)	330 (96%)	15 (4%)	0	100	100
11	h	345/451 (76%)	325 (94%)	19 (6%)	1 (0%)	41	76
11	i	345/451 (76%)	330 (96%)	15 (4%)	0	100	100
11	j	345/451 (76%)	329 (95%)	16 (5%)	0	100	100
11	k	348/451 (77%)	329 (94%)	19 (6%)	0	100	100
11	l	348/451 (77%)	329 (94%)	19 (6%)	0	100	100
11	m	345/451 (76%)	332 (96%)	13 (4%)	0	100	100
11	t	348/451 (77%)	332 (95%)	16 (5%)	0	100	100
All	All	12553/20050 (63%)	11915 (95%)	627 (5%)	11 (0%)	54	85

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	127	ASP
4	J	715	ARG
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	481/816 (59%)	479 (100%)	2 (0%)	91	94
1	C	481/816 (59%)	479 (100%)	2 (0%)	91	94
1	E	481/816 (59%)	480 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	481/816 (59%)	477 (99%)	4 (1%)	81	89
1	M	481/816 (59%)	480 (100%)	1 (0%)	93	96
2	B	519/798 (65%)	519 (100%)	0	100	100
2	D	519/798 (65%)	514 (99%)	5 (1%)	76	86
2	F	519/798 (65%)	516 (99%)	3 (1%)	86	92
2	H	519/798 (65%)	517 (100%)	2 (0%)	91	94
3	I	474/594 (80%)	466 (98%)	8 (2%)	60	78
3	K	474/594 (80%)	469 (99%)	5 (1%)	73	85
4	J	445/933 (48%)	445 (100%)	0	100	100
5	L	436/1546 (28%)	436 (100%)	0	100	100
11	a	328/400 (82%)	323 (98%)	5 (2%)	65	80
11	b	328/400 (82%)	327 (100%)	1 (0%)	92	95
11	c	328/400 (82%)	327 (100%)	1 (0%)	92	95
11	d	328/400 (82%)	326 (99%)	2 (1%)	86	92
11	e	328/400 (82%)	318 (97%)	10 (3%)	41	64
11	f	328/400 (82%)	327 (100%)	1 (0%)	92	95
11	g	328/400 (82%)	327 (100%)	1 (0%)	92	95
11	h	328/400 (82%)	324 (99%)	4 (1%)	71	84
11	i	328/400 (82%)	327 (100%)	1 (0%)	92	95
11	j	328/400 (82%)	328 (100%)	0	100	100
11	k	328/400 (82%)	327 (100%)	1 (0%)	92	95
11	l	328/400 (82%)	328 (100%)	0	100	100
11	m	328/400 (82%)	328 (100%)	0	100	100
All	All	10574/16139 (66%)	10514 (99%)	60 (1%)	86	92

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	39	THR
11	h	295	ARG
11	a	252	ASP
11	h	273	TYR
11	k	141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 201 such sidechains are listed below:

Mol	Chain	Res	Type
11	a	381	HIS
11	e	430	GLN
11	m	381	HIS
11	b	322	ASN
11	c	325	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](#)

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	$\# Z > 2$
13	GDP	h	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
13	GDP	g	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	4 (13%)
13	GDP	t	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
13	GDP	m	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.38	4 (13%)
13	GDP	f	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
13	GDP	l	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GDP	e	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.38	4 (13%)
13	GDP	j	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
13	GDP	k	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
13	GDP	c	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	4 (13%)
13	GDP	a	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.38	4 (13%)
13	GDP	b	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
13	GDP	i	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
13	GDP	d	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
12	ADP	U	800	-	24,29,29	0.69	0	29,45,45	0.84	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GDP	h	501	-	-	2/12/32/32	0/3/3/3
13	GDP	g	501	-	-	1/12/32/32	0/3/3/3
13	GDP	t	501	-	-	2/12/32/32	0/3/3/3
13	GDP	m	501	-	-	1/12/32/32	0/3/3/3
13	GDP	f	501	-	-	2/12/32/32	0/3/3/3
13	GDP	l	501	-	-	1/12/32/32	0/3/3/3
13	GDP	e	501	-	-	0/12/32/32	0/3/3/3
13	GDP	j	501	-	-	1/12/32/32	0/3/3/3
13	GDP	k	501	-	-	1/12/32/32	0/3/3/3
13	GDP	c	501	-	-	1/12/32/32	0/3/3/3
13	GDP	a	501	-	-	1/12/32/32	0/3/3/3
13	GDP	b	501	-	-	2/12/32/32	0/3/3/3
13	GDP	i	501	-	-	1/12/32/32	0/3/3/3
13	GDP	d	501	-	-	2/12/32/32	0/3/3/3
12	ADP	U	800	-	-	0/12/32/32	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)
13	e	501	GDP	C6-N1	-2.68	1.33	1.37
13	a	501	GDP	C6-N1	-2.65	1.33	1.37
13	g	501	GDP	C6-N1	-2.63	1.34	1.37
13	m	501	GDP	C6-N1	-2.61	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	501	GDP	C6-N1	-2.61	1.34	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	501	GDP	PA-O3A-PB	-4.22	118.34	132.83
13	a	501	GDP	PA-O3A-PB	-4.22	118.34	132.83
13	i	501	GDP	PA-O3A-PB	-4.06	118.90	132.83
13	c	501	GDP	PA-O3A-PB	-4.02	119.04	132.83
13	j	501	GDP	PA-O3A-PB	-4.01	119.06	132.83

There are no chirality outliers.

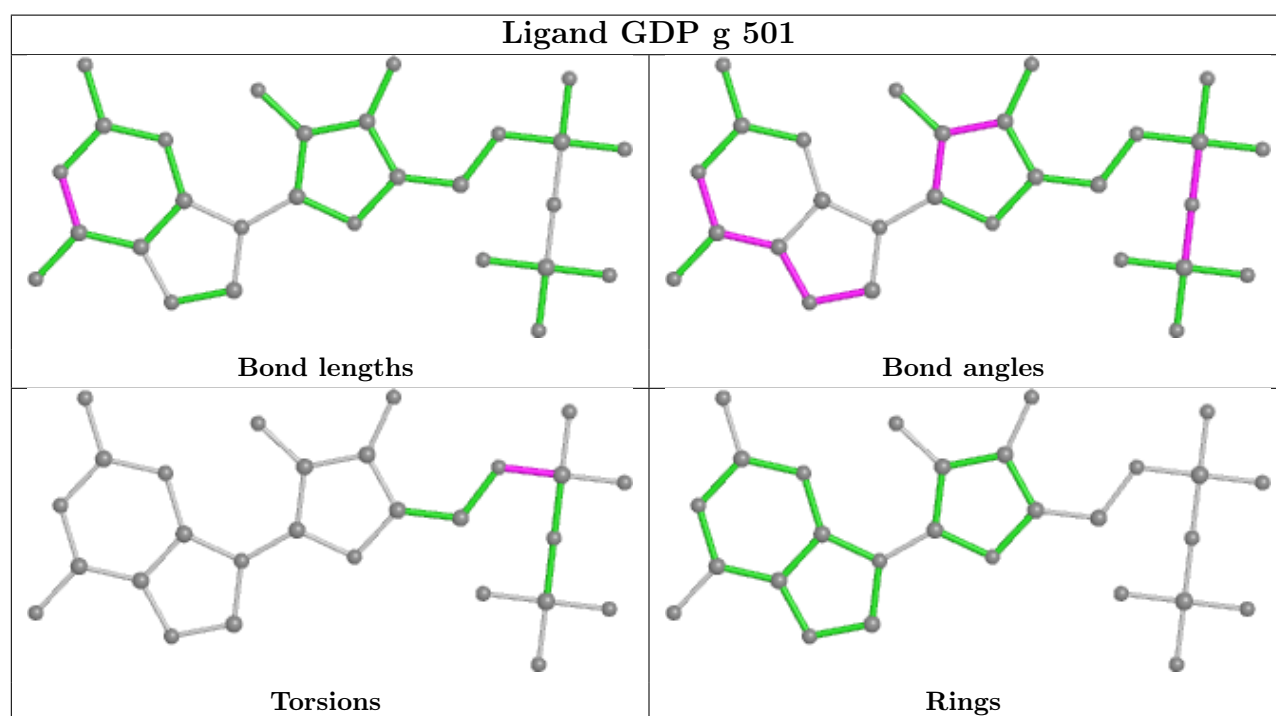
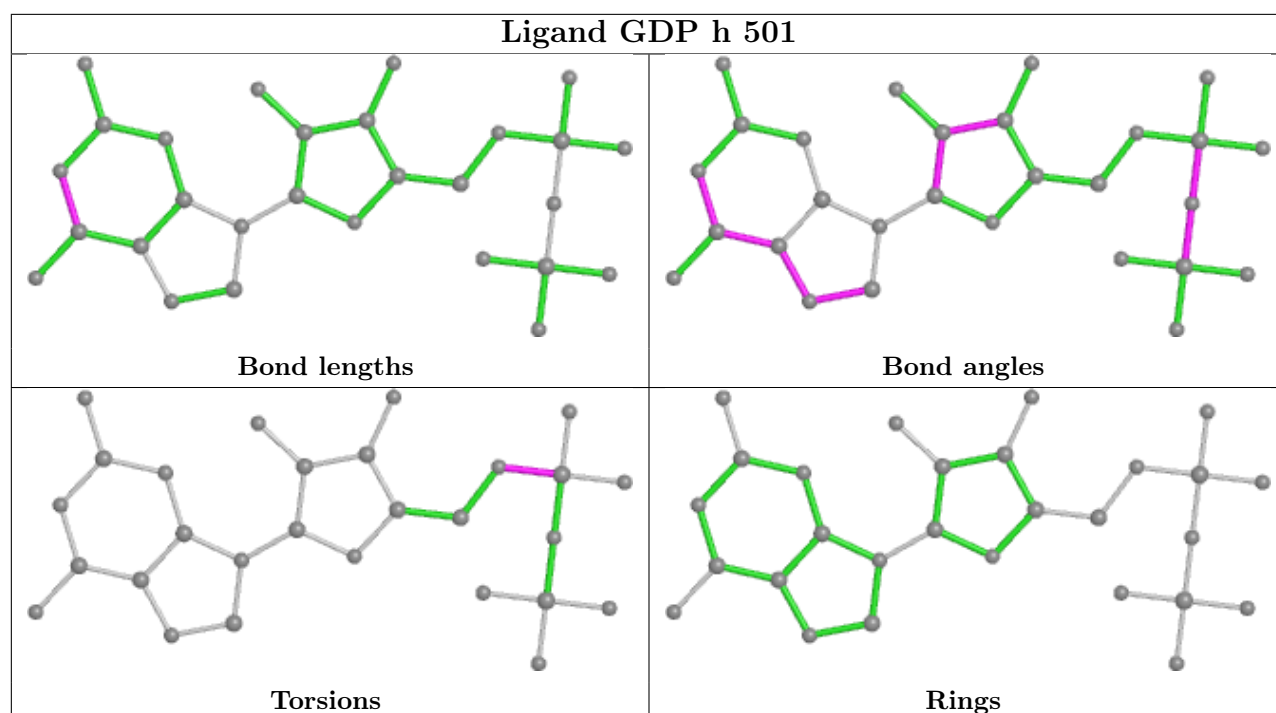
5 of 18 torsion outliers are listed below:

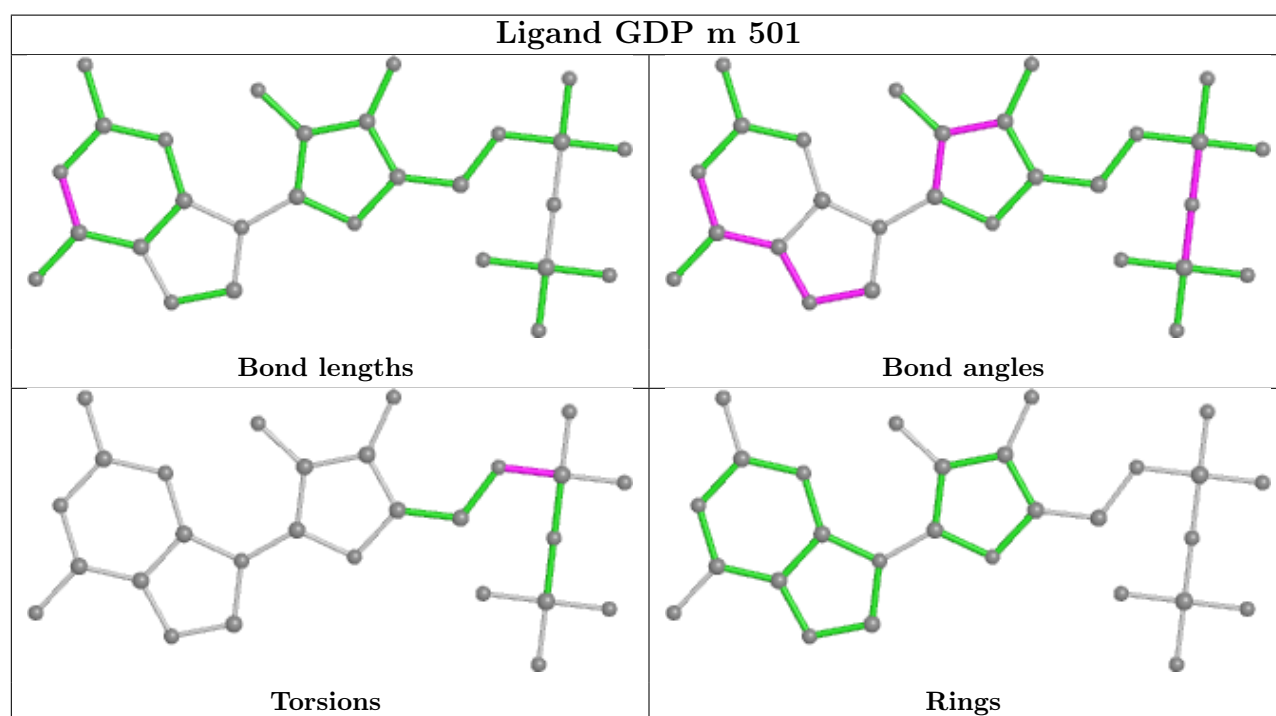
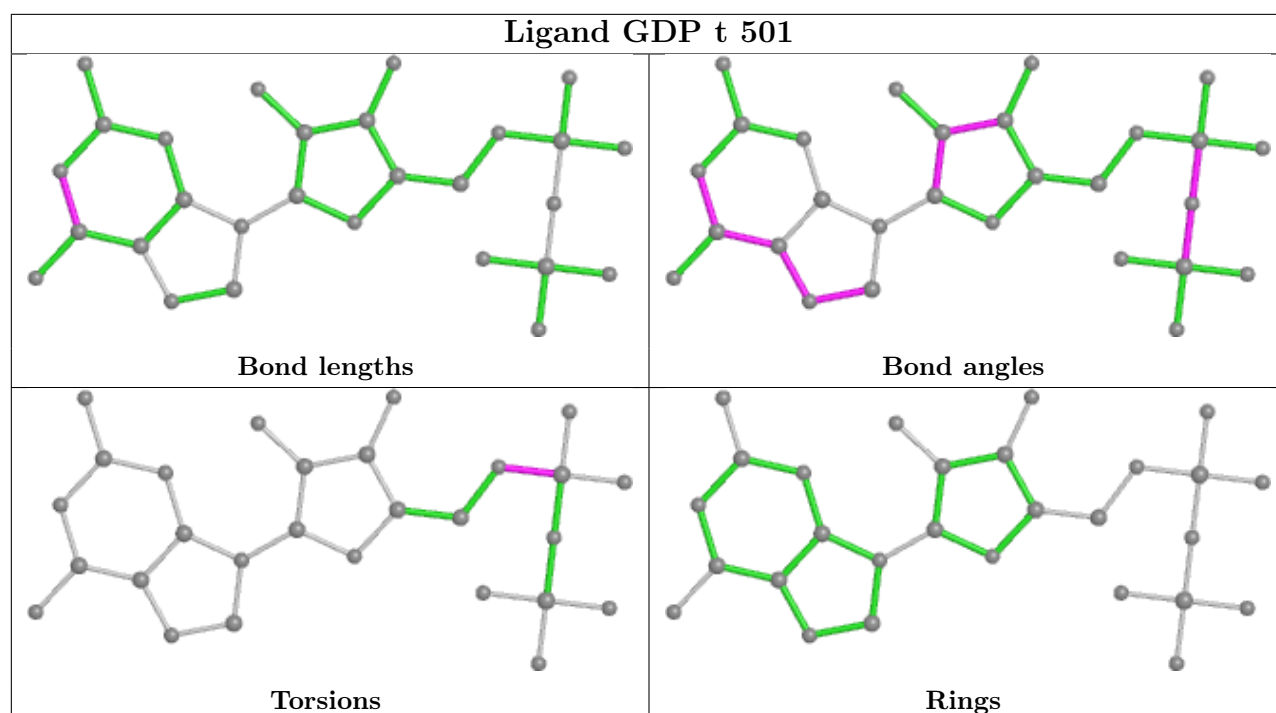
Mol	Chain	Res	Type	Atoms
13	b	501	GDP	C5'-O5'-PA-O1A
13	d	501	GDP	C5'-O5'-PA-O1A
13	f	501	GDP	C5'-O5'-PA-O1A
13	h	501	GDP	C5'-O5'-PA-O1A
13	k	501	GDP	C5'-O5'-PA-O1A

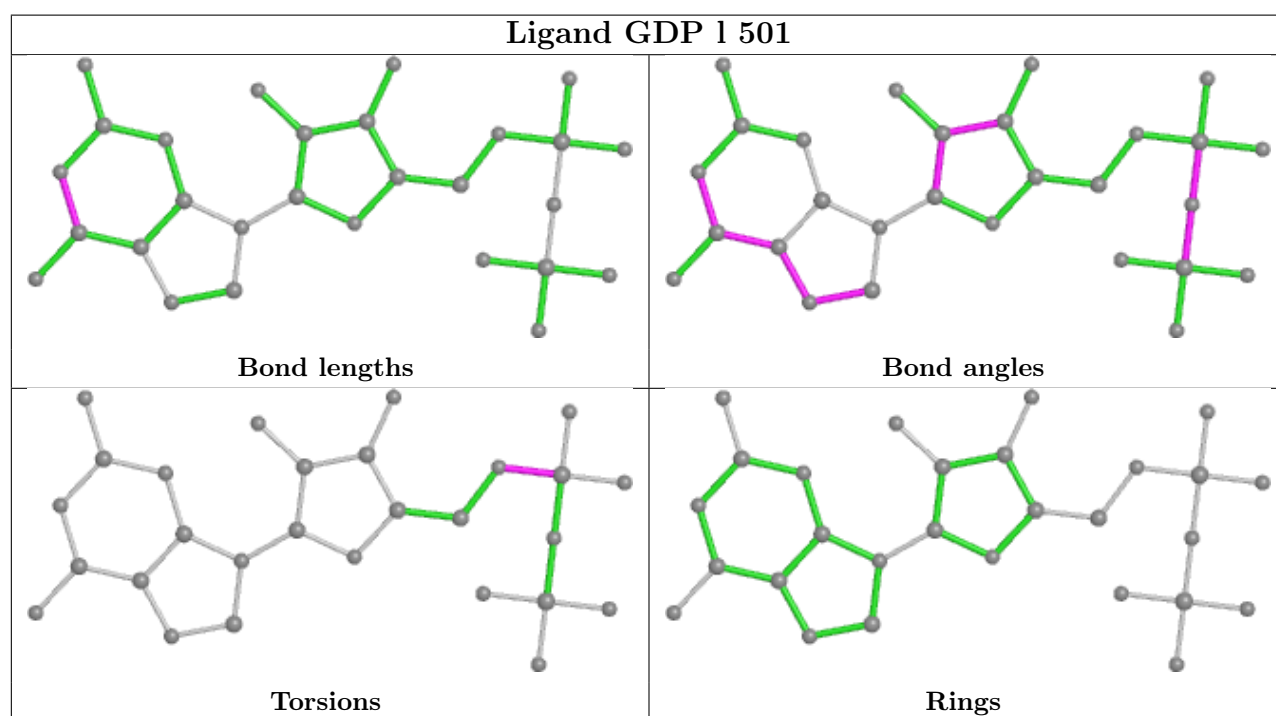
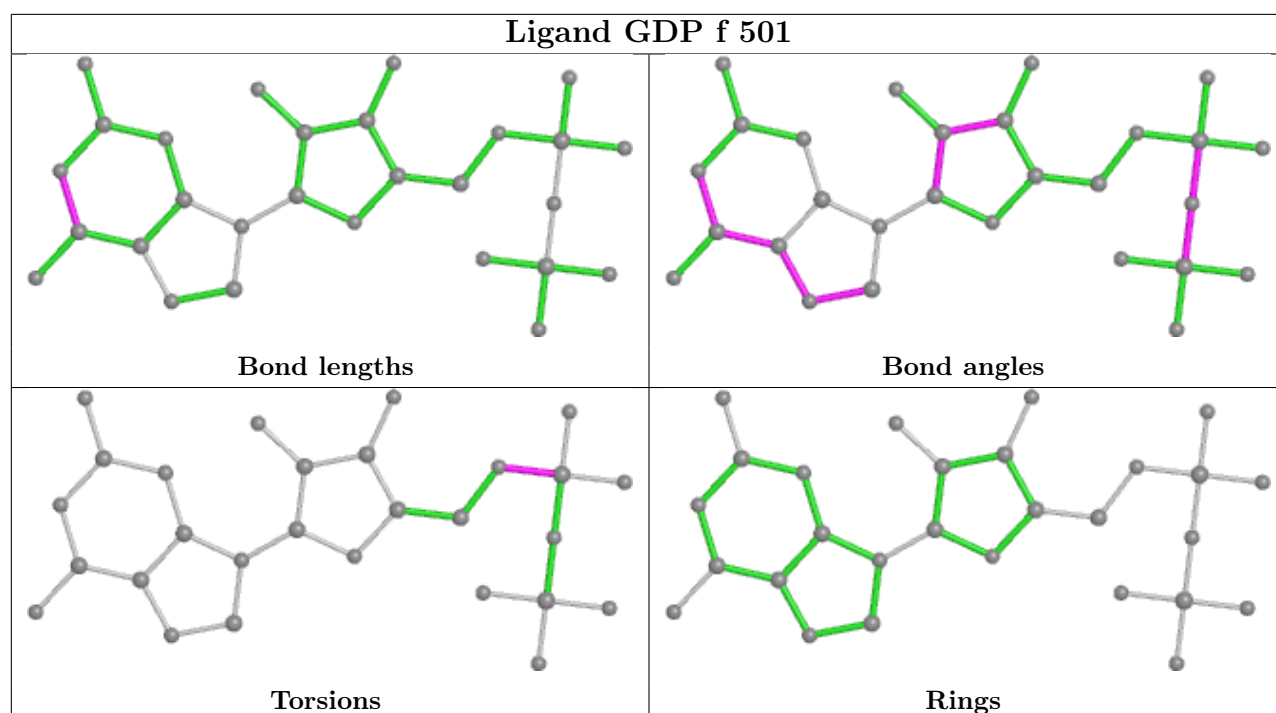
There are no ring outliers.

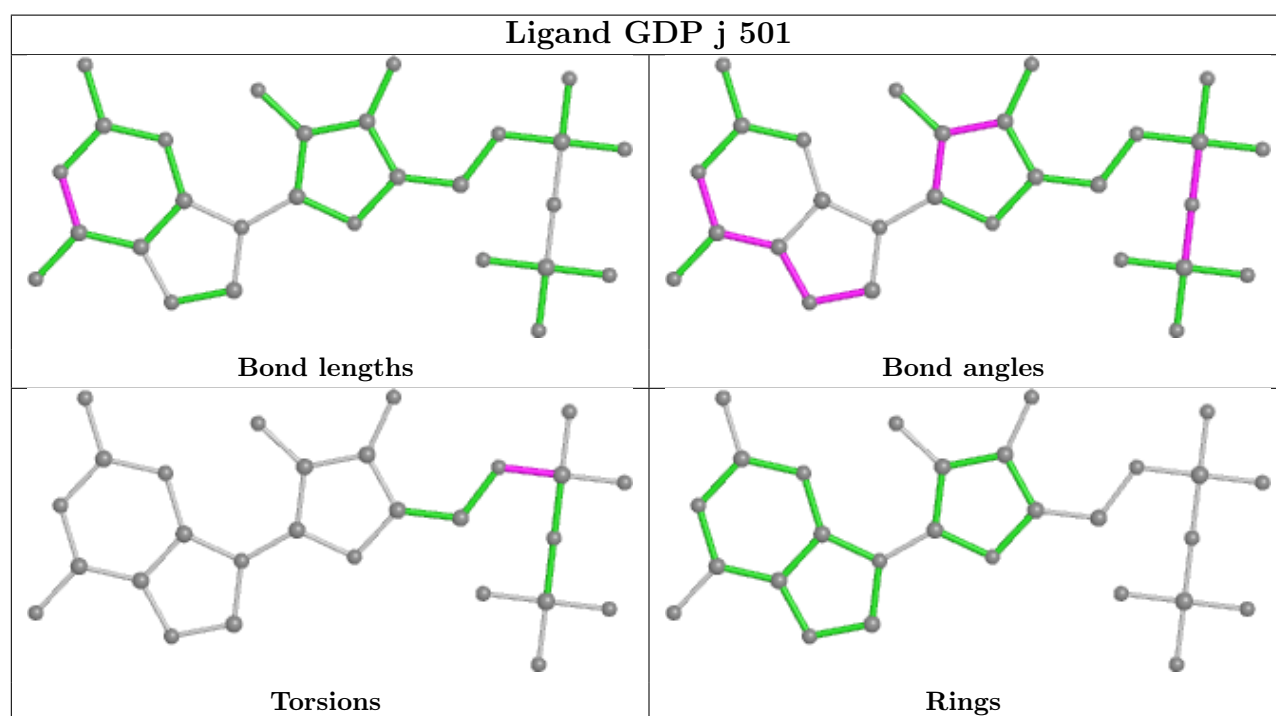
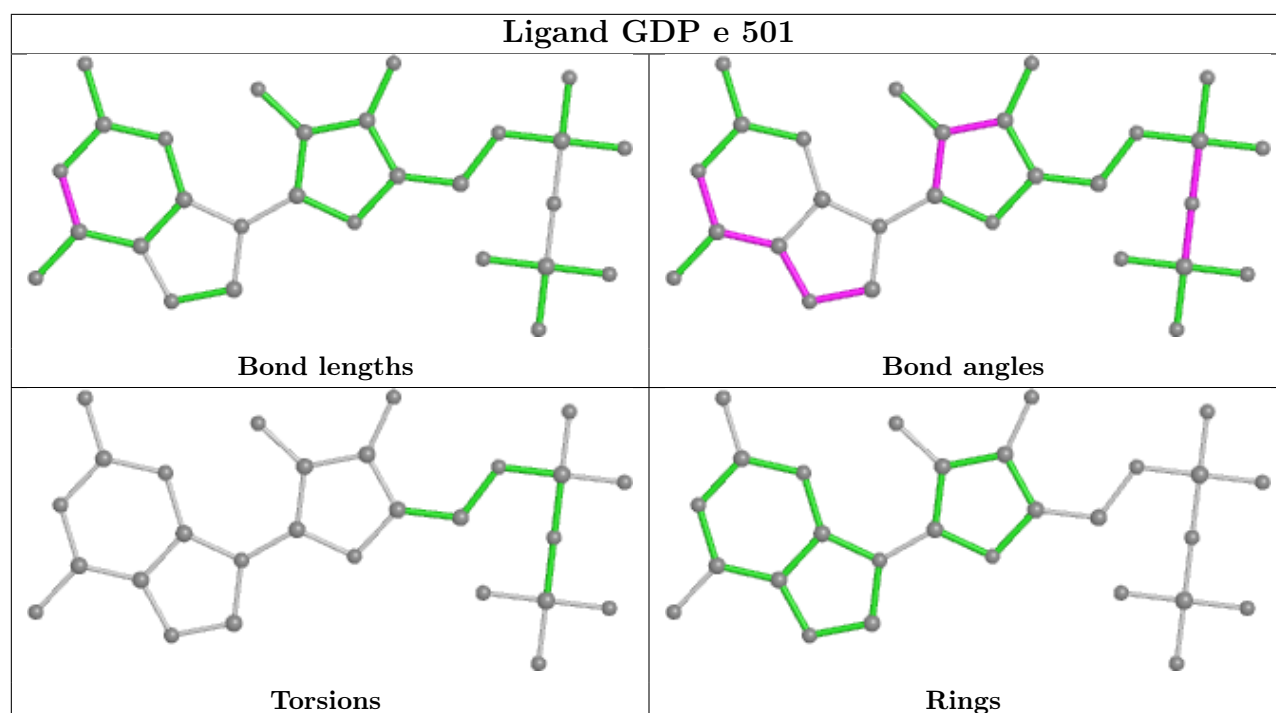
No monomer is involved in short contacts.

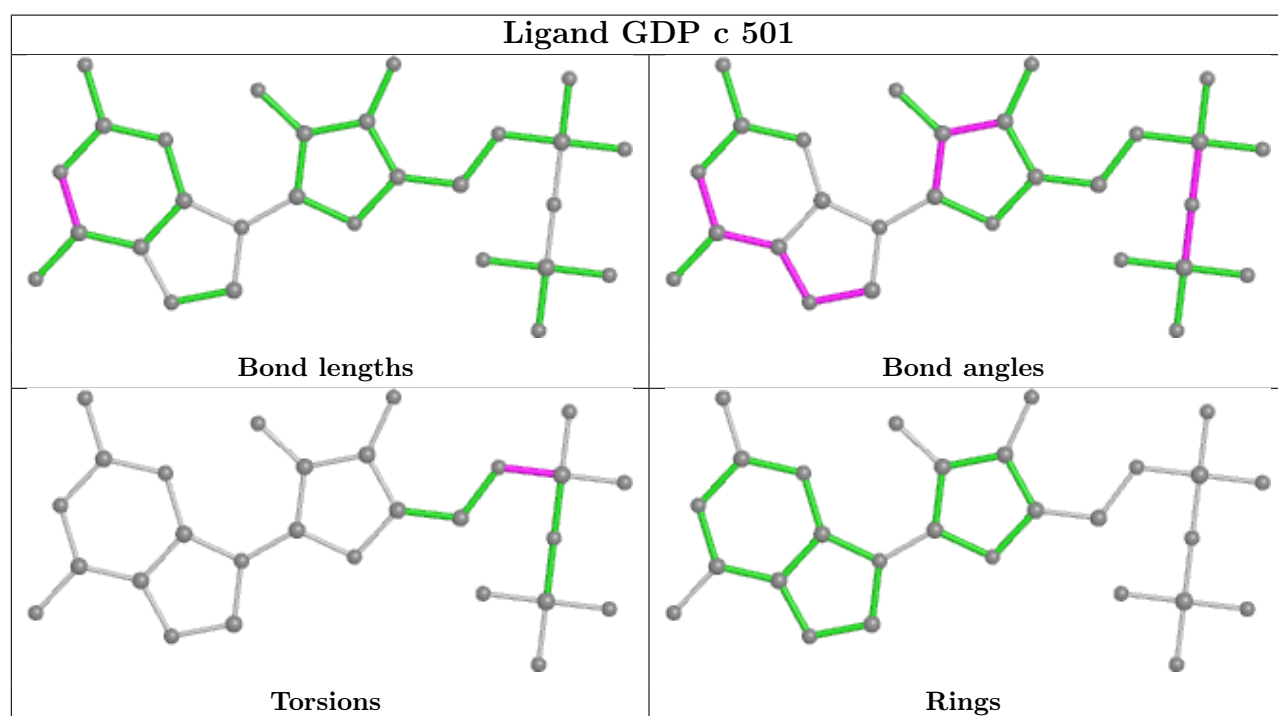
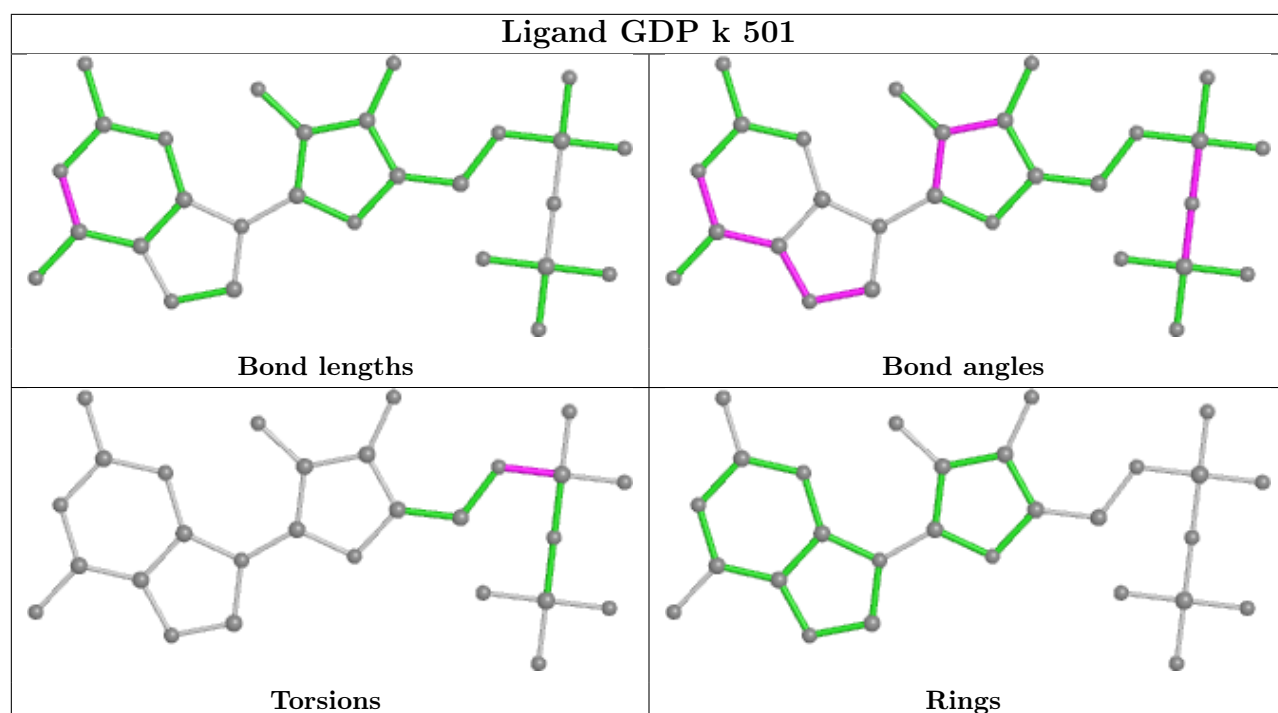
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

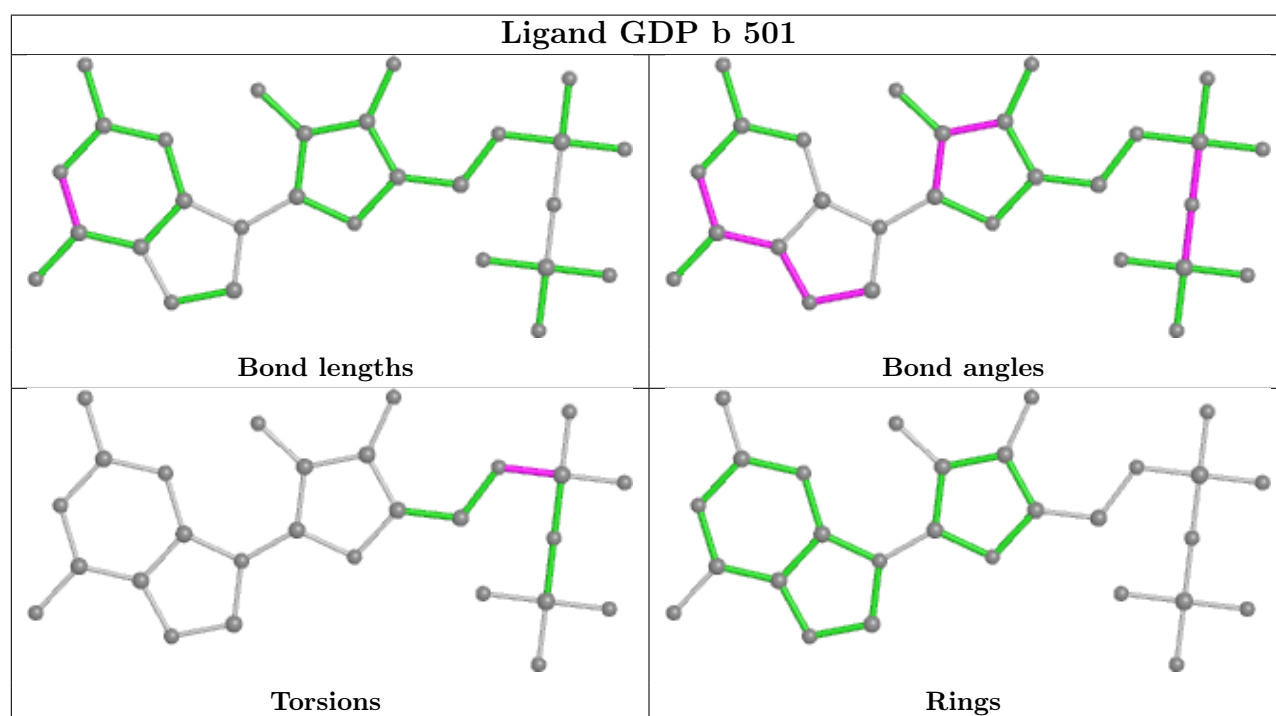
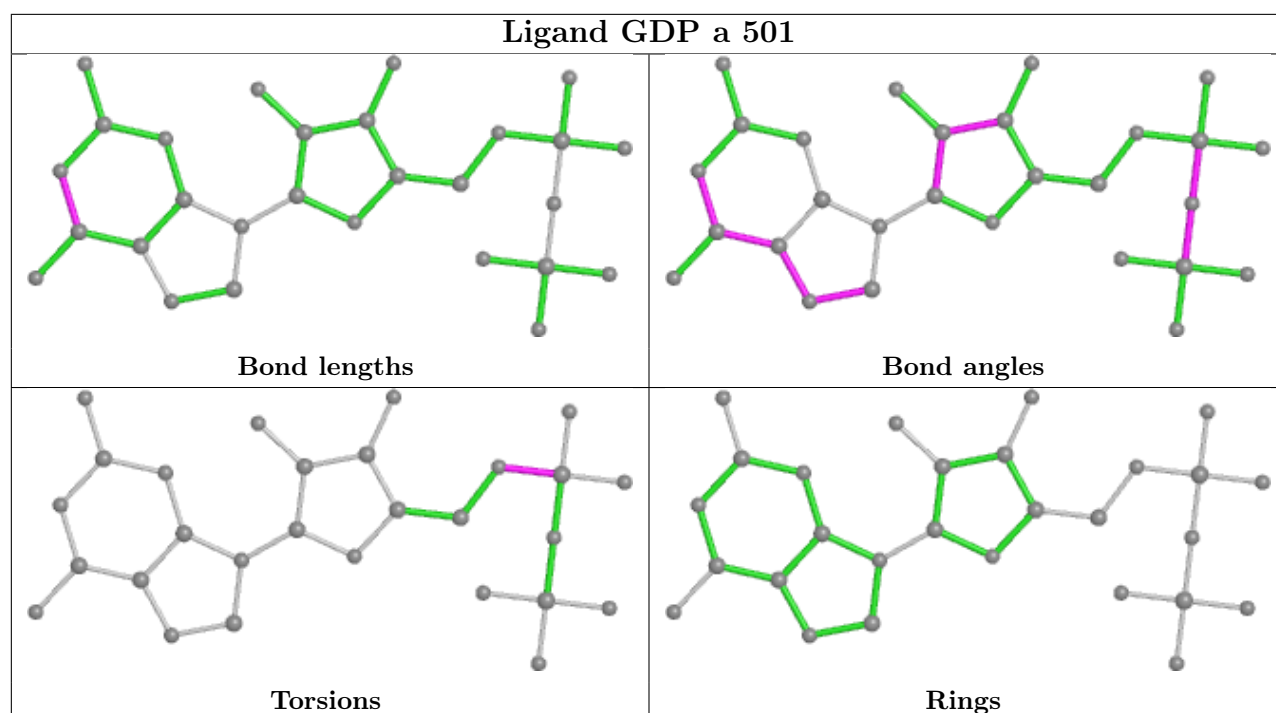


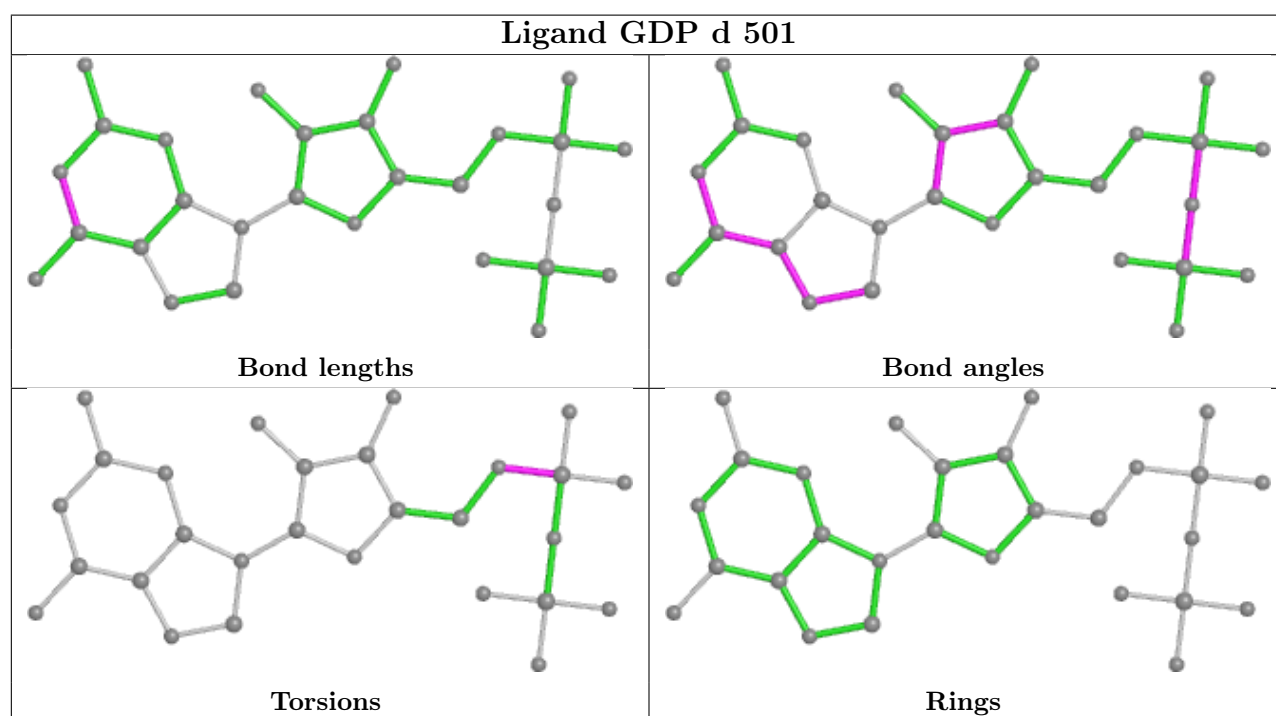
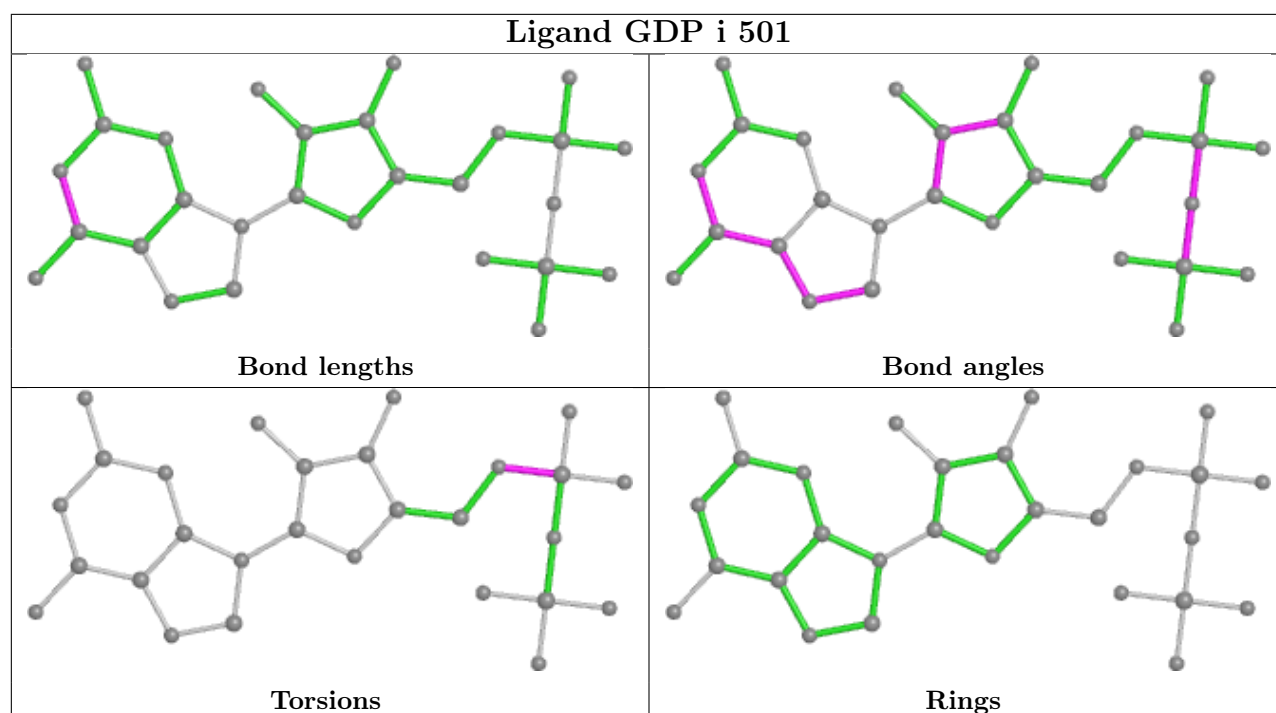


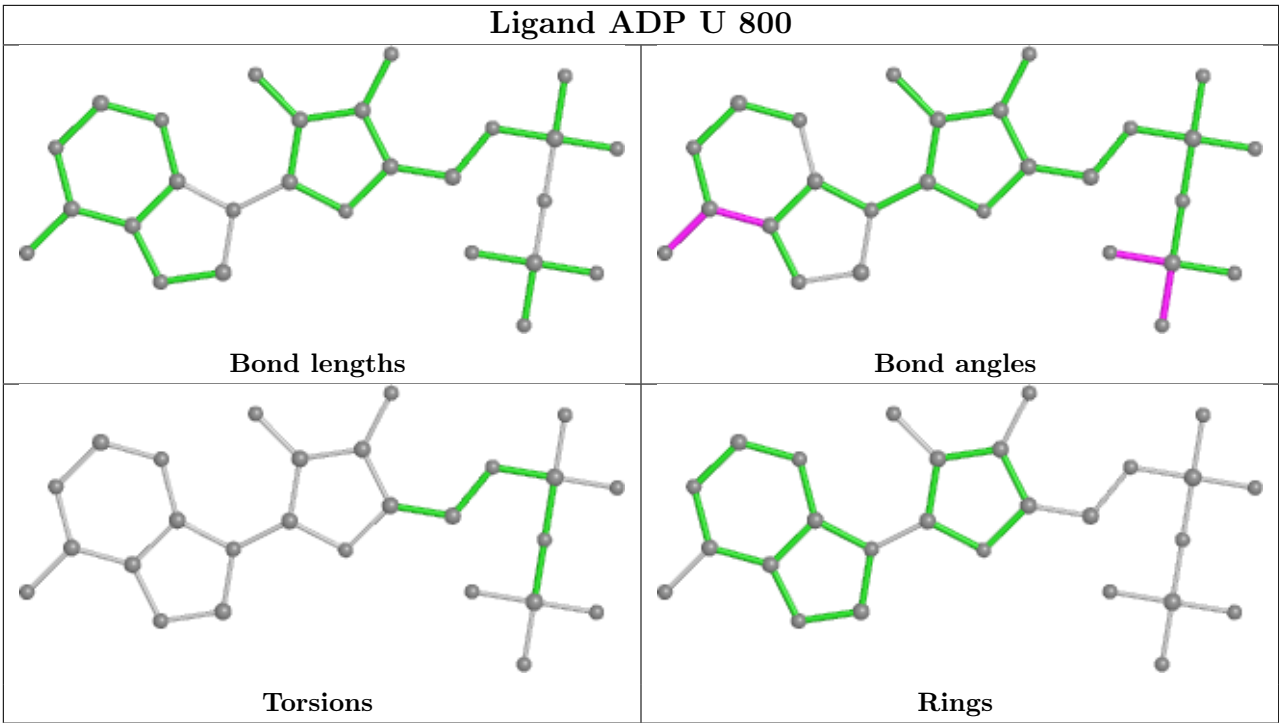












5.7 Other polymers [i](#)

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
10	X	15
9	W	8
8	V	1
6	R	1
6	N	1
6	Q	1
6	O	1
6	S	1

The worst 5 of 29 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	31:UNK	C	101:UNK	N	47.63
1	X	1115:UNK	C	1201:UNK	N	30.30
1	W	220:UNK	C	301:UNK	N	29.84

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	315:UNK	C	401:UNK	N	27.18
1	X	715:UNK	C	801:UNK	N	25.87

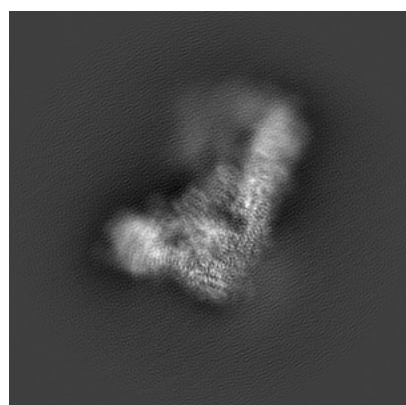
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21073. These allow visual inspection of the internal detail of the map and identification of artifacts.

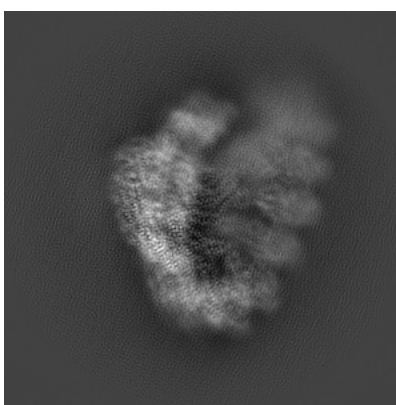
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

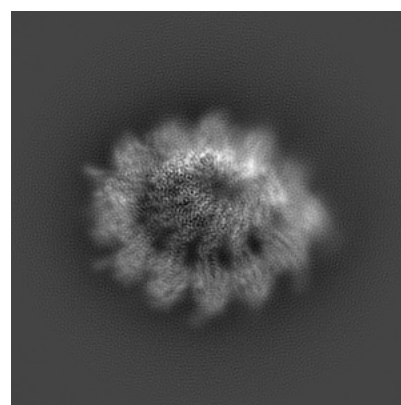
6.1.1 Primary map



X



Y



Z

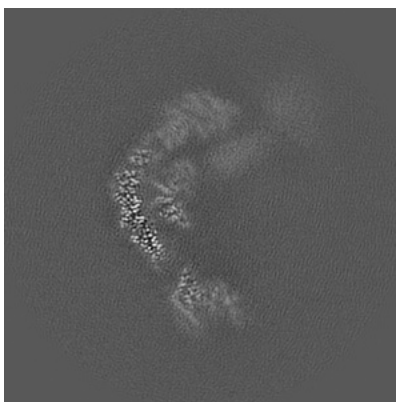
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

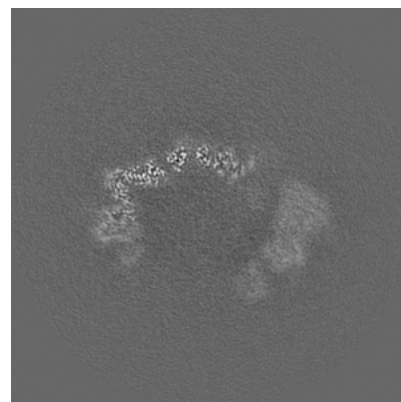
6.2.1 Primary map



X Index: 184



Y Index: 184

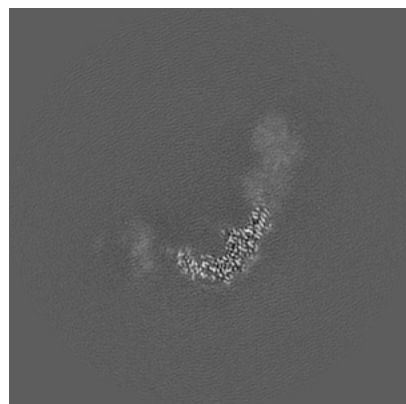


Z Index: 184

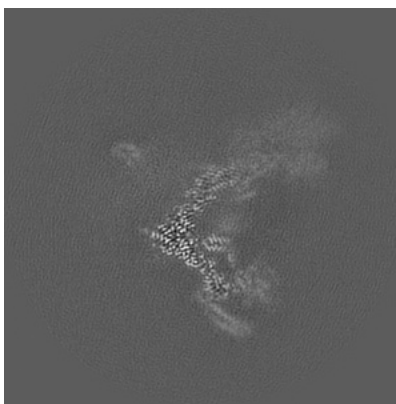
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

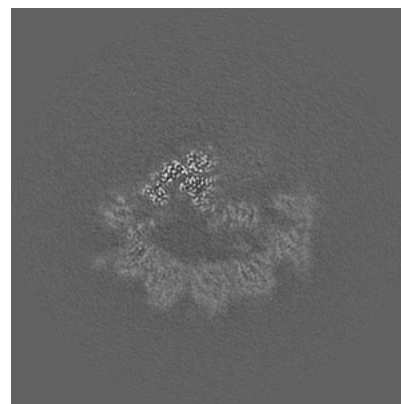
6.3.1 Primary map



X Index: 162



Y Index: 220



Z Index: 159

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

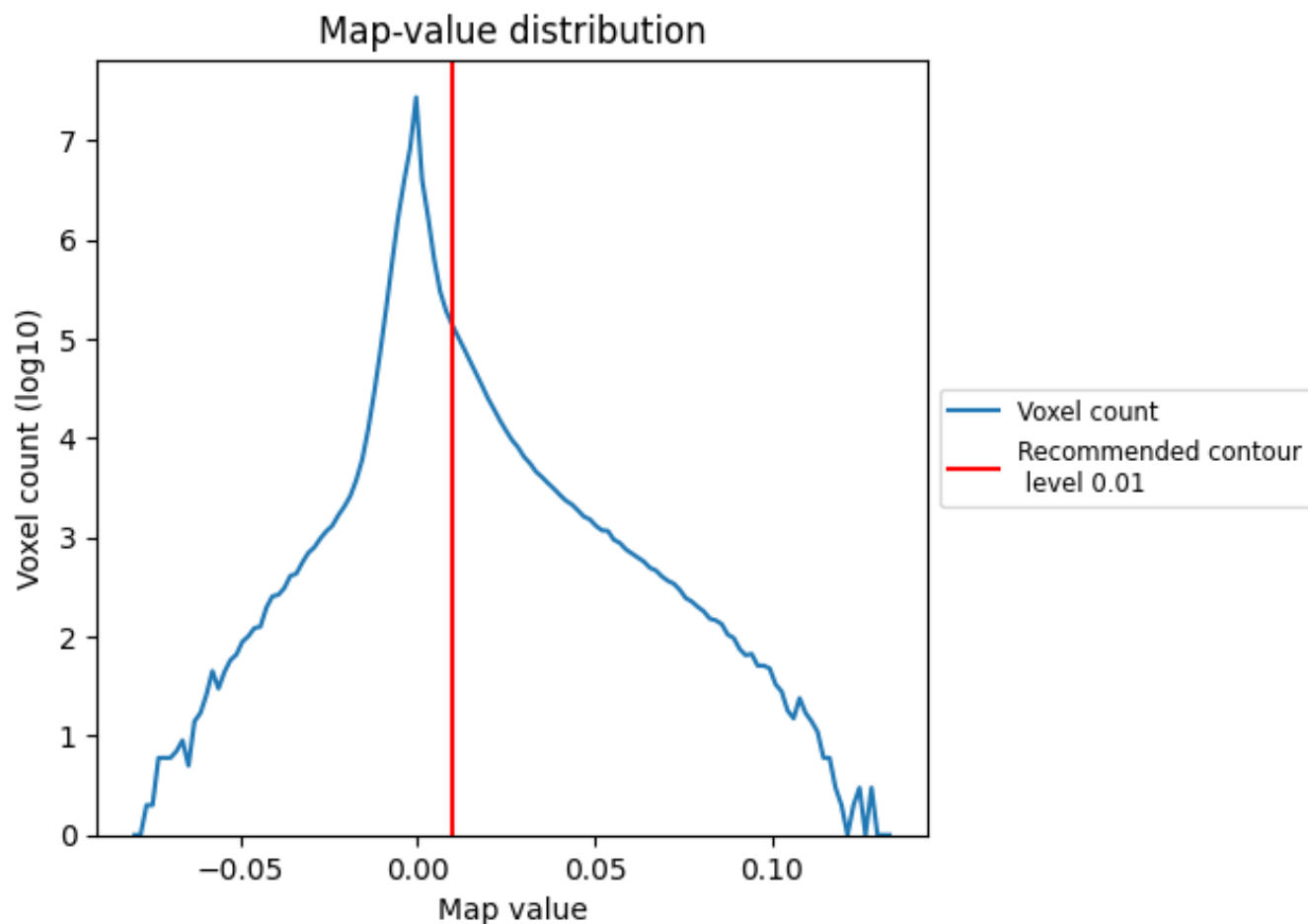
6.5 Mask visualisation

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

7 Map analysis [i](#)

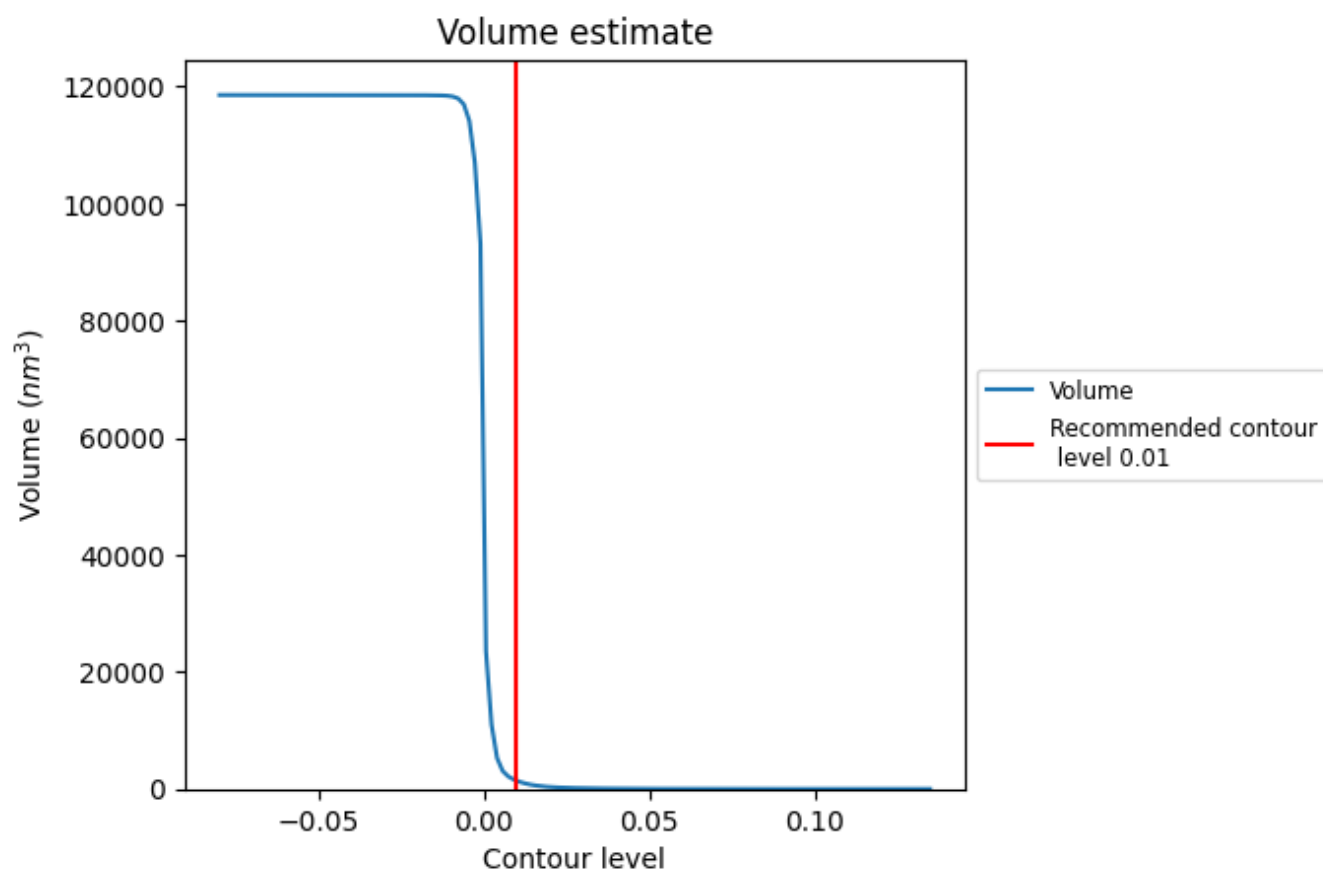
This section contains the results of statistical analysis of the map.

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.

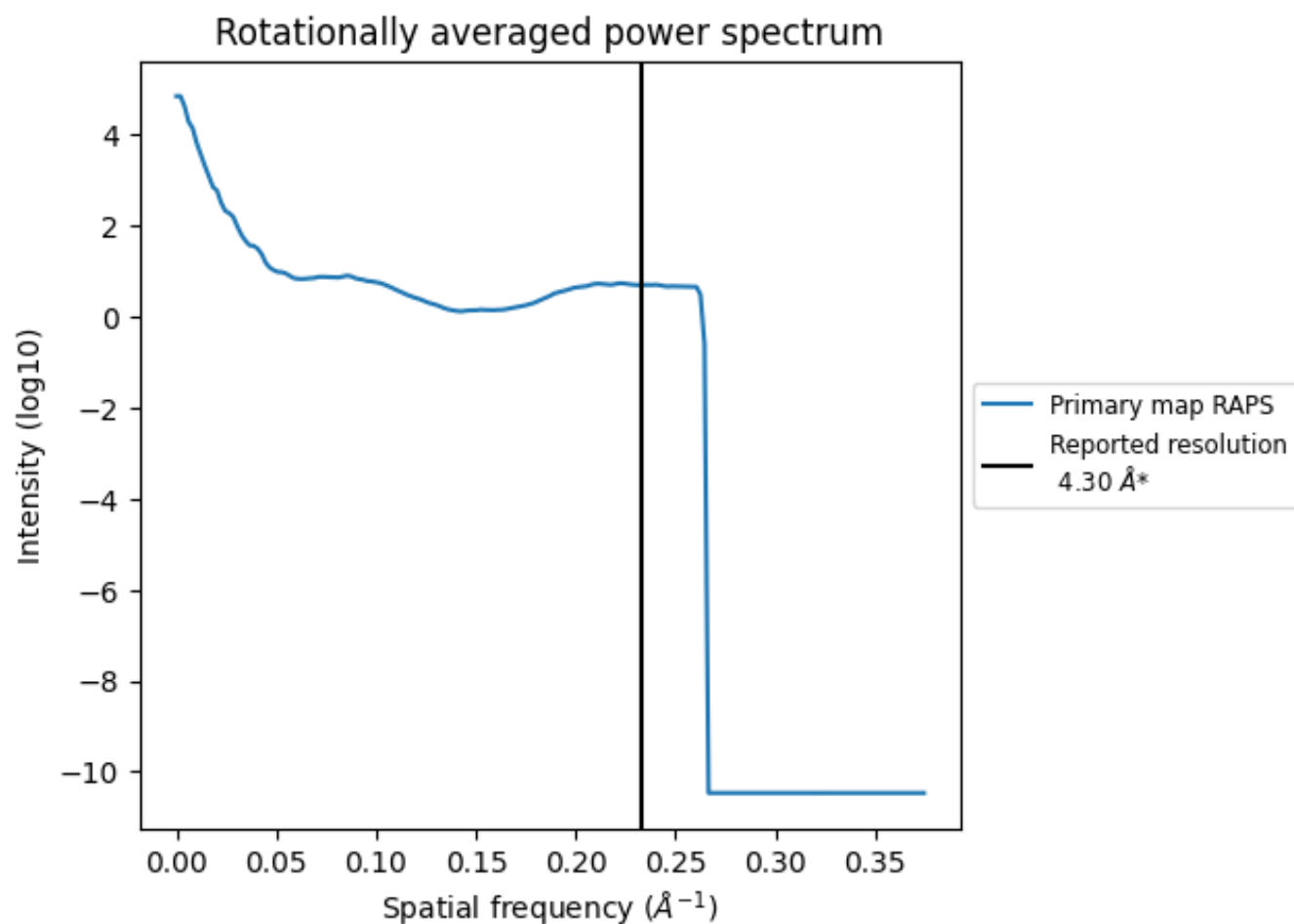
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1413 nm^3 ; this corresponds to an approximate mass of 1276 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 0.233 \AA^{-1}

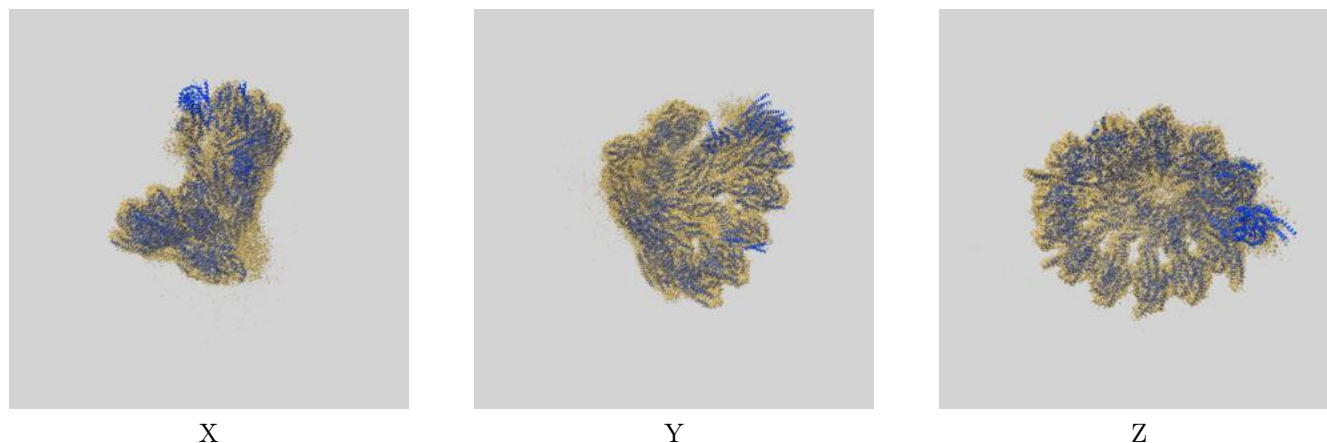
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

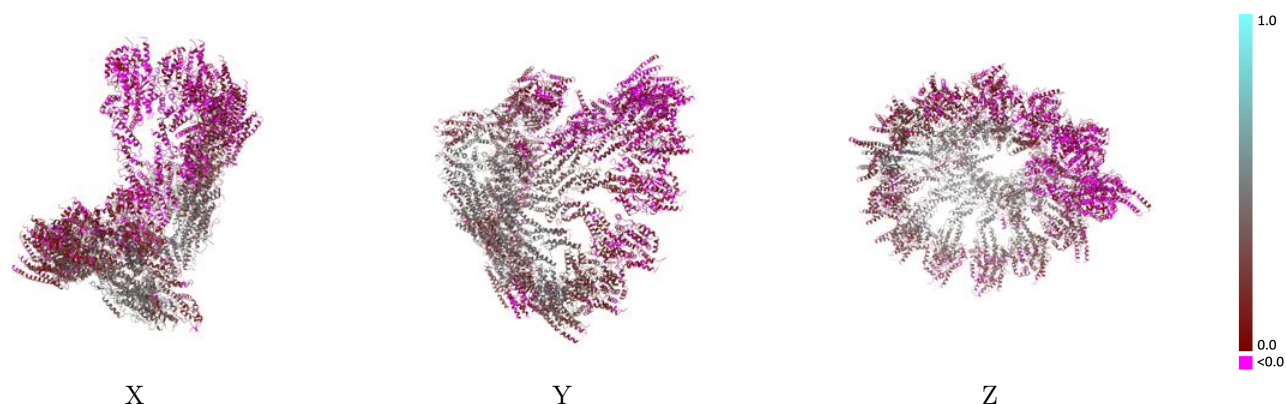
This section contains information regarding the fit between EMDB map EMD-21073 and PDB model 6V6S. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



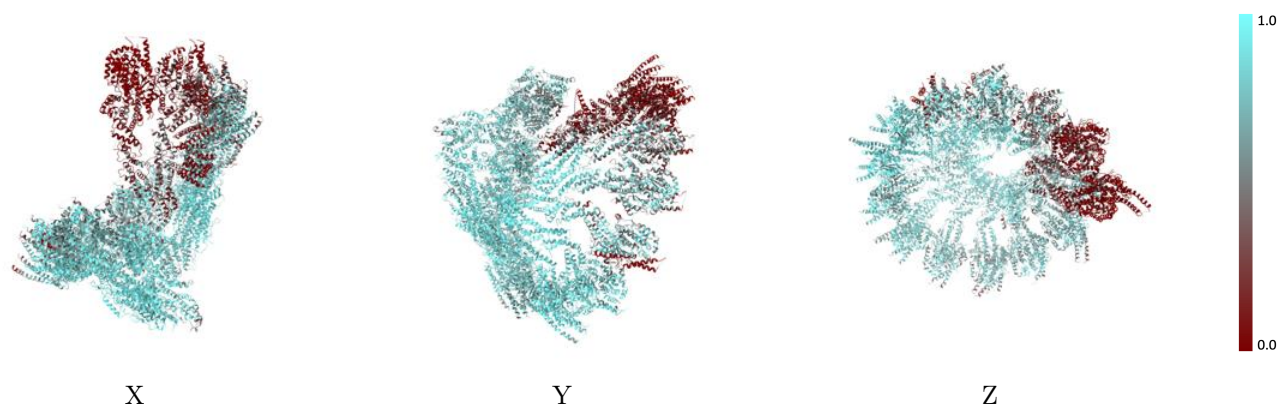
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



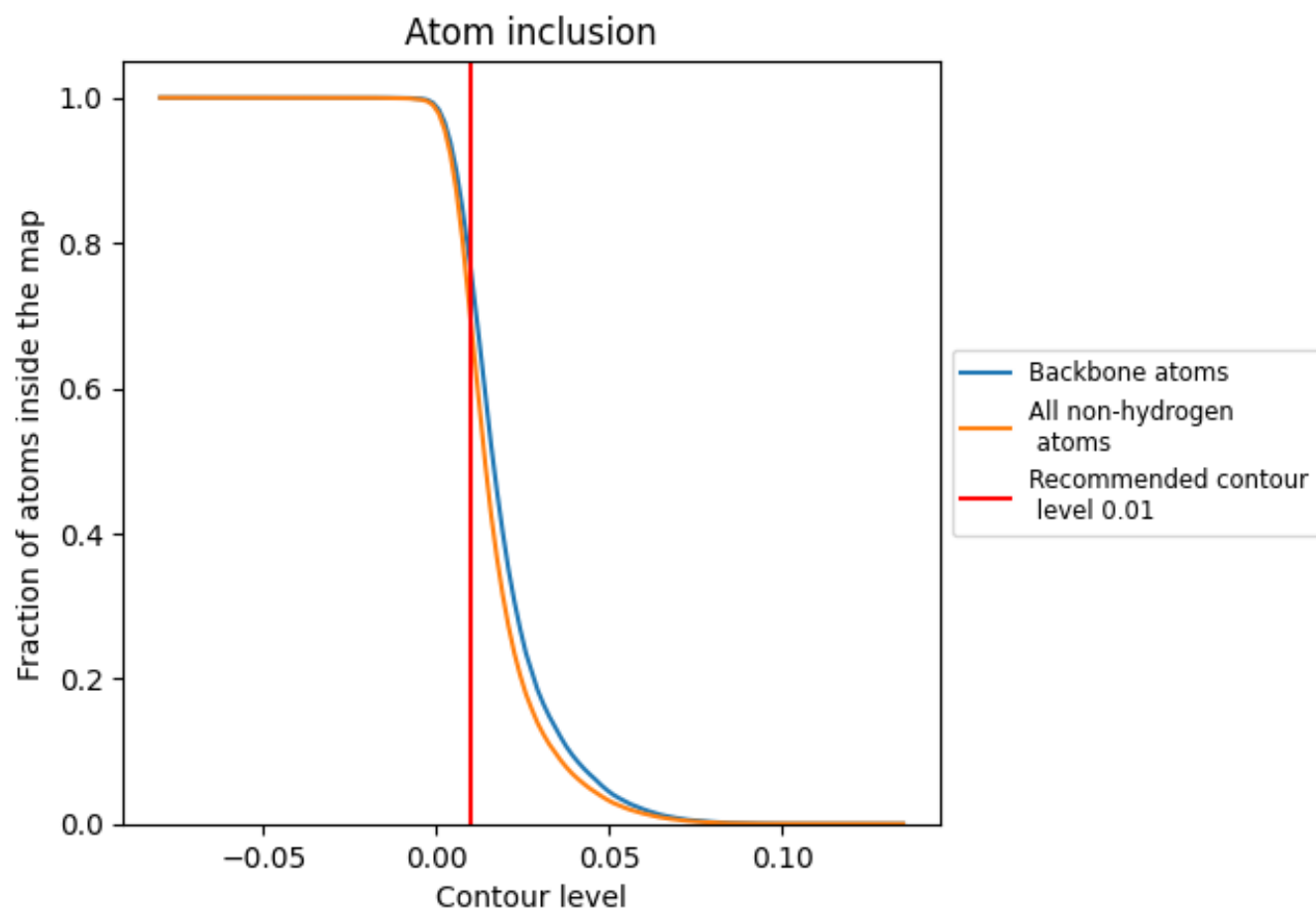
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 69% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.2180
A	 0.7333	 0.2010
B	 0.8126	 0.2940
C	 0.8837	 0.3780
D	 0.8306	 0.3150
E	 0.8548	 0.3490
F	 0.8902	 0.3850
G	 0.7350	 0.1760
H	 0.9045	 0.4000
I	 0.8831	 0.3550
J	 0.7251	 0.2400
K	 0.7615	 0.2210
L	 0.6610	 0.1540
M	 0.2410	 0.0130
N	 0.8057	 0.2690
O	 0.9450	 0.4140
Q	 0.9579	 0.4000
R	 0.9538	 0.4030
S	 0.2950	 0.0020
T	 0.1437	 0.0100
U	 0.7618	 0.2370
V	 0.1419	 0.0480
W	 0.1058	 0.0520
X	 0.9583	 0.4270
Y	 0.8947	 0.3840
a	 0.6072	 0.0740
b	 0.7223	 0.1710
c	 0.7481	 0.2060
d	 0.7100	 0.1730
e	 0.7361	 0.1750
f	 0.8340	 0.2890
g	 0.7766	 0.1980
h	 0.8914	 0.3610
i	 0.8124	 0.2160
j	 0.5388	 0.0810



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Chain	Atom inclusion	Q-score
k	 0.5933	 0.0630
l	 0.4255	 0.0450
m	 0.1055	 0.0110
t	 0.0102	 -0.0200