



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:37 AM UTC

PDB ID : 7N32 / pdb_00007n32
EMDB ID : EMD-22677
Title : protofilaments of microtubule doublets bound to outer-arm dynein
Authors : Rao, Q.; Zhang, K.
Deposited on : 2021-05-31
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation 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:

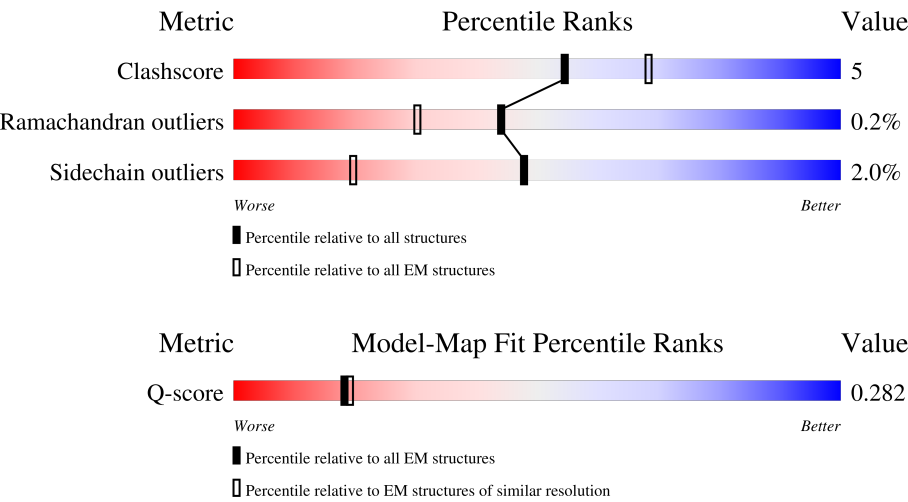
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	449	
1	c	449	
1	e	449	
1	g	449	

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Mol	Chain	Length	Quality of chain
1	i	449	58% 89% 8% ..
1	k	449	44% 82% 15% .
1	m	449	41% 82% 16% ..
1	o	449	60% 89% 9% .
1	q	449	48% 82% 16% .
1	s	449	43% 88% 9% ..
1	u	449	50% 82% 15% ..
1	w	449	67% 81% 16% ..
2	b	443	39% 80% 16% ..
2	d	443	59% 80% 19%
2	f	443	44% 84% 13% .
2	h	443	32% 86% 11% .
2	j	443	59% 89% 8% .
2	l	443	40% 87% 10% .
2	n	443	36% 83% 16% .
2	p	443	52% 87% 9% .
2	r	443	42% 86% 11% .
2	t	443	36% 88% 9% .
2	v	443	45% 85% 12% .
2	x	443	54% 87% 9% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 82021 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	w	440	Total	C	N	O	S	0	0
			3405	2152	578	653	22		
1	u	440	Total	C	N	O	S	0	0
			3409	2155	579	653	22		
1	s	440	Total	C	N	O	S	0	0
			3409	2155	579	653	22		
1	q	440	Total	C	N	O	S	0	0
			3403	2151	578	652	22		
1	o	440	Total	C	N	O	S	0	0
			3397	2146	577	652	22		
1	m	440	Total	C	N	O	S	0	0
			3409	2155	579	653	22		
1	k	440	Total	C	N	O	S	0	0
			3405	2152	578	653	22		
1	g	440	Total	C	N	O	S	0	0
			3413	2158	580	653	22		
1	e	440	Total	C	N	O	S	0	0
			3402	2149	579	652	22		
1	c	440	Total	C	N	O	S	0	0
			3402	2149	579	652	22		
1	a	440	Total	C	N	O	S	0	0
			3406	2152	580	652	22		
1	i	440	Total	C	N	O	S	0	0
			3405	2152	578	653	22		

- Molecule 2 is a protein called Tubulin beta chain.

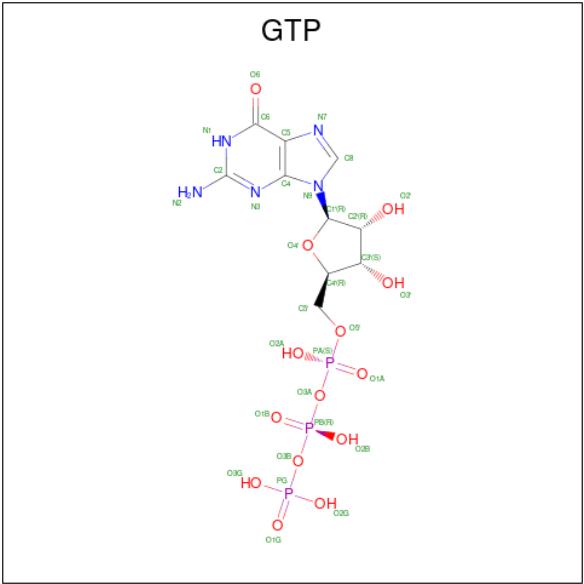
Mol	Chain	Residues	Atoms					AltConf	Trace
2	x	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	v	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	t	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	r	430	Total	C	N	O	S	0	0
			3359	2109	577	645	28		
2	p	428	Total	C	N	O	S	0	0
			3345	2101	574	642	28		
2	n	440	Total	C	N	O	S	0	0
			3412	2141	587	656	28		
2	l	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	h	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	f	430	Total	C	N	O	S	0	0
			3362	2113	576	645	28		
2	b	430	Total	C	N	O	S	0	0
			3362	2113	576	645	28		
2	d	442	Total	C	N	O	S	0	0
			3416	2145	588	655	28		
2	j	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
3	w	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	u	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
3	s	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	q	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	o	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	m	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	k	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	g	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	e	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	c	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	a	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	i	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

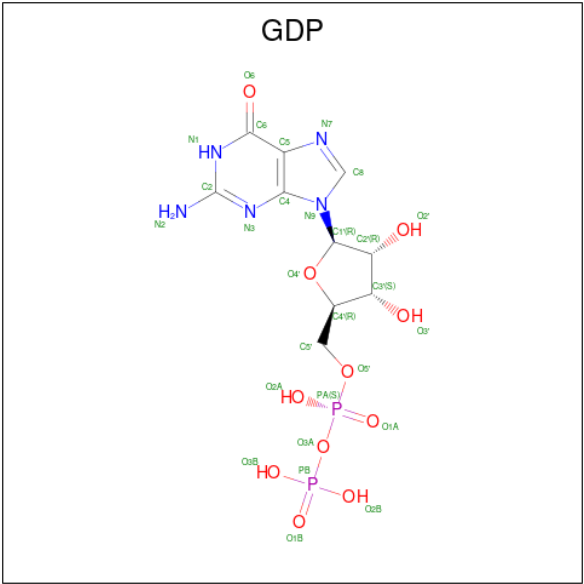
Mol	Chain	Residues	Atoms		AltConf
4	x	1	Total	Mg	0
			1	1	
4	u	1	Total	Mg	0
			1	1	
4	t	1	Total	Mg	0
			1	1	
4	q	1	Total	Mg	0
			1	1	
4	o	1	Total	Mg	0
			1	1	
4	m	1	Total	Mg	0
			1	1	
4	k	1	Total	Mg	0
			1	1	
4	g	1	Total	Mg	0
			1	1	
4	e	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	c	1	Total	Mg	0
			1	1	
4	a	1	Total	Mg	0
			1	1	
4	i	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
5	x	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	v	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	t	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	r	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	p	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	n	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	l	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	h	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

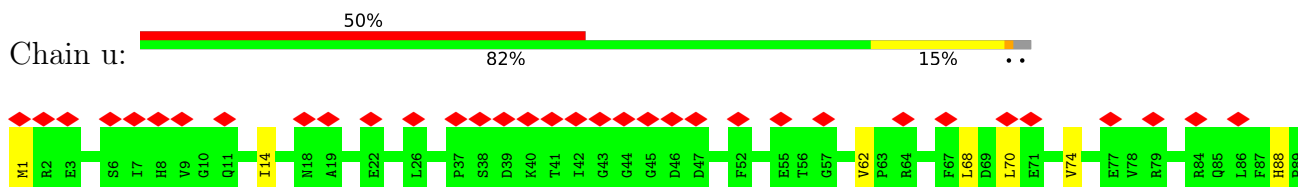
3 Residue-property plots

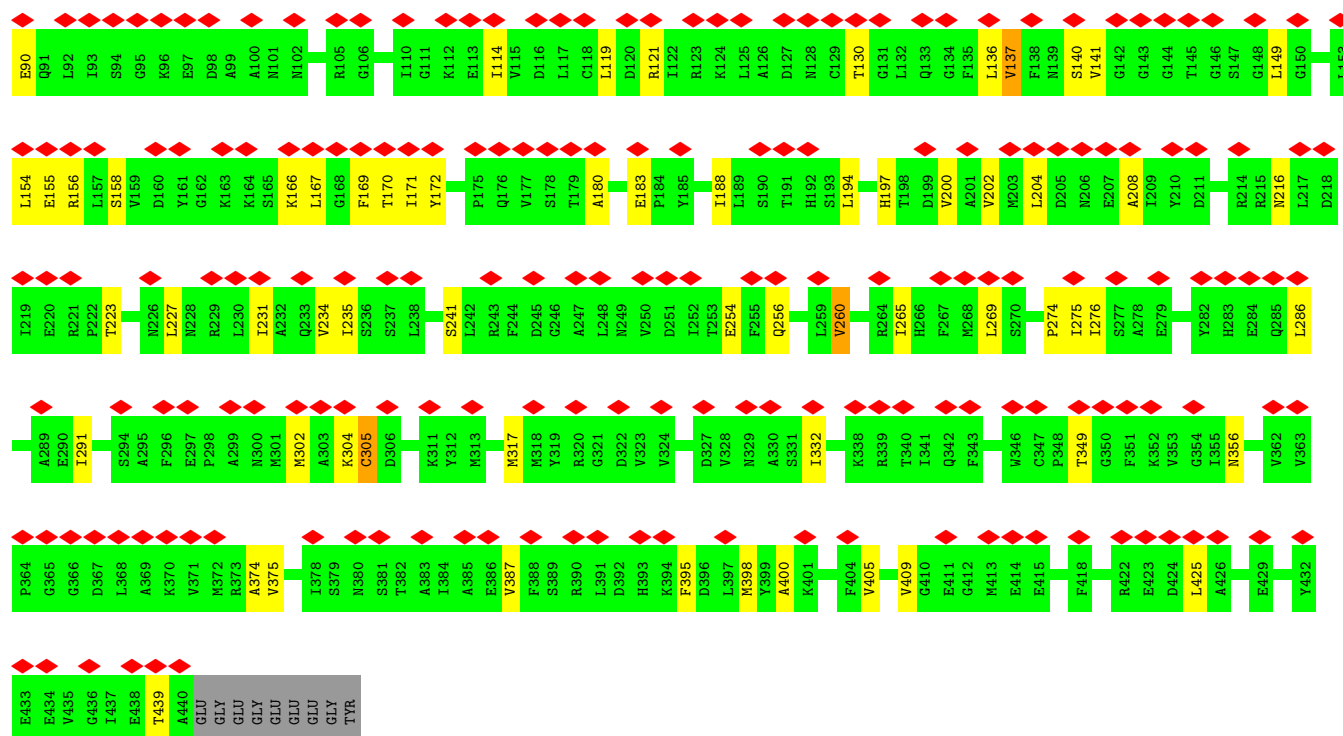
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

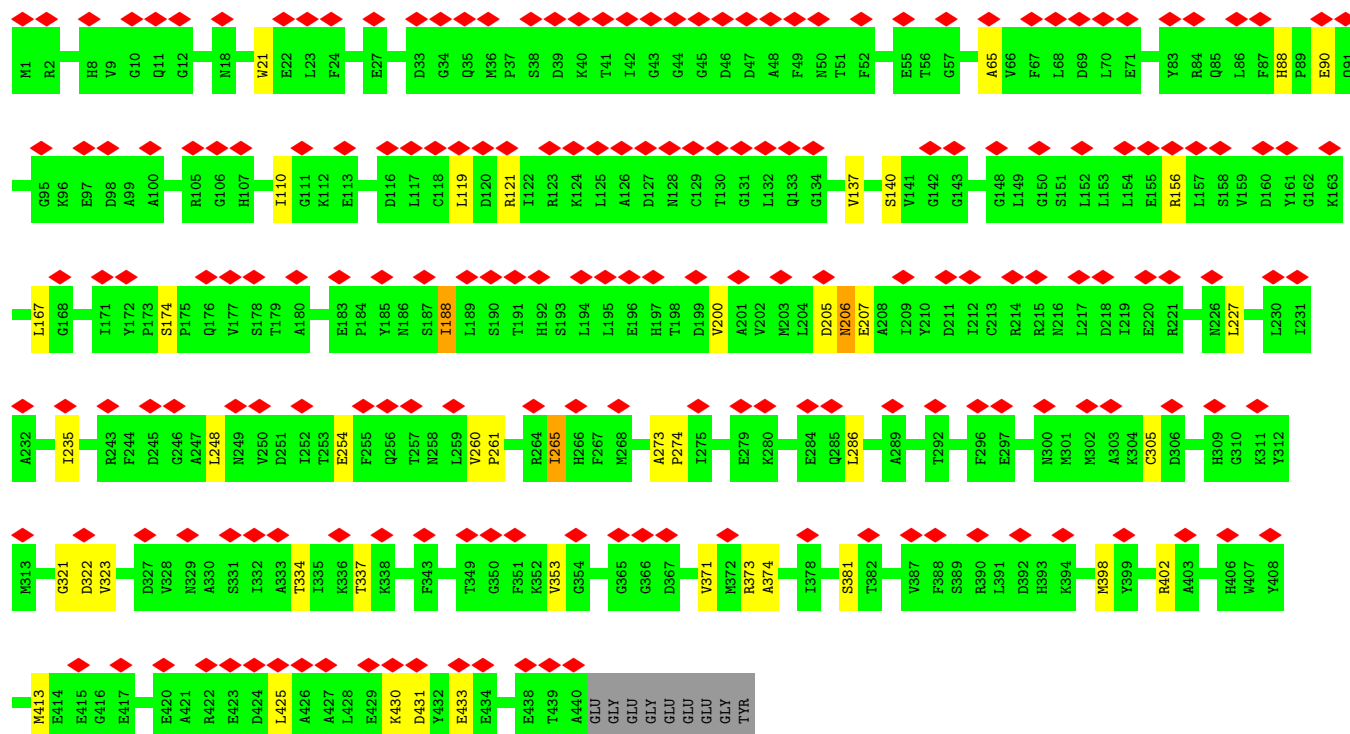
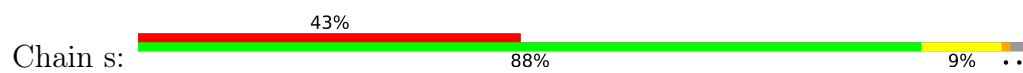


• Molecule 1: Tubulin alpha chain



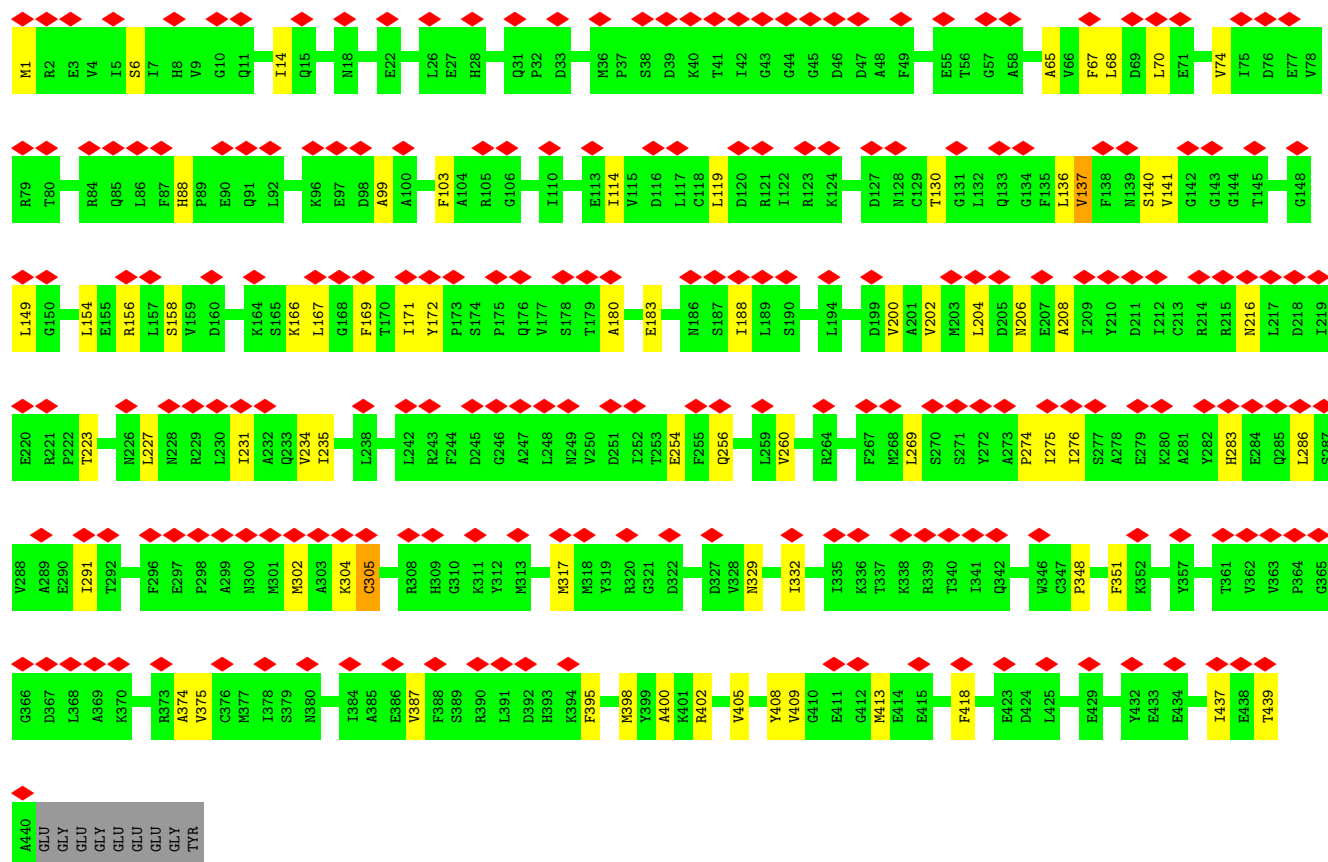


• Molecule 1: Tubulin alpha chain

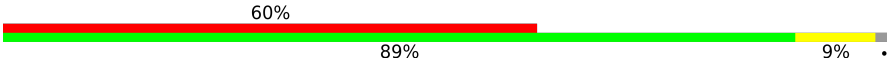


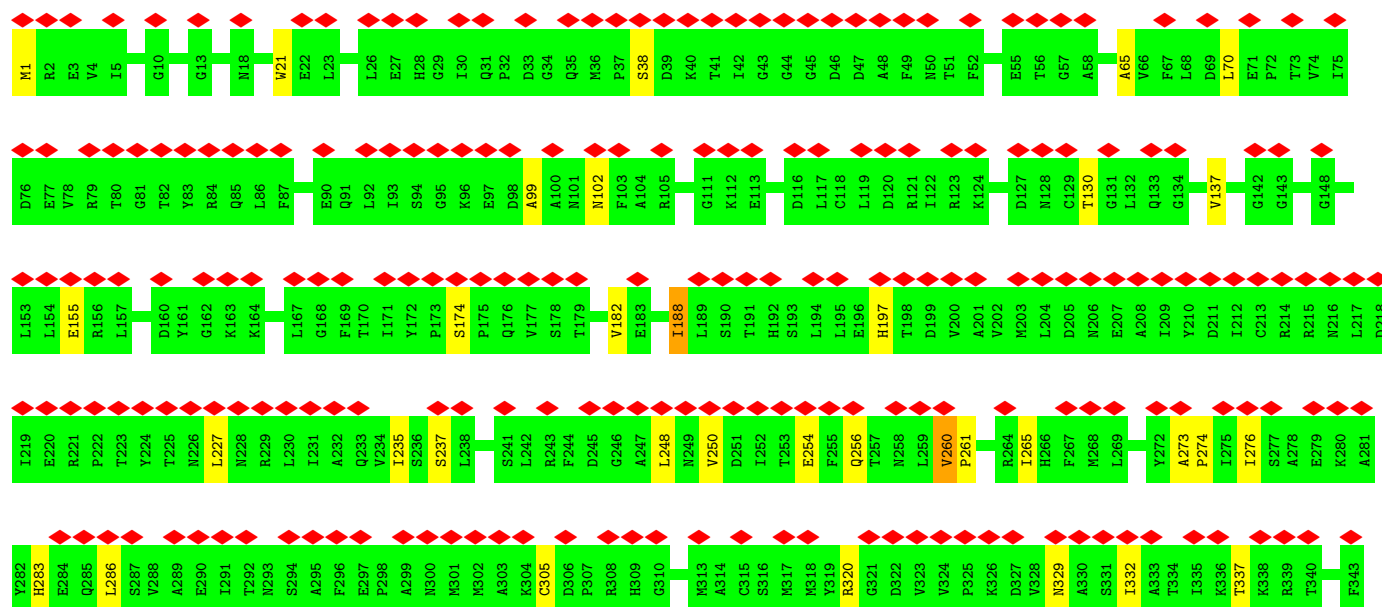
• Molecule 1: Tubulin alpha chain

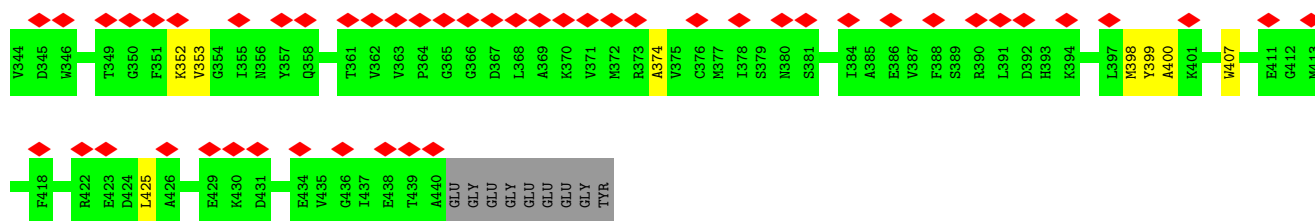
Chain q: 



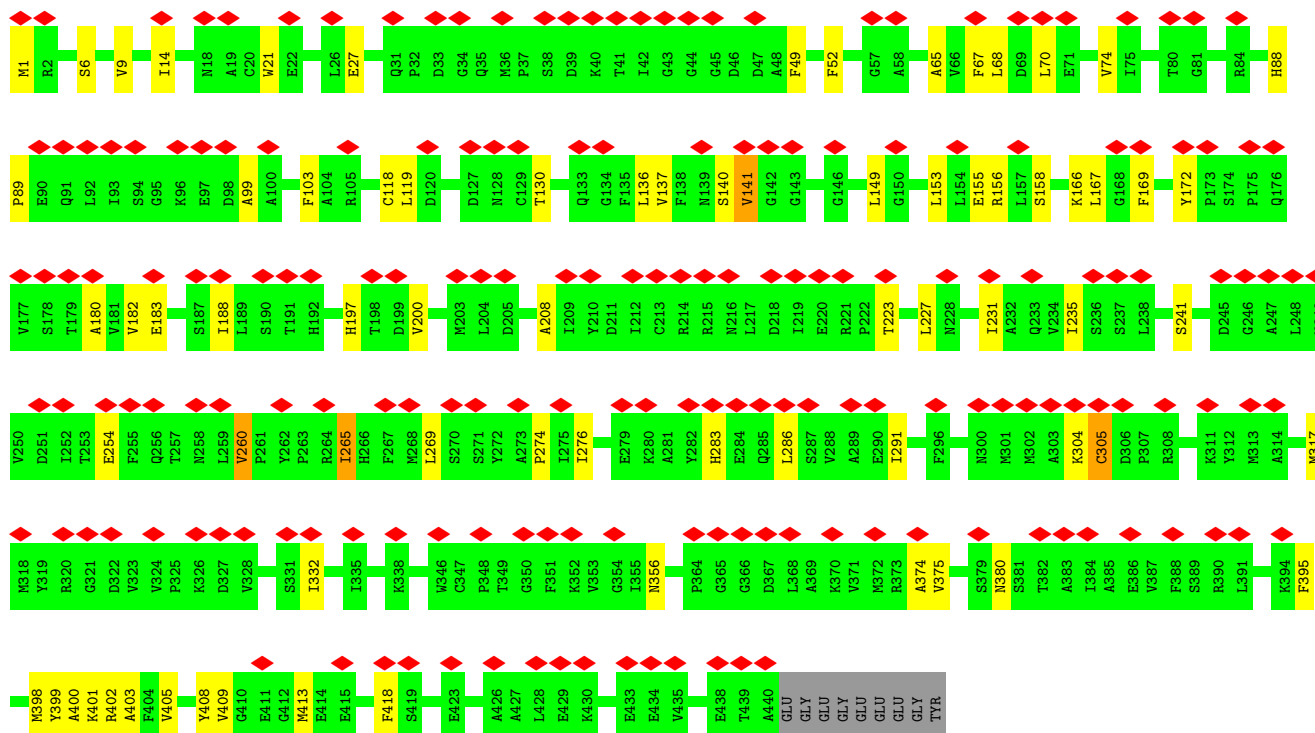
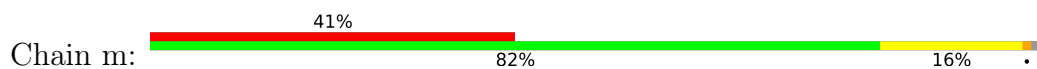
• Molecule 1: Tubulin alpha chain

Chain o: 

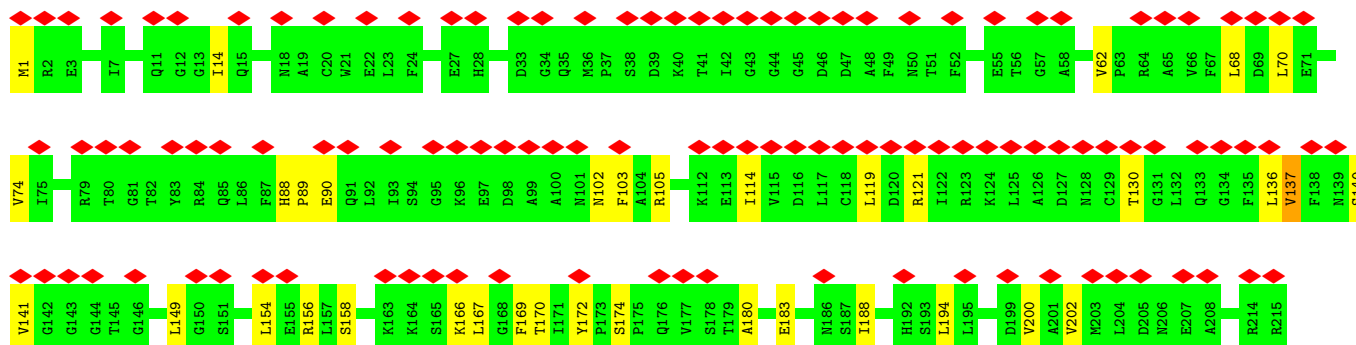
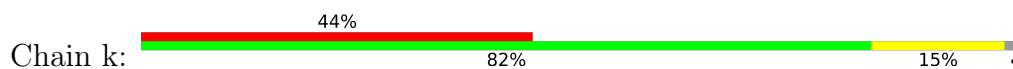


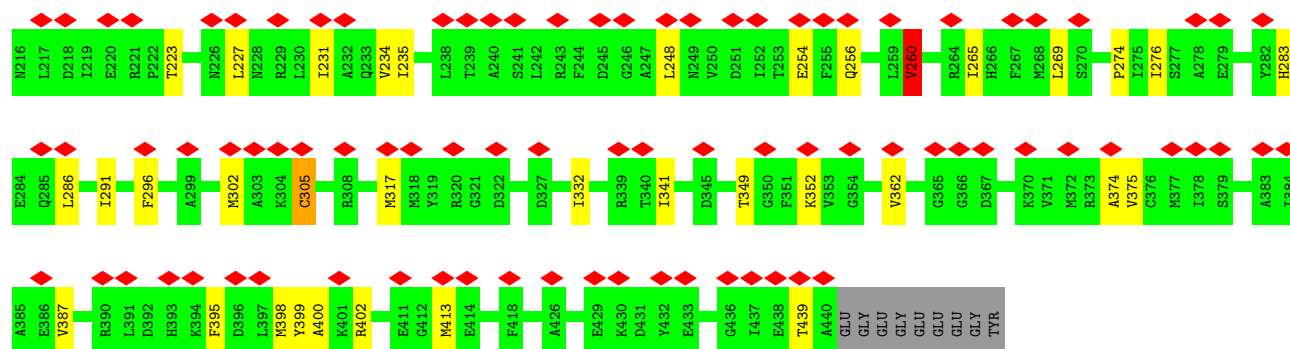


• Molecule 1: Tubulin alpha chain



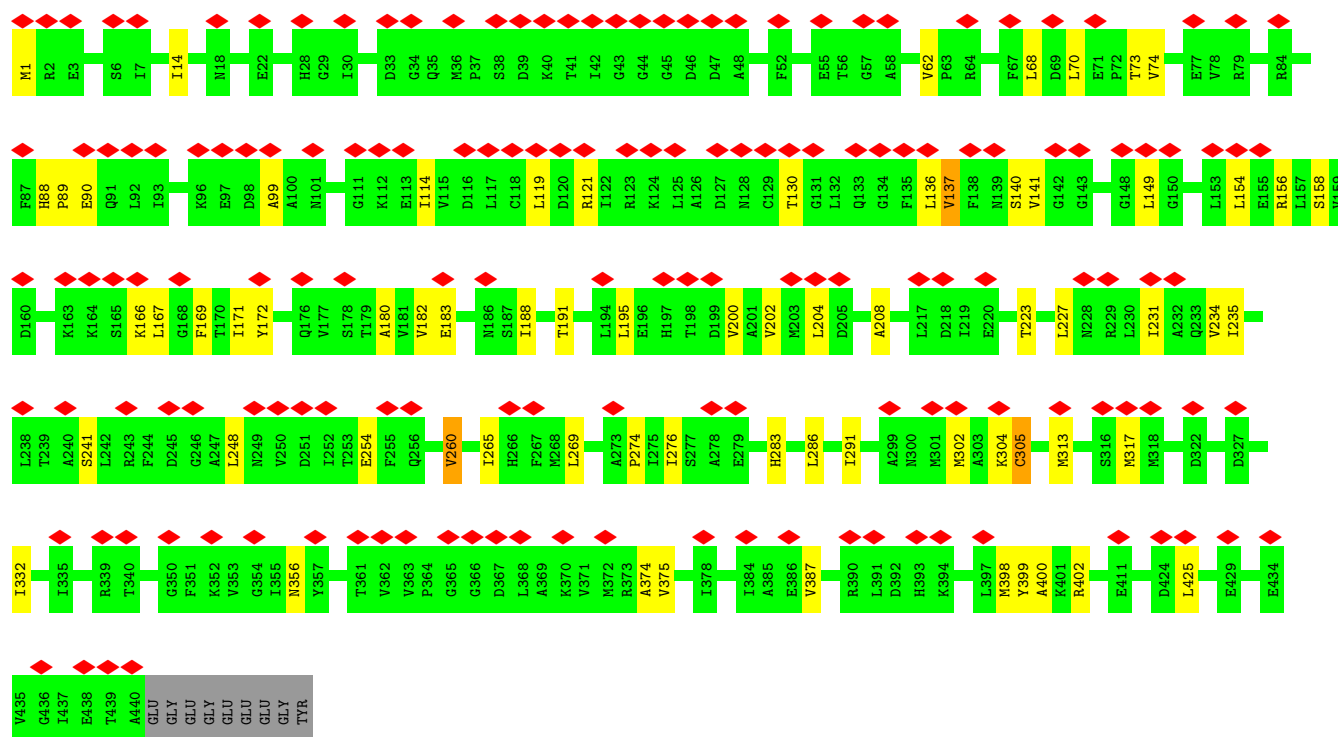
• Molecule 1: Tubulin alpha chain





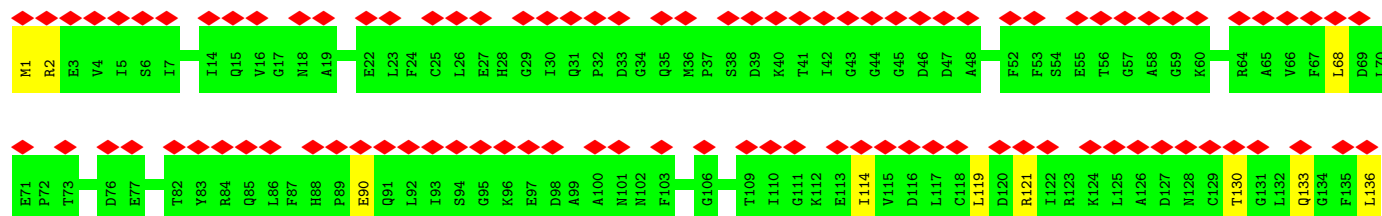
• Molecule 1: Tubulin alpha chain

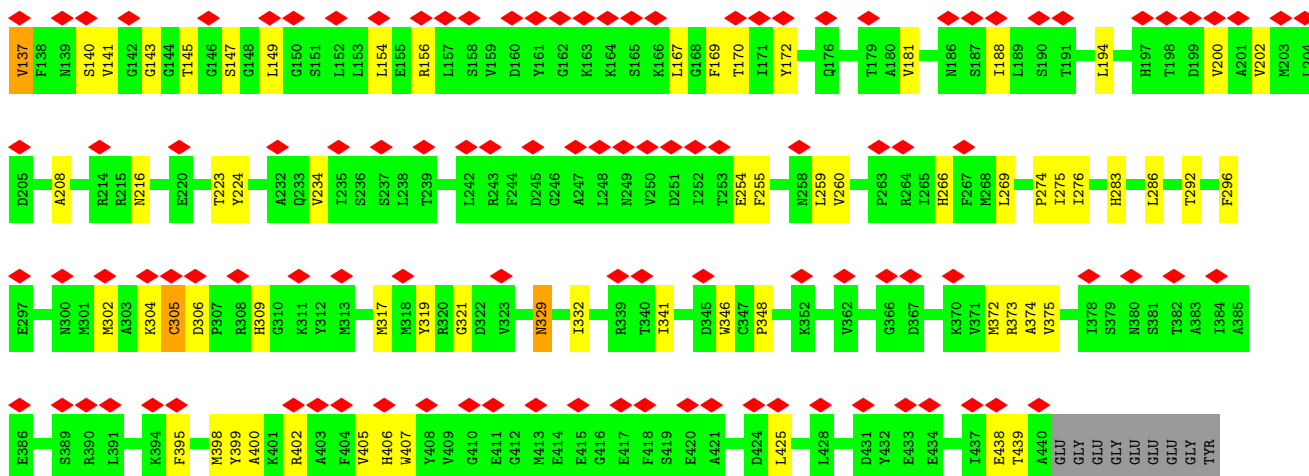
Chain g: 35% 83% 15% ..



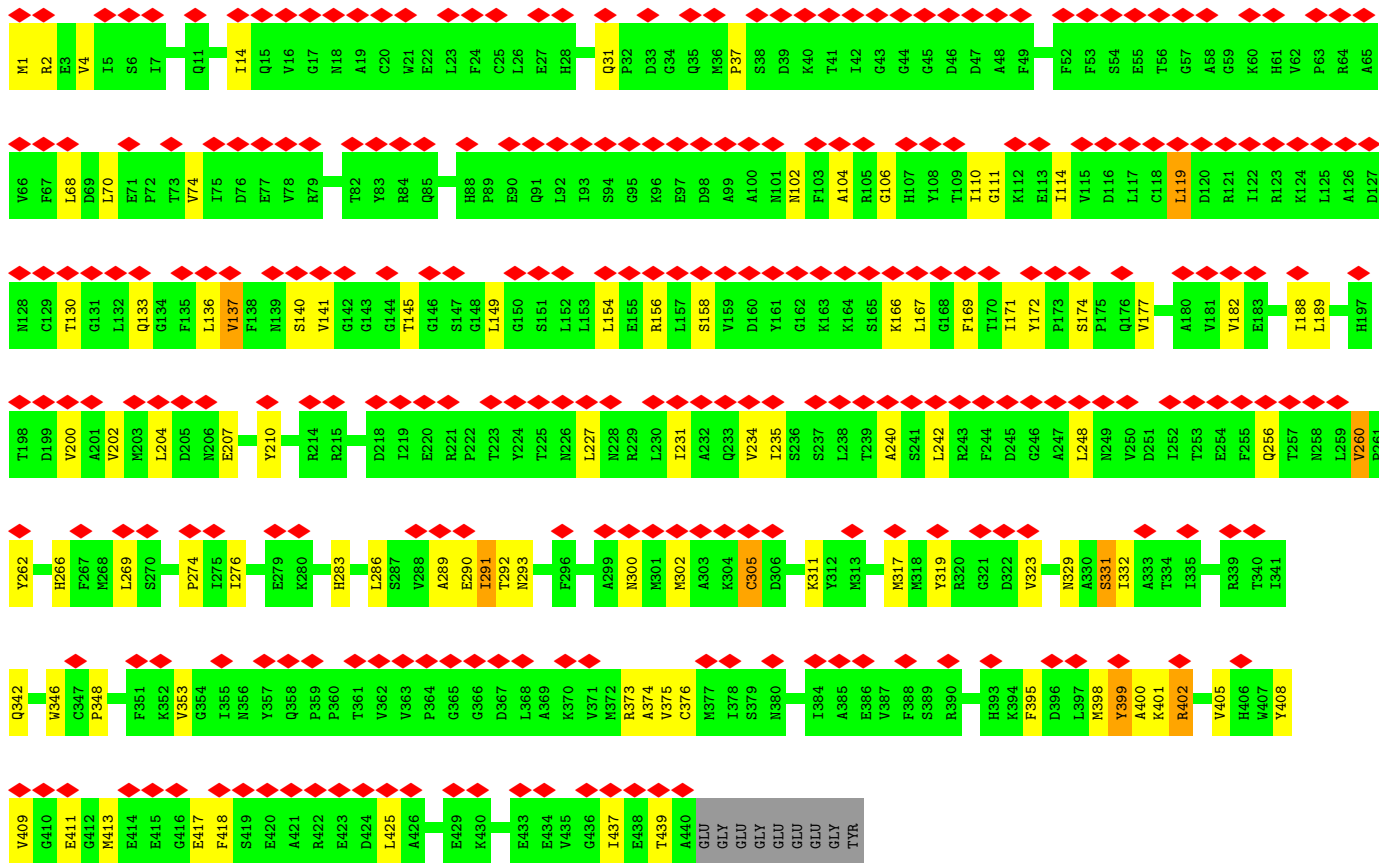
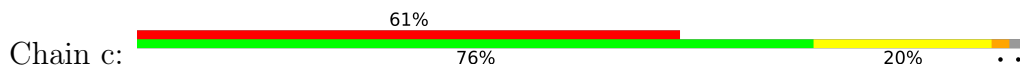
• Molecule 1: Tubulin alpha chain

Chain e: 45% 82% 16% ..

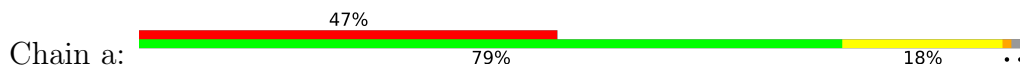


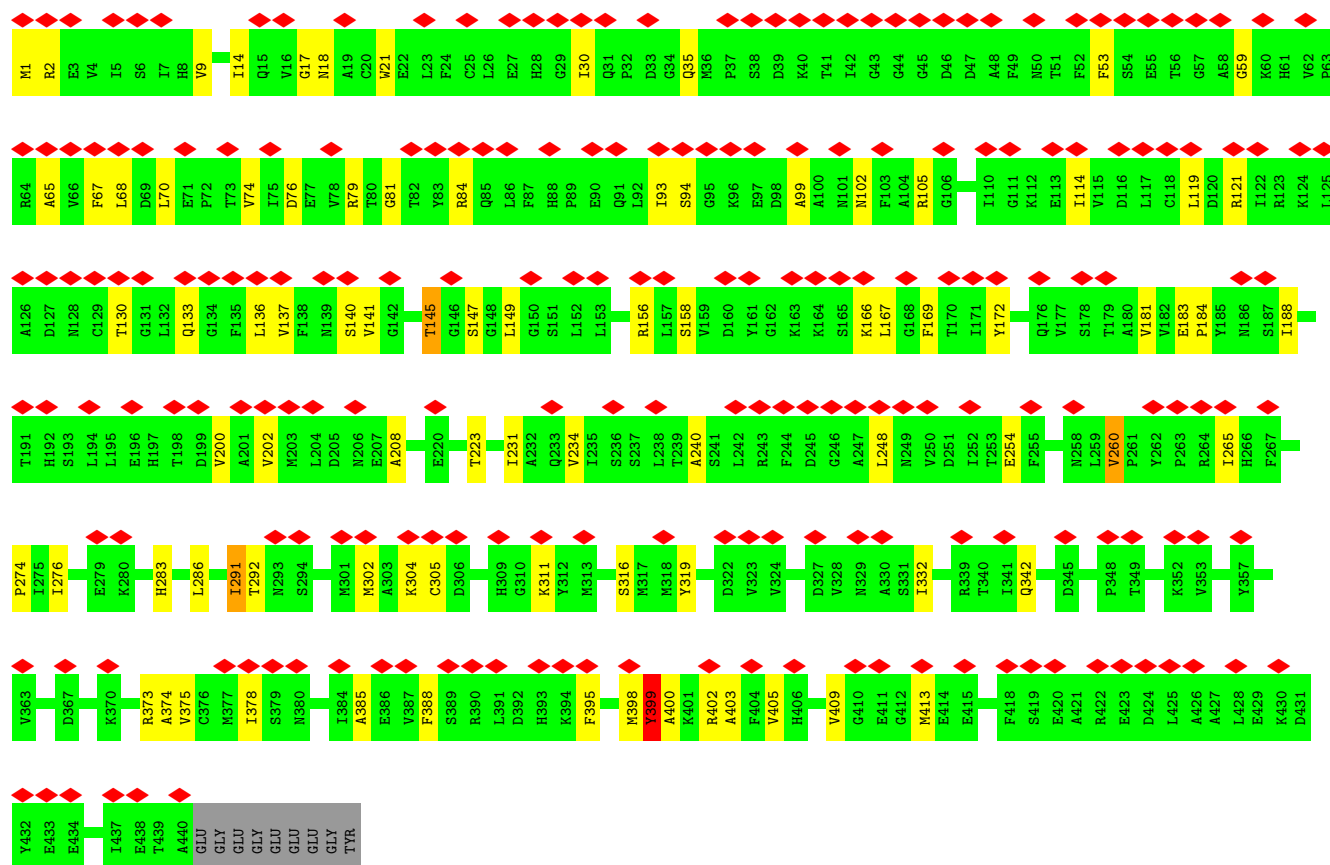


• Molecule 1: Tubulin alpha chain

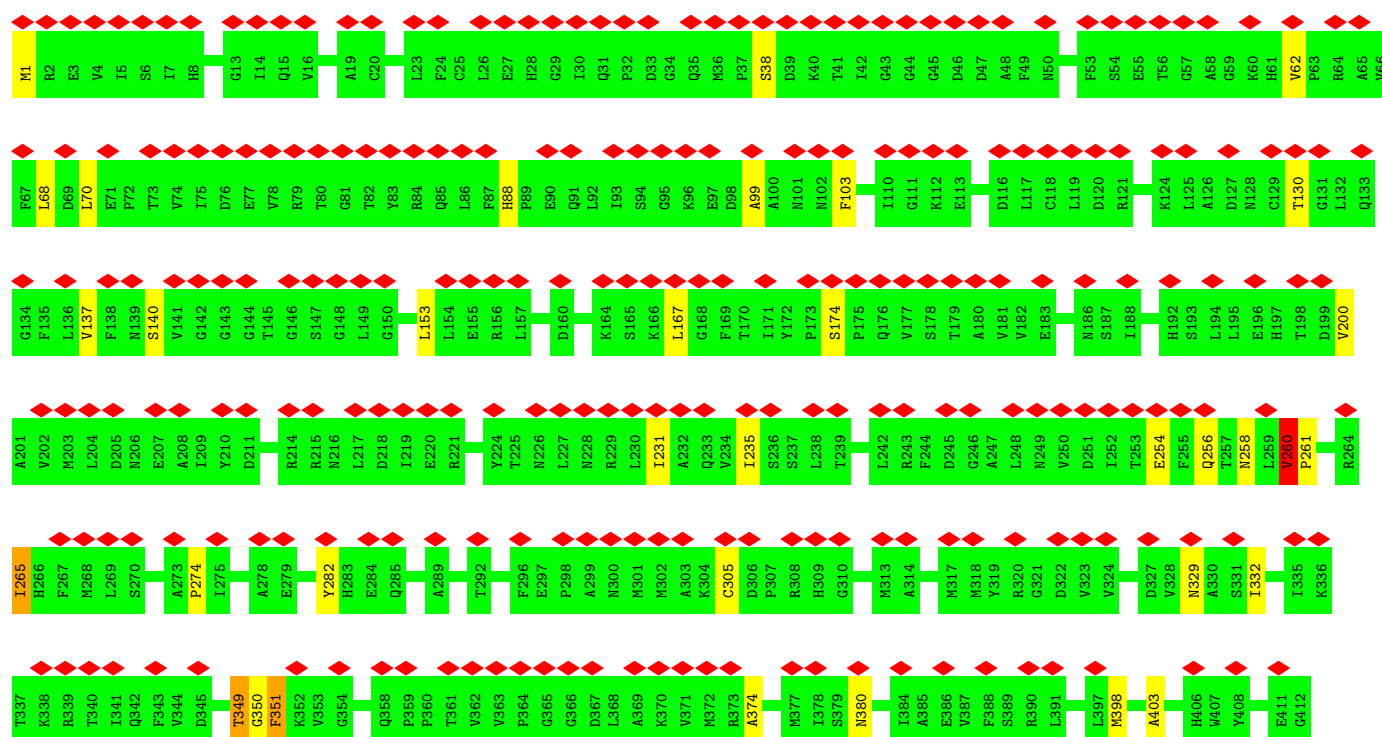
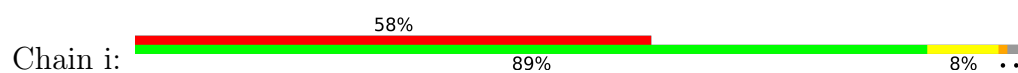


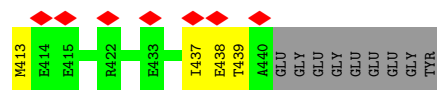
• Molecule 1: Tubulin alpha chain



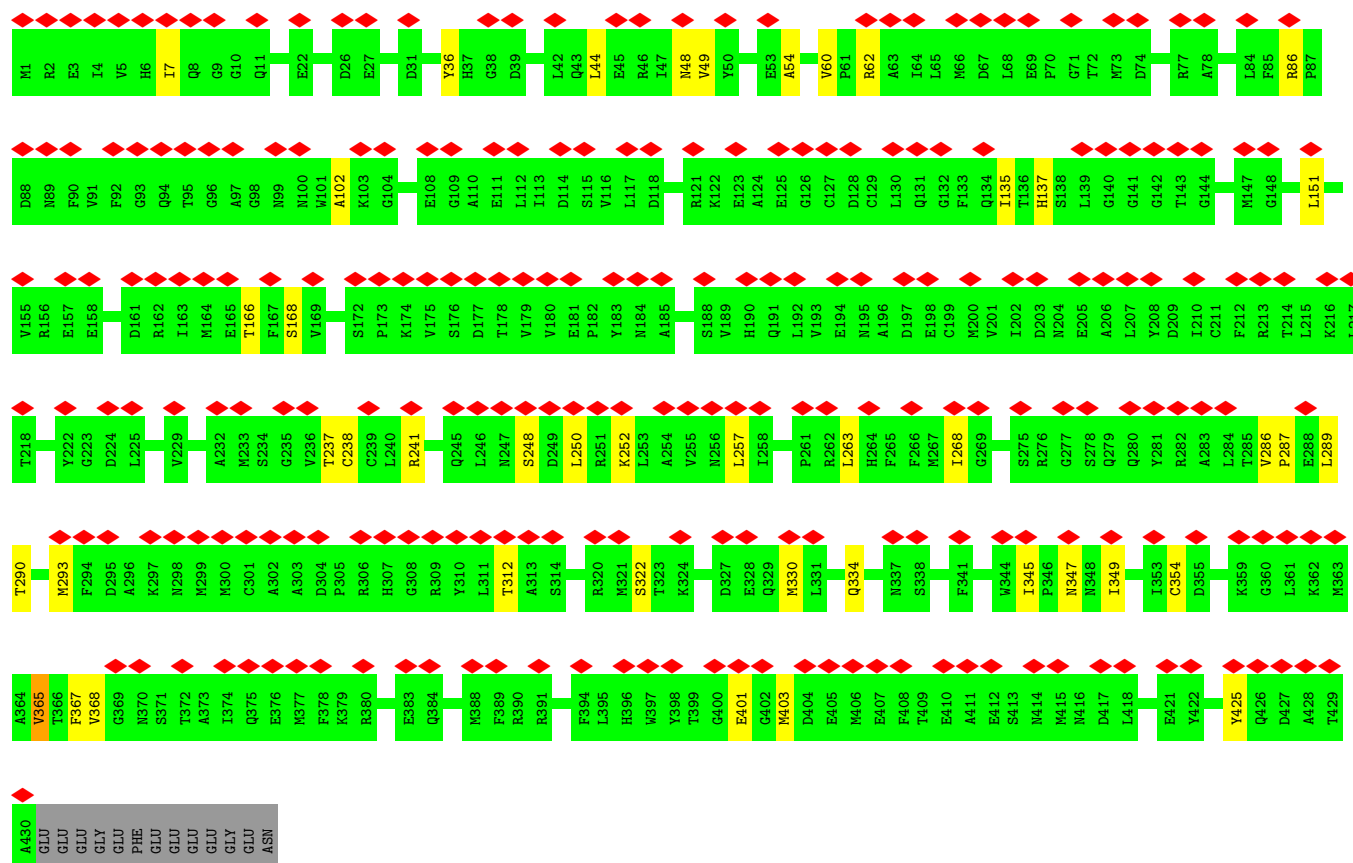
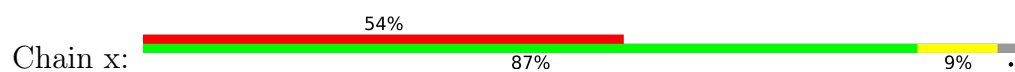


• Molecule 1: Tubulin alpha chain

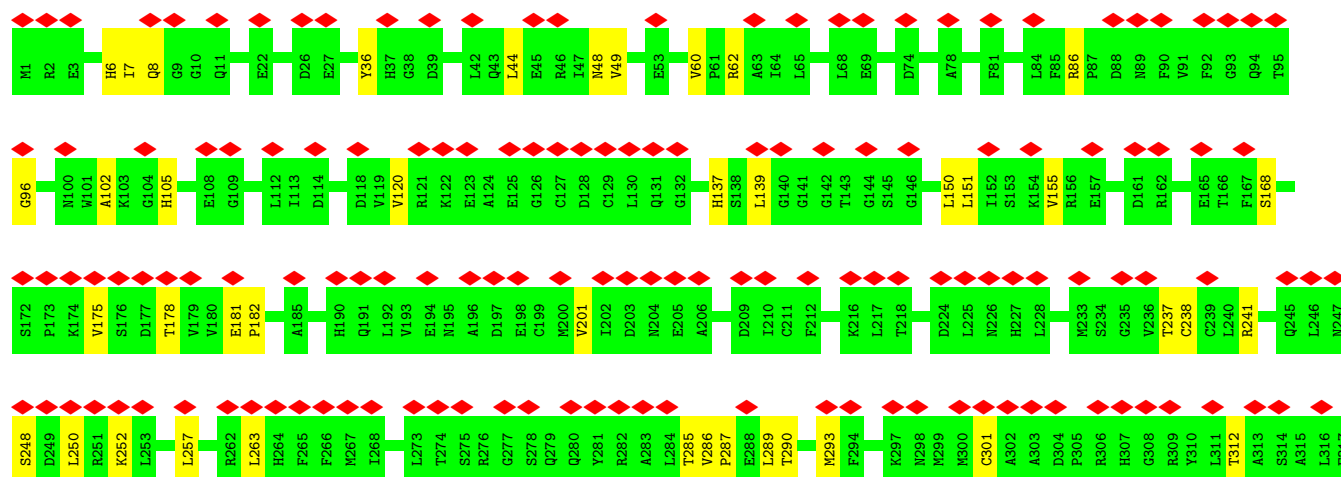
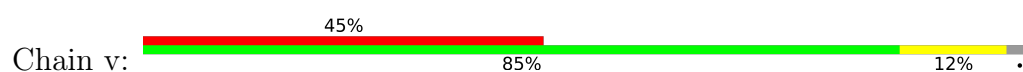


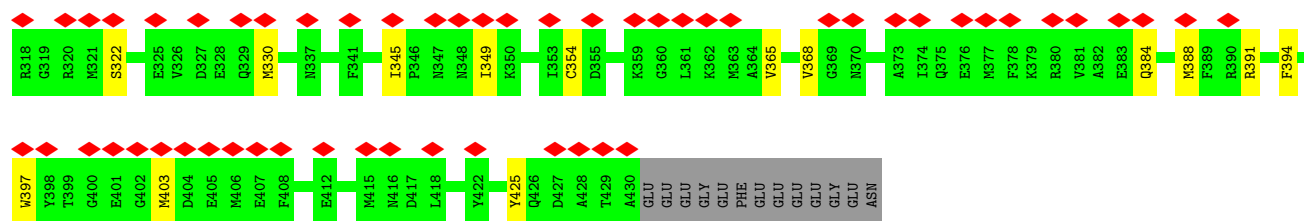


• Molecule 2: Tubulin beta chain

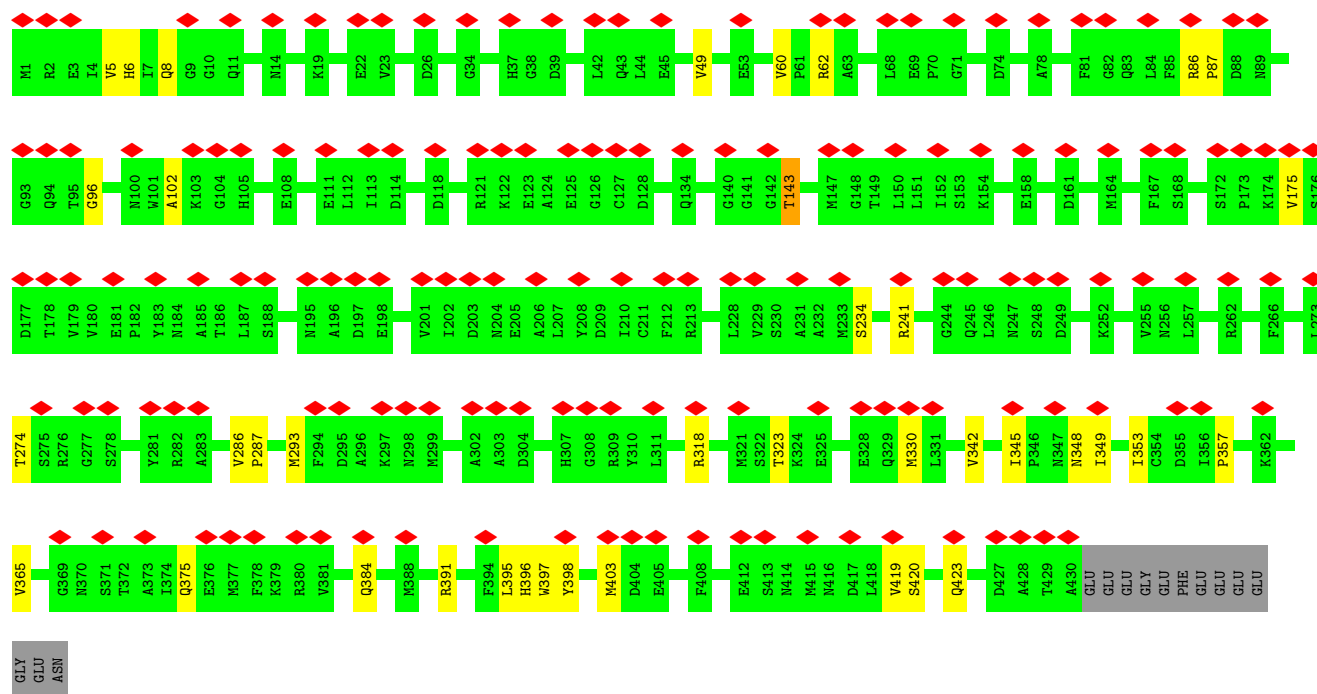
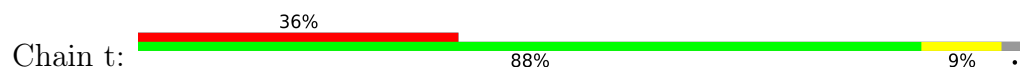


• Molecule 2: Tubulin beta chain

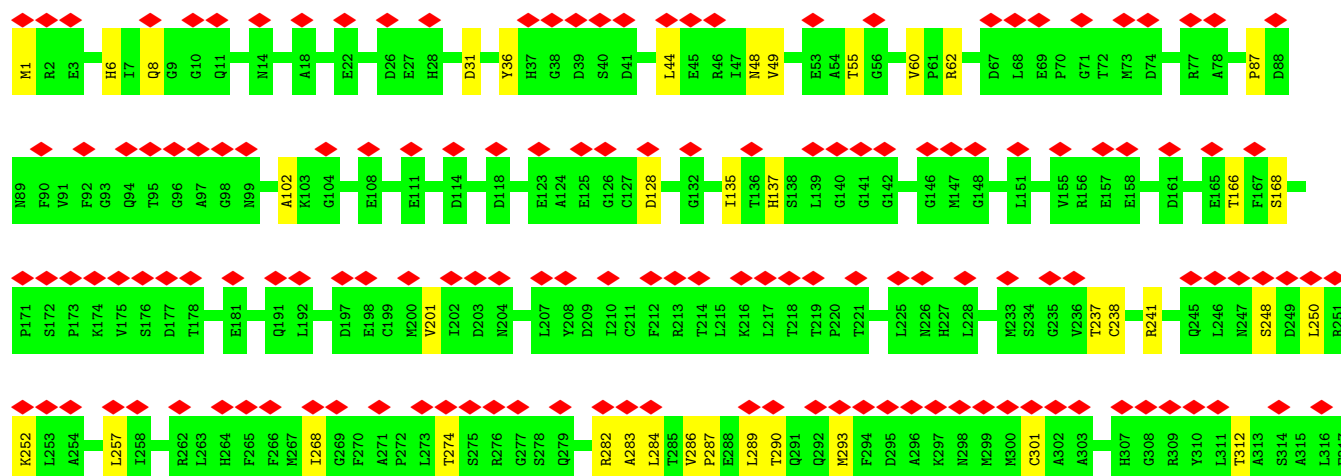
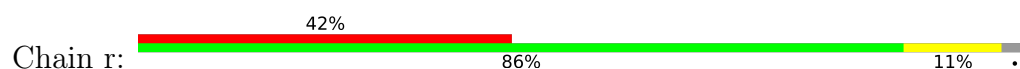


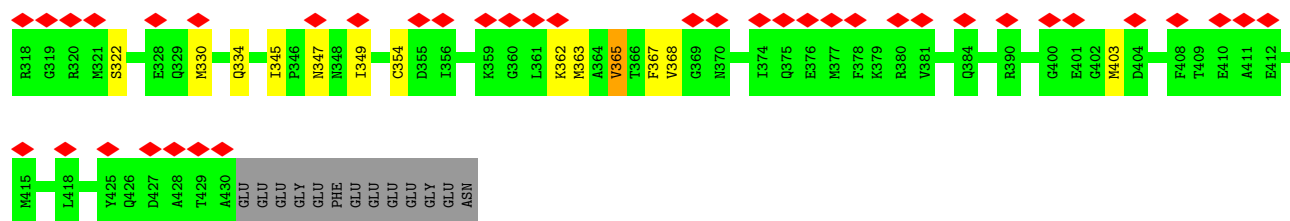


• Molecule 2: Tubulin beta chain

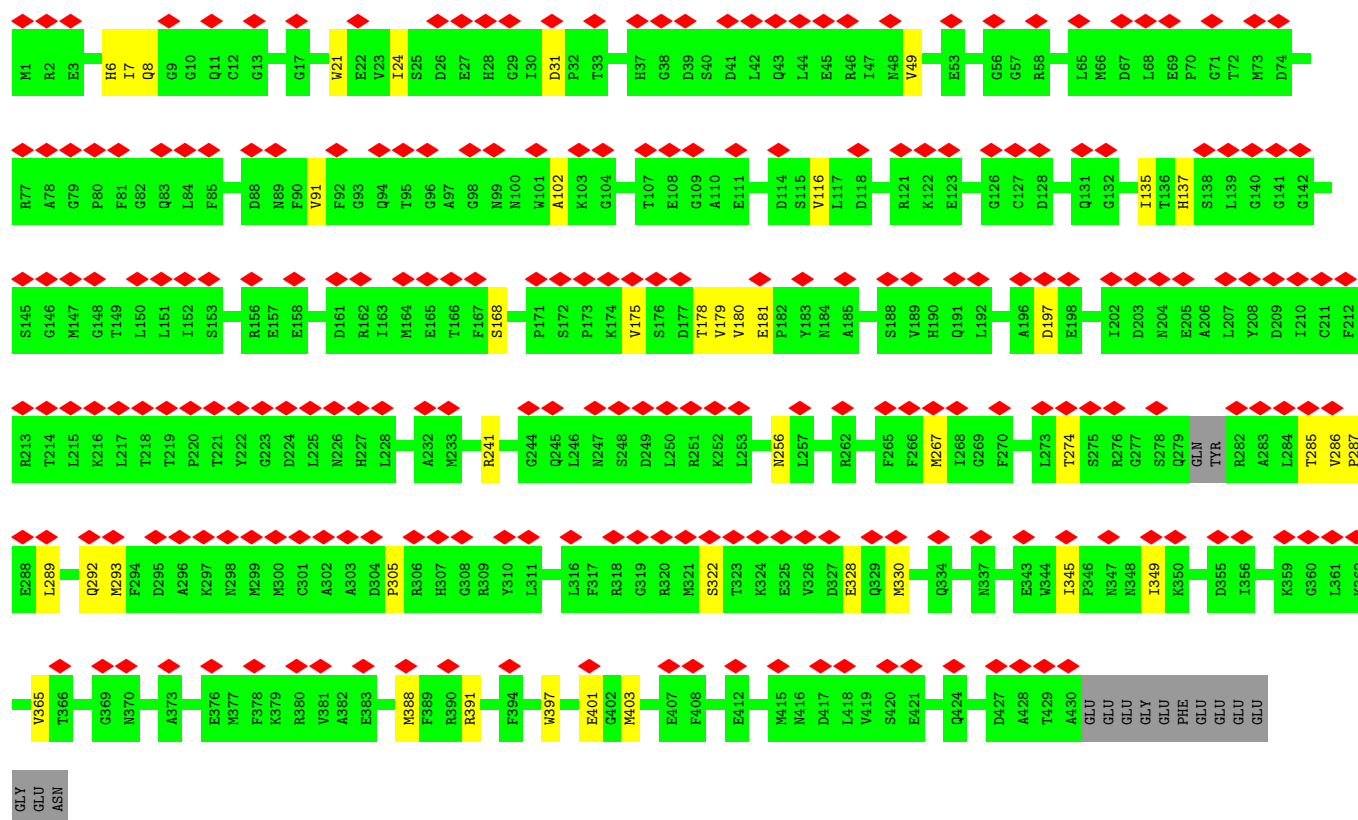
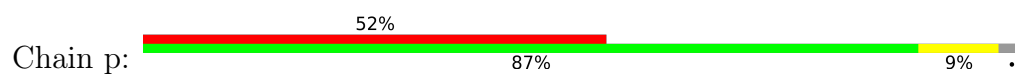


• Molecule 2: Tubulin beta chain

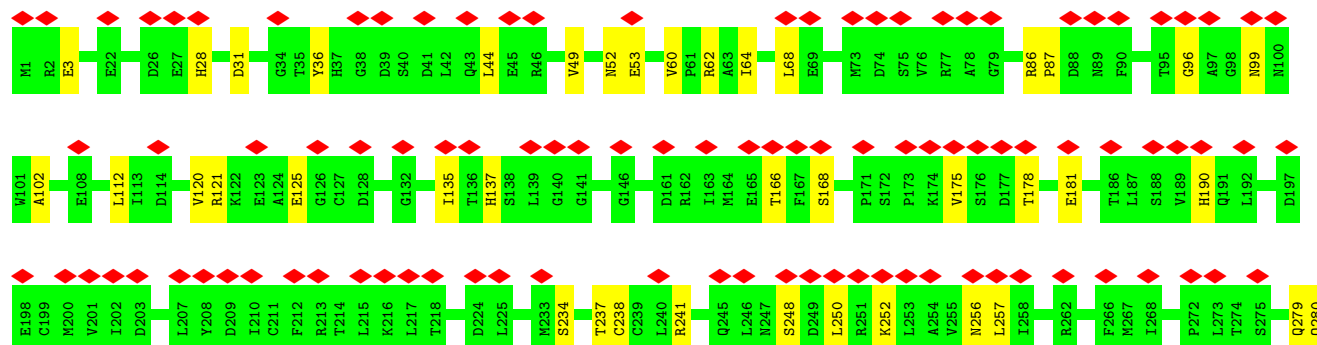
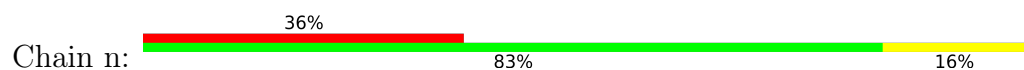


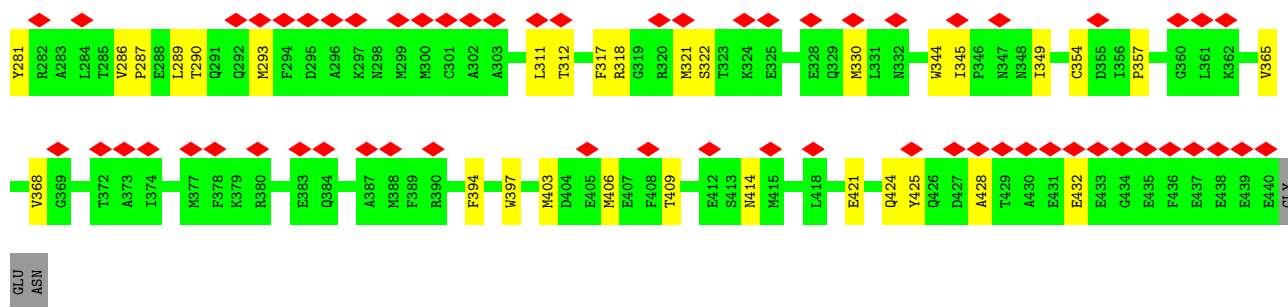


• Molecule 2: Tubulin beta chain

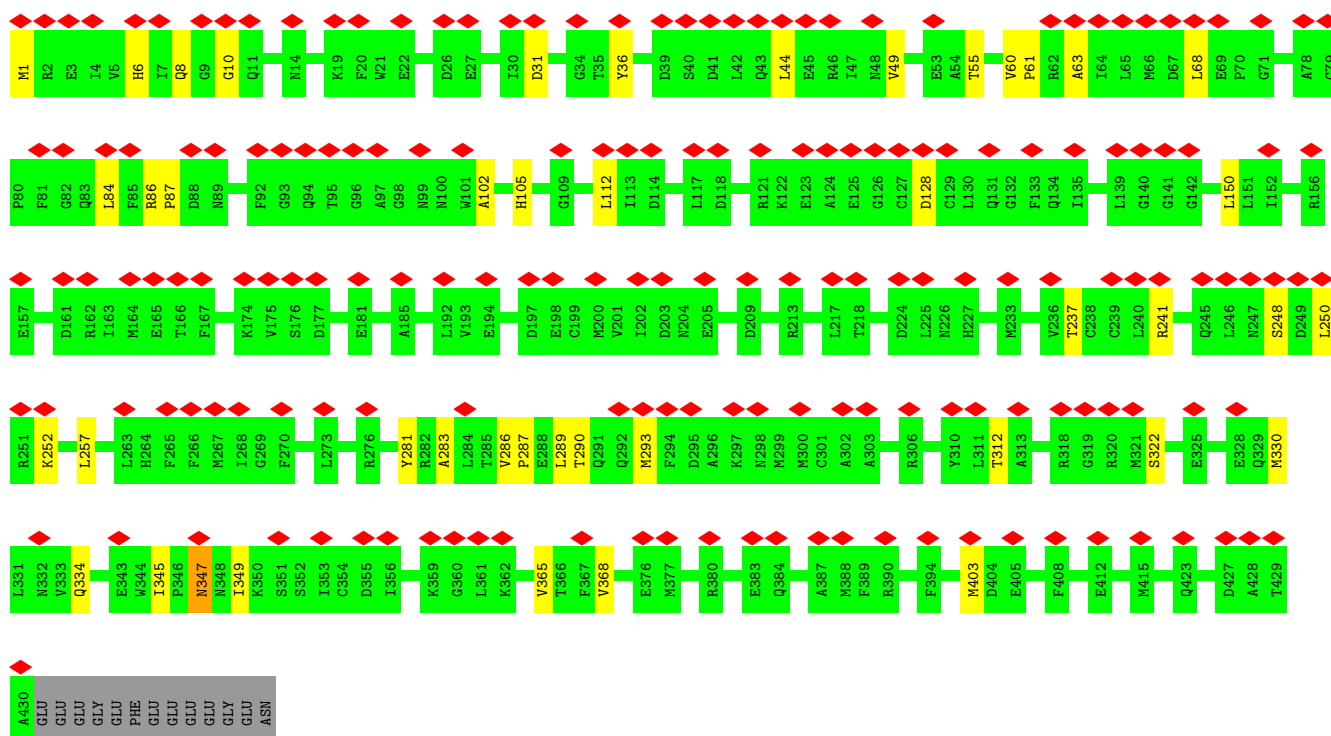
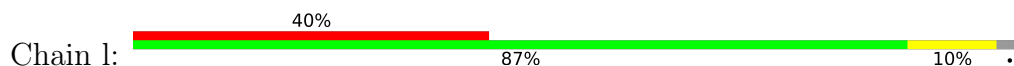


• Molecule 2: Tubulin beta chain

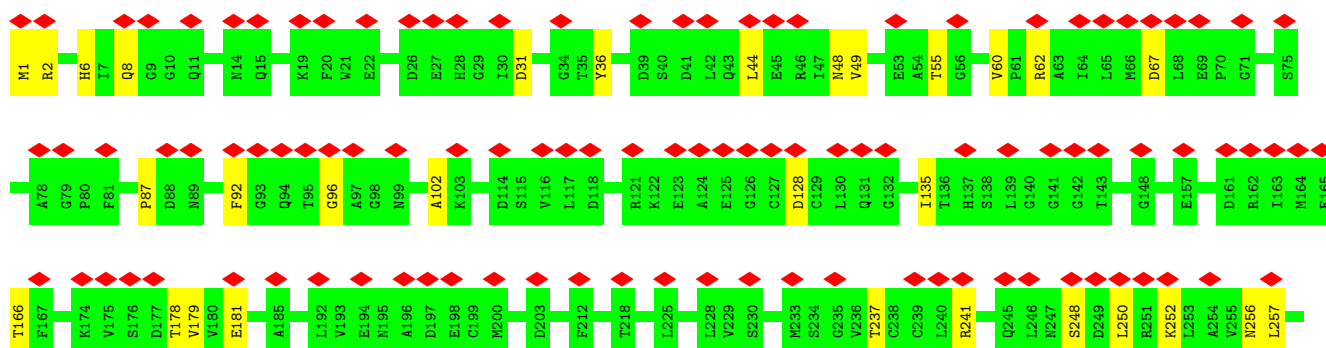
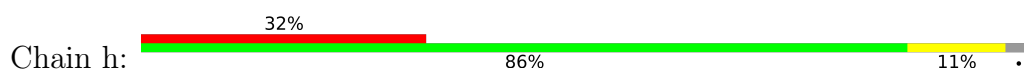


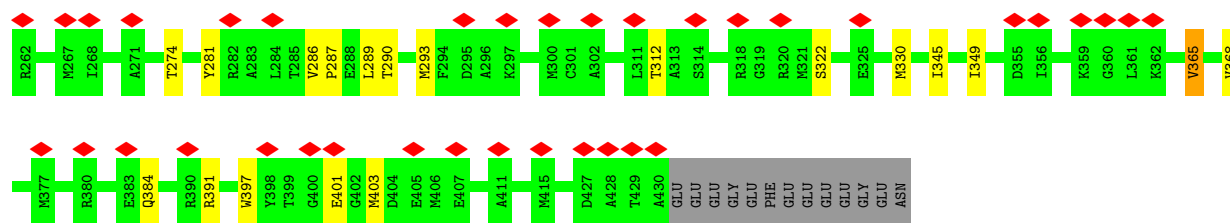


• Molecule 2: Tubulin beta chain

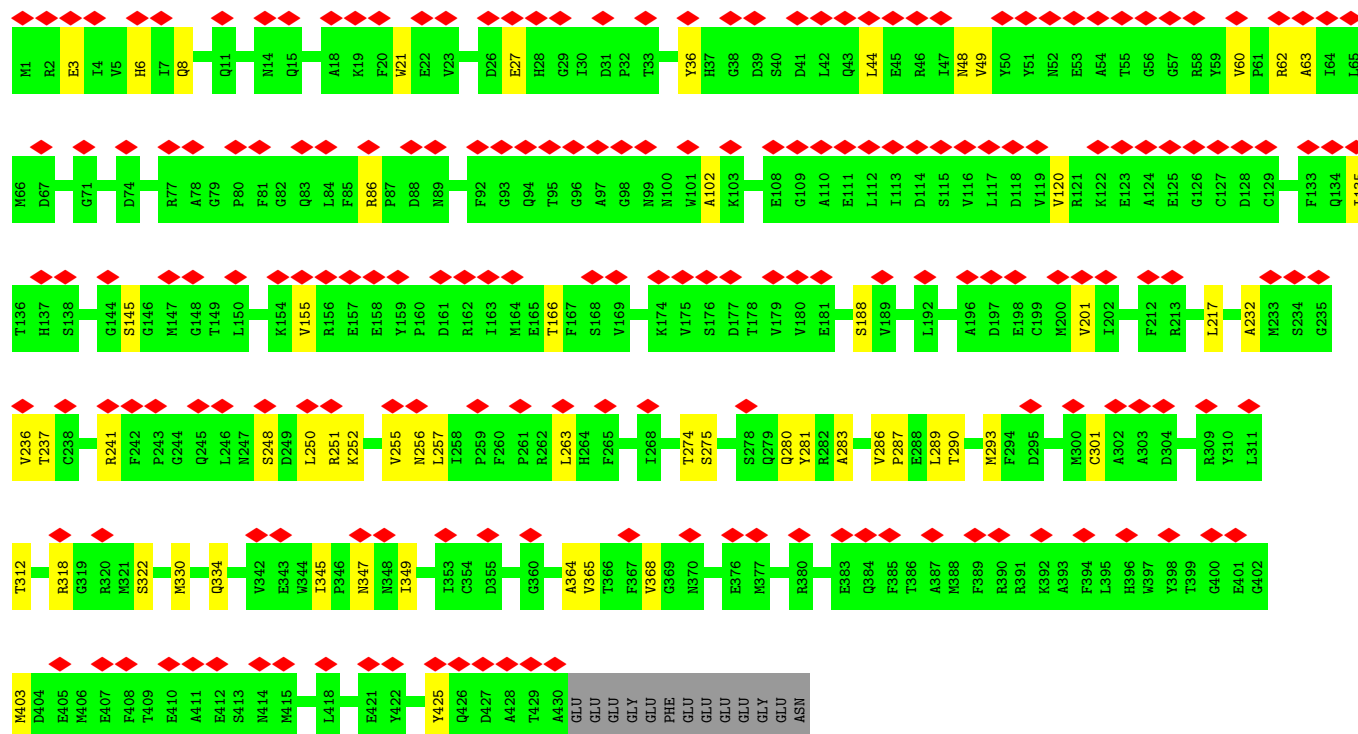
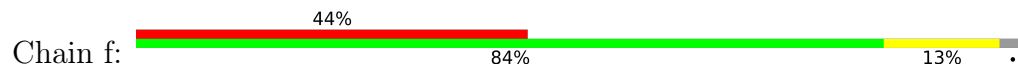


• Molecule 2: Tubulin beta chain

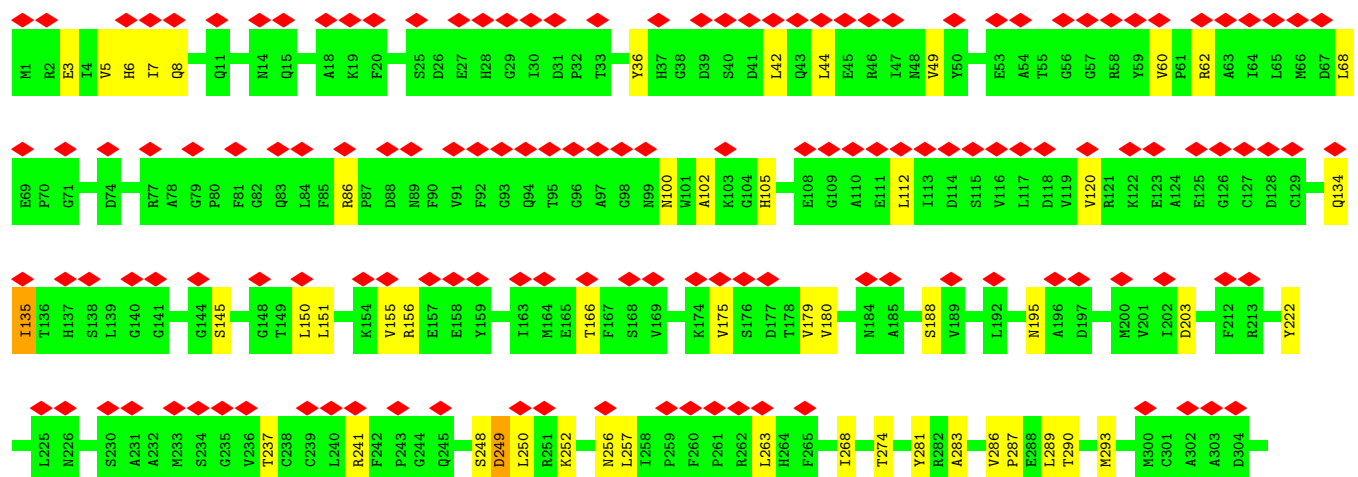
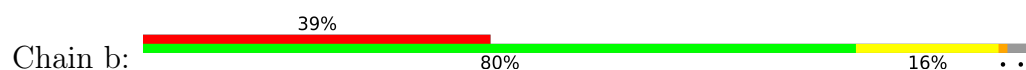


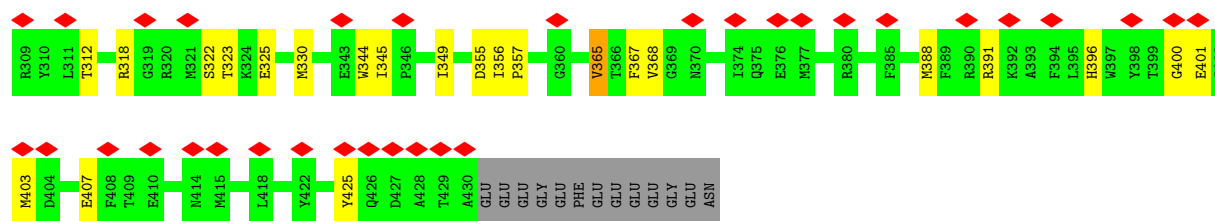


• Molecule 2: Tubulin beta chain

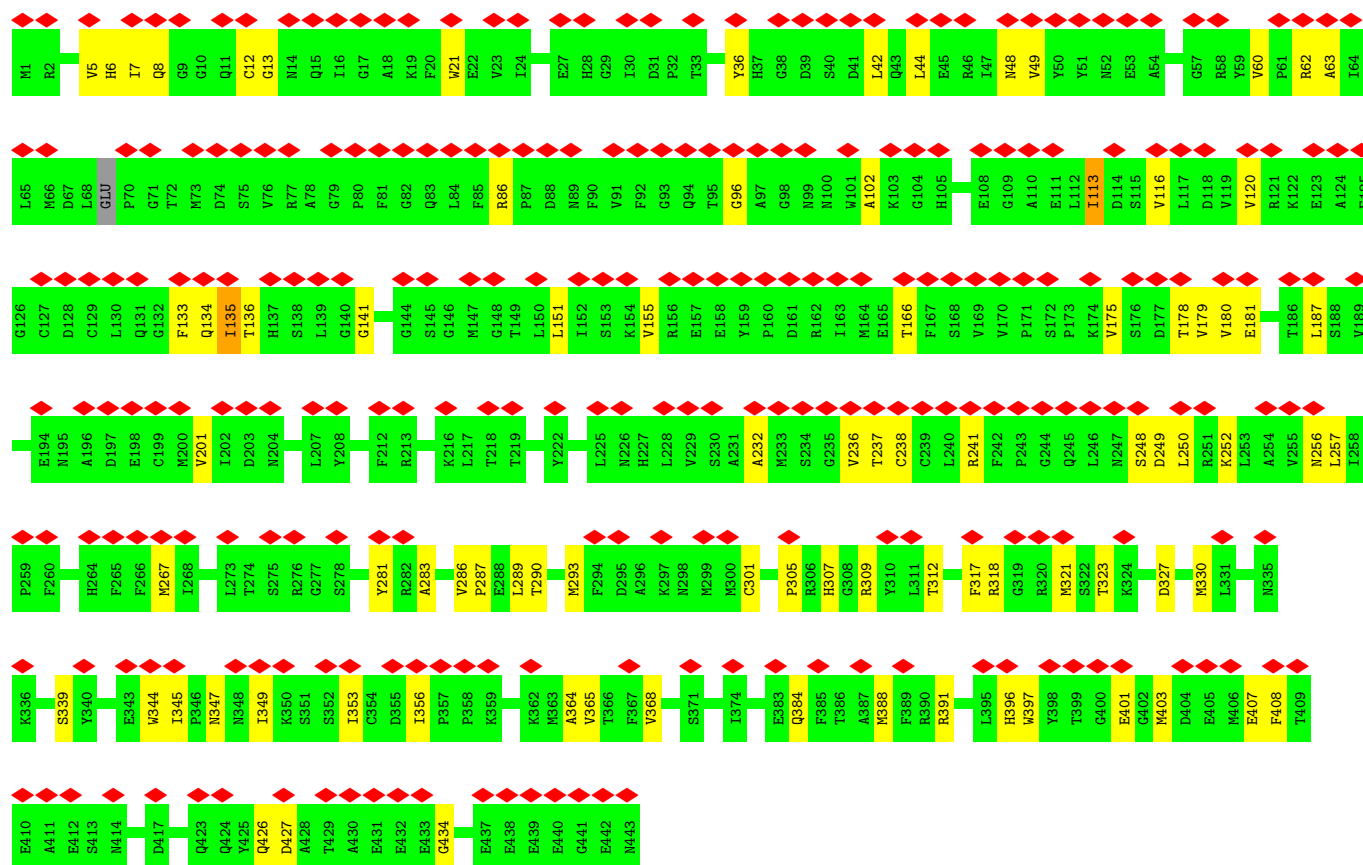
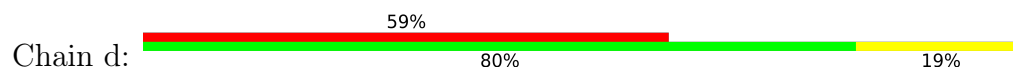


• Molecule 2: Tubulin beta chain

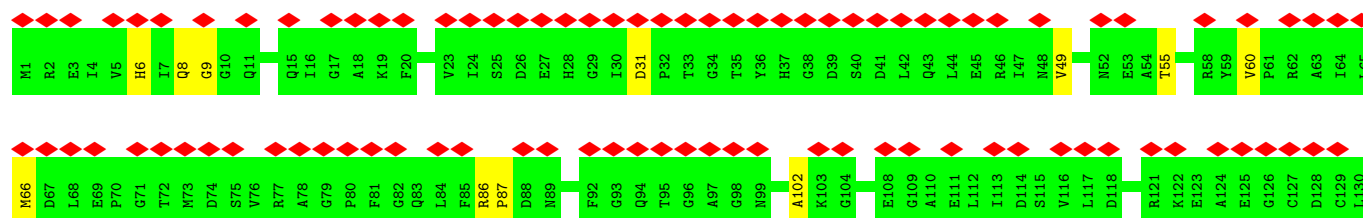
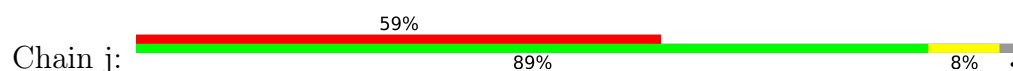




• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.012	Depositor
Minimum map value	0.000	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	530.5338, 477.21387, 449.22086	wwPDB
Map dimensions	398, 358, 337	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3329996, 1.3329996, 1.3329996	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, MG, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	1.03	1/3477 (0.0%)	1.56	4/4712 (0.1%)
1	c	1.06	0/3473	1.58	2/4708 (0.0%)
1	e	1.03	0/3473	1.56	2/4708 (0.0%)
1	g	1.02	1/3485 (0.0%)	1.55	0/4723
1	i	1.06	1/3477 (0.0%)	1.57	0/4715
1	k	1.03	1/3477 (0.0%)	1.56	0/4715
1	m	1.01	1/3481 (0.0%)	1.53	0/4719
1	o	1.05	1/3467 (0.0%)	1.56	0/4700
1	q	1.03	0/3475	1.56	0/4712
1	s	1.01	0/3481	1.51	2/4719 (0.0%)
1	u	1.03	0/3481	1.56	0/4719
1	w	1.05	0/3477	1.57	0/4715
2	b	1.00	0/3435	1.55	0/4650
2	d	1.06	0/3488	1.60	5/4721 (0.1%)
2	f	1.02	0/3435	1.56	0/4650
2	h	1.00	0/3439	1.56	1/4655 (0.0%)
2	j	1.05	0/3439	1.56	2/4655 (0.0%)
2	l	1.01	0/3439	1.57	3/4655 (0.1%)
2	n	1.00	0/3485	1.55	3/4719 (0.1%)
2	p	1.04	0/3416	1.55	2/4622 (0.0%)
2	r	1.02	0/3431	1.58	0/4644
2	t	1.00	0/3439	1.53	3/4655 (0.1%)
2	v	1.02	0/3439	1.57	5/4655 (0.1%)
2	x	1.02	0/3439	1.56	0/4655
All	All	1.03	6/83048 (0.0%)	1.56	34/112501 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
1	c	0	1
1	i	0	1
1	q	0	1
1	s	0	1
1	w	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	o	260	VAL	N-CA	5.20	1.50	1.46
1	g	260	VAL	N-CA	5.19	1.50	1.46
1	m	260	VAL	N-CA	5.16	1.50	1.46
1	i	260	VAL	N-CA	5.13	1.50	1.46
1	k	260	VAL	N-CA	5.06	1.50	1.46
1	a	260	VAL	N-CA	5.00	1.50	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	96	GLY	CA-C-O	-5.61	118.36	122.23
2	v	96	GLY	CA-C-O	-5.59	118.38	122.23
2	n	96	GLY	CA-C-O	-5.58	118.38	122.23
2	v	285	THR	CA-C-N	5.57	124.78	120.33
2	v	285	THR	C-N-CA	5.57	124.78	120.33
2	d	96	GLY	CA-C-O	-5.53	118.15	122.52
2	d	347	ASN	CA-C-N	5.43	127.56	120.28
2	d	347	ASN	C-N-CA	5.43	127.56	120.28
2	t	234	SER	CA-C-N	5.43	126.11	120.03
2	t	234	SER	C-N-CA	5.43	126.11	120.03
2	t	96	GLY	CA-C-O	-5.39	118.72	122.22
1	a	145	THR	CA-C-N	5.33	125.86	119.94
1	a	145	THR	C-N-CA	5.33	125.86	119.94
1	a	94	SER	CA-C-N	5.18	125.60	121.61
1	a	94	SER	C-N-CA	5.18	125.60	121.61
2	v	139	LEU	CA-C-N	5.17	125.58	119.94
2	v	139	LEU	C-N-CA	5.17	125.58	119.94
2	p	285	THR	CA-C-N	5.16	125.38	120.43
2	p	285	THR	C-N-CA	5.16	125.38	120.43
2	l	347	ASN	CA-C-N	5.15	127.18	120.28
2	l	347	ASN	C-N-CA	5.15	127.18	120.28
2	d	141	GLY	CA-C-N	5.11	126.57	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	141	GLY	C-N-CA	5.11	126.57	120.13
2	l	10	GLY	CA-C-O	-5.09	118.16	122.29
1	e	145	THR	CA-C-N	5.07	125.61	119.98
1	e	145	THR	C-N-CA	5.07	125.61	119.98
2	j	234	SER	CA-C-N	5.04	125.54	119.94
2	j	234	SER	C-N-CA	5.04	125.54	119.94
2	n	234	SER	CA-C-N	5.04	125.68	119.99
2	n	234	SER	C-N-CA	5.04	125.68	119.99
1	c	240	ALA	CA-C-N	5.02	127.01	120.28
1	c	240	ALA	C-N-CA	5.02	127.01	120.28
1	s	110	ILE	CA-C-N	5.02	125.65	120.03
1	s	110	ILE	C-N-CA	5.02	125.65	120.03

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	399	TYR	Peptide
1	c	402	ARG	Peptide
1	i	349	THR	Peptide
1	q	402	ARG	Peptide
1	s	402	ARG	Peptide
1	w	402	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3406	0	3345	51	0
1	c	3402	0	3334	72	0
1	e	3402	0	3334	49	0
1	g	3413	0	3352	44	0
1	i	3405	0	3330	21	0
1	k	3405	0	3330	43	0
1	m	3409	0	3341	42	0
1	o	3397	0	3329	21	0
1	q	3403	0	3325	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	s	3409	0	3341	20	0
1	u	3409	0	3341	40	0
1	w	3405	0	3330	50	0
2	b	3362	0	3251	56	0
2	d	3416	0	3273	63	0
2	f	3362	0	3251	47	0
2	h	3366	0	3257	40	0
2	j	3366	0	3257	28	0
2	l	3366	0	3257	35	0
2	n	3412	0	3269	49	0
2	p	3345	0	3239	24	0
2	r	3359	0	3250	35	0
2	t	3366	0	3257	25	0
2	v	3366	0	3257	39	0
2	x	3366	0	3257	30	0
3	a	32	0	12	0	0
3	c	32	0	12	1	0
3	e	32	0	12	2	0
3	g	32	0	12	0	0
3	i	32	0	12	0	0
3	k	32	0	12	0	0
3	m	32	0	12	0	0
3	o	32	0	12	0	0
3	q	32	0	12	1	0
3	s	32	0	12	0	0
3	u	32	0	12	0	0
3	w	32	0	12	1	0
4	a	1	0	0	0	0
4	c	1	0	0	0	0
4	e	1	0	0	0	0
4	g	1	0	0	0	0
4	i	1	0	0	0	0
4	k	1	0	0	0	0
4	m	1	0	0	0	0
4	o	1	0	0	0	0
4	q	1	0	0	0	0
4	t	1	0	0	0	0
4	u	1	0	0	0	0
4	x	1	0	0	0	0
5	b	28	0	12	0	0
5	f	28	0	12	0	0
5	h	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	j	28	0	12	0	0
5	l	28	0	12	0	0
5	n	28	0	12	0	0
5	p	28	0	12	0	0
5	r	28	0	12	0	0
5	t	28	0	12	1	0
5	v	28	0	12	0	0
5	x	28	0	12	0	0
All	All	82021	0	79383	824	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:293:MET:HE1	2:n:330:MET:HE1	1.51	0.92
2:f:293:MET:HE1	2:f:330:MET:HE1	1.51	0.90
2:b:293:MET:HE1	2:b:330:MET:HE1	1.51	0.89
2:v:293:MET:HE1	2:v:330:MET:HE1	1.54	0.88
2:r:293:MET:HE1	2:r:330:MET:HE1	1.56	0.87
2:h:293:MET:HE1	2:h:330:MET:HE1	1.57	0.83
2:x:293:MET:HE1	2:x:330:MET:HE1	1.57	0.83
1:a:398:MET:HG2	2:b:345:ILE:HD11	1.59	0.83
2:l:293:MET:HE1	2:l:330:MET:HE1	1.59	0.82
2:l:330:MET:HE3	2:l:349:ILE:HG21	1.63	0.80
2:f:330:MET:HE3	2:f:349:ILE:HG21	1.64	0.80
2:r:330:MET:HE3	2:r:349:ILE:HG21	1.63	0.79
2:n:330:MET:HE3	2:n:349:ILE:HG21	1.63	0.79
2:h:330:MET:HE3	2:h:349:ILE:HG21	1.64	0.79
2:b:330:MET:HE3	2:b:349:ILE:HG21	1.65	0.79
2:l:87:PRO:HD3	2:f:281:TYR:CE1	2.18	0.78
2:x:330:MET:HE3	2:x:349:ILE:HG21	1.65	0.78
1:c:283:HIS:HB2	1:i:88:HIS:ND1	2.00	0.77
2:v:330:MET:HE3	2:v:349:ILE:HG21	1.65	0.76
2:t:330:MET:HE3	2:t:349:ILE:HG21	1.67	0.76
2:j:293:MET:HE1	2:j:330:MET:HE1	1.69	0.74
2:t:375:GLN:HE22	2:t:423:GLN:HB2	1.53	0.72
2:f:102:ALA:HB2	2:f:403:MET:HE2	1.71	0.72
1:c:317:MET:HE3	1:c:375:VAL:HG21	1.71	0.72
2:b:102:ALA:HB2	2:b:403:MET:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:87:PRO:HD3	2:f:281:TYR:CD1	2.26	0.71
2:d:293:MET:HE1	2:d:330:MET:HE1	1.73	0.71
2:d:330:MET:HE3	2:d:349:ILE:HG21	1.73	0.69
1:k:398:MET:HE3	2:l:345:ILE:HD11	1.74	0.69
1:a:286:LEU:O	1:a:373:ARG:NH1	2.26	0.68
2:d:237:THR:O	2:d:241:ARG:NH1	2.27	0.67
1:c:119:LEU:HD11	1:c:156:ARG:HB3	1.77	0.67
1:a:274:PRO:HG3	1:a:374:ALA:HA	1.77	0.66
1:c:401:LYS:HG3	2:d:344:TRP:CD1	2.30	0.66
2:d:281:TYR:CE2	2:j:87:PRO:HD3	2.31	0.66
2:n:344:TRP:CZ3	2:n:428:ALA:HB3	2.30	0.66
1:e:398:MET:HG2	2:f:345:ILE:HD11	1.77	0.66
2:p:102:ALA:HB2	2:p:403:MET:HE2	1.78	0.65
2:f:257:LEU:HA	2:f:312:THR:HG21	1.78	0.65
1:u:439:THR:HG22	2:t:391:ARG:HD2	1.78	0.65
1:c:283:HIS:HB2	1:i:88:HIS:HD1	1.62	0.65
1:o:102:ASN:HD21	1:o:407:TRP:HB3	1.61	0.65
1:w:317:MET:HE3	1:w:375:VAL:HG21	1.79	0.64
1:q:398:MET:HE3	2:r:345:ILE:HD11	1.79	0.64
2:j:330:MET:HE3	2:j:349:ILE:HG21	1.78	0.64
2:f:201:VAL:HG23	2:f:301:CYS:SG	2.37	0.64
2:p:330:MET:HE3	2:p:349:ILE:HG21	1.80	0.64
1:e:274:PRO:HG3	1:e:374:ALA:HA	1.80	0.64
1:w:88:HIS:ND1	1:q:283:HIS:HB2	2.13	0.64
1:k:119:LEU:HD11	1:k:156:ARG:HB3	1.81	0.63
1:c:398:MET:HG2	2:d:345:ILE:CD1	2.28	0.63
1:w:437:ILE:O	2:v:391:ARG:NH1	2.32	0.63
2:h:87:PRO:HD3	2:b:281:TYR:CE1	2.34	0.62
1:e:346:TRP:HB3	2:d:391:ARG:HG3	1.82	0.62
1:c:188:ILE:HD12	1:c:395:PHE:CG	2.34	0.62
1:s:119:LEU:HD11	1:s:156:ARG:HB3	1.79	0.62
1:g:398:MET:HE3	2:h:345:ILE:HD11	1.81	0.62
1:w:398:MET:HE3	2:x:345:ILE:HD11	1.81	0.62
1:u:119:LEU:HD11	1:u:156:ARG:HB3	1.81	0.62
2:d:257:LEU:HA	2:d:312:THR:HG21	1.82	0.62
1:a:398:MET:HG2	2:b:345:ILE:CD1	2.29	0.62
2:d:248:SER:HA	2:d:252:LYS:HD3	1.82	0.62
1:e:346:TRP:CD1	2:d:391:ARG:HD3	2.35	0.61
1:g:223:THR:HG22	2:h:322:SER:HA	1.80	0.61
1:o:182:VAL:HG12	2:p:256:ASN:HD21	1.66	0.61
1:g:62:VAL:HG21	1:a:283:HIS:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:317:MET:HE3	1:q:375:VAL:HG21	1.83	0.61
2:f:36:TYR:CG	2:f:44:LEU:HD11	2.36	0.61
1:k:88:HIS:ND1	1:e:283:HIS:HB2	2.16	0.61
1:g:188:ILE:HD12	1:g:425:LEU:CD1	2.31	0.61
2:d:36:TYR:CG	2:d:44:LEU:HD11	2.35	0.60
1:m:398:MET:HE3	2:n:345:ILE:HD11	1.82	0.60
2:b:36:TYR:CG	2:b:44:LEU:HD11	2.36	0.60
1:w:274:PRO:HG3	1:w:374:ALA:HA	1.82	0.60
1:g:1:MET:N	1:g:130:THR:O	2.34	0.60
1:c:398:MET:HG2	2:d:345:ILE:HD11	1.82	0.60
1:w:119:LEU:HD11	1:w:156:ARG:HB3	1.83	0.60
1:u:317:MET:HE3	1:u:375:VAL:HG21	1.83	0.60
1:u:274:PRO:HG3	1:u:374:ALA:HA	1.83	0.60
1:s:265:ILE:CG2	1:s:265:ILE:O	2.49	0.60
1:a:188:ILE:HD12	1:a:395:PHE:CG	2.37	0.60
2:n:36:TYR:CG	2:n:44:LEU:HD11	2.36	0.60
2:h:6:HIS:HE2	2:h:8:GLN:HB3	1.66	0.59
2:n:87:PRO:HD3	2:h:281:TYR:CE1	2.37	0.59
1:w:1:MET:N	1:w:130:THR:O	2.36	0.59
2:l:60:VAL:HG21	2:f:281:TYR:HA	1.84	0.59
1:g:88:HIS:ND1	1:a:283:HIS:HB2	2.18	0.59
2:v:290:THR:HG23	2:v:293:MET:HE2	1.85	0.59
2:x:36:TYR:CG	2:x:44:LEU:HD11	2.38	0.59
1:m:317:MET:HE3	1:m:375:VAL:HG21	1.84	0.59
1:e:317:MET:HE3	1:e:375:VAL:HG21	1.83	0.59
2:b:248:SER:HA	2:b:252:LYS:HD3	1.85	0.59
1:m:119:LEU:HD11	1:m:156:ARG:HB3	1.85	0.59
2:b:257:LEU:HA	2:b:312:THR:HG21	1.85	0.59
2:n:257:LEU:HA	2:n:312:THR:HG21	1.85	0.58
1:k:399:TYR:O	1:k:402:ARG:NH1	2.36	0.58
1:e:167:LEU:HD22	1:e:200:VAL:HB	1.84	0.58
1:k:1:MET:N	1:k:130:THR:O	2.36	0.58
1:k:317:MET:HE3	1:k:375:VAL:HG21	1.85	0.58
1:g:276:ILE:CD1	1:g:286:LEU:HD21	2.33	0.58
1:w:167:LEU:HD22	1:w:200:VAL:HB	1.85	0.58
1:g:317:MET:HE3	1:g:375:VAL:HG21	1.84	0.58
1:e:399:TYR:O	1:e:402:ARG:NH1	2.36	0.58
1:a:1:MET:N	1:a:130:THR:O	2.36	0.58
2:r:102:ALA:HB2	2:r:403:MET:HE2	1.85	0.58
1:m:88:HIS:ND1	1:g:283:HIS:HB2	2.18	0.58
1:k:274:PRO:HG3	1:k:374:ALA:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:36:TYR:CG	2:r:44:LEU:HD11	2.39	0.57
1:m:274:PRO:HG3	1:m:374:ALA:HA	1.86	0.57
2:d:187:LEU:HD11	2:d:408:PHE:CE2	2.39	0.57
1:w:269:LEU:HD21	1:w:305:CYS:SG	2.44	0.57
2:x:102:ALA:HB2	2:x:403:MET:HE2	1.85	0.57
1:k:167:LEU:HD22	1:k:200:VAL:HB	1.85	0.57
1:e:119:LEU:HD11	1:e:156:ARG:HB3	1.87	0.57
2:v:36:TYR:CG	2:v:44:LEU:HD11	2.40	0.57
1:c:274:PRO:HG3	1:c:374:ALA:HA	1.86	0.57
1:m:276:ILE:CD1	1:m:286:LEU:HD21	2.34	0.57
1:q:274:PRO:HG3	1:q:374:ALA:HA	1.85	0.57
1:u:188:ILE:HD12	1:u:395:PHE:CG	2.40	0.56
2:h:102:ALA:HB2	2:h:403:MET:HE2	1.87	0.56
1:c:437:ILE:O	2:b:391:ARG:NH1	2.38	0.56
1:a:167:LEU:HD22	1:a:200:VAL:HB	1.86	0.56
2:v:102:ALA:HB2	2:v:403:MET:HE2	1.86	0.56
1:q:256:GLN:HG2	2:p:397:TRP:CH2	2.40	0.56
1:s:188:ILE:HG13	1:s:425:LEU:HD12	1.87	0.56
1:q:1:MET:N	1:q:130:THR:O	2.38	0.56
2:h:87:PRO:HD3	2:b:281:TYR:CD1	2.41	0.56
1:e:188:ILE:HD12	1:e:395:PHE:CG	2.41	0.56
1:c:167:LEU:HD22	1:c:200:VAL:HB	1.86	0.56
1:u:167:LEU:HD22	1:u:200:VAL:HB	1.87	0.56
1:a:399:TYR:O	1:a:402:ARG:NH1	2.38	0.56
1:c:260:VAL:HG23	1:c:262:TYR:O	2.06	0.56
1:w:329:ASN:HD21	2:v:175:VAL:HG22	1.70	0.56
1:w:346:TRP:CD1	2:v:391:ARG:HD3	2.41	0.56
1:q:119:LEU:HD11	1:q:156:ARG:HB3	1.88	0.56
1:g:399:TYR:O	1:g:402:ARG:NH1	2.39	0.56
1:g:188:ILE:HG23	1:g:425:LEU:HD12	1.86	0.56
2:h:55:THR:HG23	2:b:283:ALA:HA	1.86	0.56
2:r:257:LEU:HA	2:r:312:THR:HG21	1.88	0.56
1:w:256:GLN:HG2	2:v:397:TRP:CH2	2.41	0.56
1:q:276:ILE:CD1	1:q:286:LEU:HD21	2.36	0.56
1:q:398:MET:C	1:q:400:ALA:H	2.14	0.56
2:r:284:LEU:HD23	2:r:362:LYS:HB2	1.88	0.55
1:o:256:GLN:HG2	2:n:397:TRP:CH2	2.41	0.55
1:g:398:MET:HG2	2:h:345:ILE:HD11	1.88	0.55
1:c:292:THR:HG21	1:c:331:SER:CB	2.37	0.55
2:t:375:GLN:NE2	2:t:419:VAL:O	2.39	0.55
1:q:269:LEU:HD21	1:q:305:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:119:LEU:HD11	1:g:156:ARG:HB3	1.89	0.55
2:r:274:THR:HG21	2:r:282:ARG:HD2	1.87	0.55
1:u:1:MET:N	1:u:130:THR:O	2.39	0.55
2:l:55:THR:HG23	2:f:283:ALA:HA	1.89	0.55
1:c:399:TYR:O	1:c:402:ARG:NH1	2.40	0.55
1:c:1:MET:N	1:c:130:THR:O	2.40	0.55
1:c:402:ARG:C	1:c:405:VAL:HG23	2.31	0.55
2:l:36:TYR:CG	2:l:44:LEU:HD11	2.42	0.55
2:t:87:PRO:HD3	2:n:281:TYR:CE2	2.41	0.55
1:q:437:ILE:O	2:p:391:ARG:NH1	2.40	0.55
1:g:167:LEU:HD22	1:g:200:VAL:HB	1.87	0.55
1:s:265:ILE:O	1:s:265:ILE:HG22	2.06	0.55
2:l:102:ALA:HB2	2:l:403:MET:HE2	1.87	0.55
1:k:349:THR:HB	2:j:176:SER:OG	2.07	0.54
1:k:62:VAL:HG21	1:e:283:HIS:HA	1.89	0.54
2:f:49:VAL:HG11	2:f:241:ARG:HG2	1.89	0.54
1:w:188:ILE:HD12	1:w:395:PHE:CG	2.42	0.54
2:n:60:VAL:HG21	2:h:281:TYR:HA	1.89	0.54
1:s:334:THR:O	1:s:337:THR:N	2.41	0.54
2:n:49:VAL:HG11	2:n:241:ARG:HG2	1.89	0.54
2:l:49:VAL:HG11	2:l:241:ARG:HG2	1.90	0.54
1:c:286:LEU:O	1:c:373:ARG:NH1	2.41	0.54
1:m:241:SER:HA	1:m:356:ASN:HD21	1.72	0.54
2:h:36:TYR:CG	2:h:44:LEU:HD11	2.43	0.54
2:x:237:THR:O	2:x:241:ARG:NH1	2.41	0.54
2:l:6:HIS:HE2	2:l:8:GLN:HB3	1.72	0.54
1:c:182:VAL:HG12	2:d:256:ASN:HD21	1.73	0.54
1:w:398:MET:C	1:w:400:ALA:H	2.16	0.54
2:t:102:ALA:HB2	2:t:403:MET:HE2	1.89	0.54
1:m:155:GLU:HG2	1:m:197:HIS:CD2	2.43	0.54
2:n:102:ALA:HB2	2:n:403:MET:HE2	1.89	0.54
1:g:274:PRO:HG3	1:g:374:ALA:HA	1.88	0.54
2:h:290:THR:HG23	2:h:293:MET:HE2	1.89	0.54
1:u:276:ILE:CD1	1:u:286:LEU:HD21	2.37	0.54
2:d:201:VAL:HG23	2:d:301:CYS:SG	2.48	0.54
1:q:223:THR:HG22	2:r:322:SER:HA	1.90	0.53
1:o:265:ILE:O	1:o:265:ILE:CG2	2.56	0.53
2:x:290:THR:HG23	2:x:293:MET:HE2	1.90	0.53
1:s:205:ASP:O	1:s:206:ASN:C	2.51	0.53
2:l:237:THR:O	2:l:241:ARG:NH1	2.41	0.53
2:r:137:HIS:O	2:r:168:SER:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:234:VAL:HG21	1:e:302:MET:SD	2.48	0.53
2:b:290:THR:HG23	2:b:293:MET:HE2	1.89	0.53
2:p:293:MET:HE1	2:p:330:MET:HE1	1.89	0.53
1:m:399:TYR:O	1:m:402:ARG:NH1	2.41	0.53
2:d:49:VAL:HG11	2:d:241:ARG:HG2	1.90	0.53
2:n:137:HIS:O	2:n:168:SER:HA	2.09	0.53
2:n:190:HIS:CD2	2:n:414:ASN:HD22	2.26	0.53
2:r:290:THR:HG23	2:r:293:MET:HE2	1.90	0.53
2:l:289:LEU:HD23	2:l:365:VAL:HG23	1.91	0.53
1:c:70:LEU:HD22	1:c:110:ILE:HG22	1.90	0.53
2:v:49:VAL:HG11	2:v:241:ARG:HG2	1.91	0.53
1:s:88:HIS:ND1	1:m:283:HIS:HB2	2.24	0.53
1:s:273:ALA:HB3	1:s:274:PRO:HD3	1.91	0.53
2:r:284:LEU:HD21	2:r:363:MET:N	2.24	0.53
1:o:274:PRO:HG3	1:o:374:ALA:HA	1.91	0.53
1:c:276:ILE:CD1	1:c:286:LEU:HD21	2.38	0.53
2:j:345:ILE:O	2:j:345:ILE:HG22	2.08	0.53
2:x:257:LEU:HA	2:x:312:THR:HG21	1.90	0.52
1:a:76:ASP:O	1:a:79:ARG:N	2.42	0.52
1:u:158:SER:HA	1:u:166:LYS:HE2	1.91	0.52
2:v:48:ASN:O	2:v:62:ARG:NH2	2.35	0.52
2:v:257:LEU:HA	2:v:312:THR:HG21	1.90	0.52
2:r:49:VAL:HG11	2:r:241:ARG:HG2	1.90	0.52
2:p:345:ILE:HG22	2:p:345:ILE:O	2.09	0.52
1:c:289:ALA:O	1:c:292:THR:OG1	2.26	0.52
2:d:102:ALA:HB2	2:d:403:MET:HE2	1.90	0.52
2:x:54:ALA:HA	2:r:283:ALA:HB2	1.92	0.52
1:a:398:MET:C	1:a:400:ALA:H	2.16	0.52
1:u:256:GLN:HG2	2:t:397:TRP:CH2	2.43	0.52
1:q:329:ASN:HD21	2:p:175:VAL:HG22	1.75	0.52
2:n:87:PRO:HD3	2:h:281:TYR:CD1	2.44	0.52
2:r:238:CYS:SG	2:r:354:CYS:SG	3.07	0.52
2:f:36:TYR:CD2	2:f:44:LEU:HD11	2.44	0.52
2:x:334:GLN:HE22	2:x:347:ASN:H	1.56	0.52
1:e:398:MET:C	1:e:400:ALA:H	2.18	0.52
1:i:265:ILE:CG2	1:i:380:ASN:HD21	2.23	0.52
2:t:6:HIS:HE2	2:t:8:GLN:HB3	1.75	0.52
2:n:290:THR:HG23	2:n:293:MET:HE2	1.92	0.52
1:c:189:LEU:HD11	1:c:418:PHE:CE1	2.44	0.52
2:f:145:SER:OG	2:f:188:SER:HB3	2.10	0.52
2:d:403:MET:SD	2:d:407:GLU:HG2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:269:LEU:HD21	1:m:305:CYS:SG	2.50	0.51
1:k:352:LYS:HA	2:j:177:ASP:O	2.10	0.51
2:f:6:HIS:CD2	2:f:21:TRP:HE1	2.28	0.51
1:u:398:MET:HE3	2:v:345:ILE:HD11	1.92	0.51
1:o:188:ILE:HG13	1:o:425:LEU:HD12	1.90	0.51
1:m:188:ILE:HD12	1:m:395:PHE:CG	2.45	0.51
1:k:141:VAL:HG22	1:k:172:TYR:HA	1.91	0.51
2:h:49:VAL:HG11	2:h:241:ARG:HG2	1.92	0.51
1:g:269:LEU:HD21	1:g:305:CYS:SG	2.50	0.51
1:g:398:MET:C	1:g:400:ALA:H	2.19	0.51
2:d:289:LEU:HD23	2:d:365:VAL:HG23	1.93	0.51
1:w:206:ASN:HD21	3:w:501:GTP:HN22	1.59	0.51
1:q:158:SER:HA	1:q:166:LYS:HE2	1.92	0.51
1:m:141:VAL:HG22	1:m:172:TYR:HA	1.93	0.51
1:k:223:THR:HG22	2:l:322:SER:HA	1.93	0.51
2:f:290:THR:HG23	2:f:293:MET:HE2	1.92	0.51
1:a:158:SER:HA	1:a:166:LYS:HE2	1.92	0.51
2:b:237:THR:O	2:b:241:ARG:NH1	2.44	0.51
1:e:208:ALA:HB2	1:e:304:LYS:HB2	1.93	0.51
1:q:167:LEU:HD22	1:q:200:VAL:HB	1.92	0.51
1:k:234:VAL:HG21	1:k:302:MET:SD	2.51	0.51
1:g:234:VAL:HG21	1:g:302:MET:SD	2.51	0.51
1:u:234:VAL:HG21	1:u:302:MET:SD	2.51	0.51
2:b:49:VAL:HG11	2:b:241:ARG:HG2	1.92	0.51
1:c:102:ASN:ND2	1:c:411:GLU:OE1	2.44	0.50
1:w:276:ILE:CD1	1:w:286:LEU:HD21	2.40	0.50
1:w:296:PHE:CZ	1:w:351:PHE:CE2	2.99	0.50
2:f:6:HIS:HE2	2:f:8:GLN:HB3	1.76	0.50
2:b:403:MET:SD	2:b:407:GLU:HG2	2.50	0.50
2:d:309:ARG:NE	2:d:339:SER:O	2.44	0.50
2:x:49:VAL:HG11	2:x:241:ARG:HG2	1.93	0.50
1:m:398:MET:C	1:m:400:ALA:H	2.18	0.50
2:l:257:LEU:HA	2:l:312:THR:HG21	1.92	0.50
1:c:375:VAL:HG22	1:c:376:CYS:O	2.11	0.50
1:a:208:ALA:HB3	1:a:302:MET:O	2.12	0.50
1:a:231:ILE:O	1:a:234:VAL:HB	2.11	0.50
2:v:6:HIS:HE2	2:v:8:GLN:HB3	1.76	0.50
1:m:158:SER:HA	1:m:166:LYS:HE2	1.94	0.50
1:w:158:SER:HA	1:w:166:LYS:HE2	1.92	0.50
2:n:330:MET:HE3	2:n:349:ILE:CG2	2.40	0.50
1:g:158:SER:HA	1:g:166:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:398:MET:HG2	2:v:345:ILE:CD1	2.42	0.50
2:r:48:ASN:O	2:r:62:ARG:NH2	2.40	0.50
2:f:248:SER:HA	2:f:252:LYS:HD3	1.94	0.50
2:j:102:ALA:HB2	2:j:403:MET:HE2	1.93	0.50
1:m:398:MET:HG2	2:n:345:ILE:HD11	1.93	0.50
1:e:141:VAL:HG22	1:e:172:TYR:HA	1.93	0.50
2:d:6:HIS:O	2:d:63:ALA:HA	2.11	0.50
1:k:269:LEU:HD21	1:k:305:CYS:SG	2.52	0.49
2:h:345:ILE:O	2:h:345:ILE:HG22	2.12	0.49
1:e:329:ASN:HD21	2:d:175:VAL:HG22	1.77	0.49
1:a:234:VAL:HG21	1:a:302:MET:SD	2.53	0.49
2:j:201:VAL:O	2:j:301:CYS:SG	2.70	0.49
1:e:1:MET:N	1:e:130:THR:O	2.45	0.49
2:d:6:HIS:CD2	2:d:21:TRP:HE1	2.30	0.49
1:w:296:PHE:HB3	1:w:341:ILE:HD11	1.94	0.49
2:d:345:ILE:HG22	2:d:345:ILE:O	2.12	0.49
2:r:135:ILE:HB	2:r:166:THR:HG22	1.93	0.49
2:l:87:PRO:CD	2:f:281:TYR:CD1	2.94	0.49
2:l:345:ILE:HG22	2:l:345:ILE:O	2.11	0.49
2:t:293:MET:HE1	2:t:330:MET:HE1	1.94	0.49
1:q:188:ILE:HD12	1:q:395:PHE:CG	2.48	0.49
2:h:289:LEU:HD23	2:h:365:VAL:HG23	1.95	0.49
1:c:346:TRP:HB3	2:b:391:ARG:HG3	1.95	0.49
1:a:119:LEU:HD11	1:a:156:ARG:HB3	1.94	0.49
1:a:276:ILE:CD1	1:a:286:LEU:HD21	2.43	0.49
2:d:48:ASN:O	2:d:62:ARG:NH2	2.41	0.49
2:j:289:LEU:HD23	2:j:365:VAL:HG23	1.94	0.49
1:o:188:ILE:CG1	1:o:425:LEU:HD12	2.43	0.49
1:a:81:GLY:O	1:a:84:ARG:N	2.46	0.49
2:v:289:LEU:HD23	2:v:365:VAL:HG23	1.94	0.48
2:p:286:VAL:N	2:p:287:PRO:HD2	2.28	0.48
1:k:276:ILE:CD1	1:k:286:LEU:HD21	2.43	0.48
1:e:439:THR:HG22	2:d:391:ARG:CG	2.43	0.48
1:u:241:SER:HA	1:u:356:ASN:HD21	1.78	0.48
2:n:286:VAL:N	2:n:287:PRO:HD2	2.28	0.48
1:k:256:GLN:O	1:k:260:VAL:HG13	2.12	0.48
2:h:391:ARG:NH1	1:i:437:ILE:O	2.46	0.48
2:d:283:ALA:HA	2:j:55:THR:HG23	1.94	0.48
1:q:234:VAL:HG21	1:q:302:MET:SD	2.54	0.48
1:e:286:LEU:O	1:e:373:ARG:NH1	2.46	0.48
2:h:257:LEU:HA	2:h:312:THR:HG21	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:318:ARG:N	2:f:364:ALA:O	2.46	0.48
1:e:143:GLY:HA3	3:e:501:GTP:O3A	2.13	0.48
1:c:102:ASN:CG	1:c:411:GLU:OE1	2.56	0.48
2:v:137:HIS:O	2:v:168:SER:HA	2.14	0.48
1:a:136:LEU:HD22	1:a:169:PHE:HE1	1.78	0.48
2:d:281:TYR:CD1	2:j:86:ARG:HA	2.48	0.48
2:d:317:PHE:HB3	2:d:321:MET:SD	2.54	0.48
2:j:257:LEU:HA	2:j:312:THR:HG21	1.96	0.48
2:x:137:HIS:O	2:x:168:SER:HA	2.13	0.48
1:u:141:VAL:HG22	1:u:172:TYR:HA	1.95	0.48
1:o:329:ASN:HD21	2:n:175:VAL:HG22	1.79	0.48
2:p:49:VAL:HG11	2:p:241:ARG:HG2	1.95	0.48
1:k:248:LEU:HD21	2:j:177:ASP:CG	2.39	0.48
2:h:397:TRP:CH2	1:i:256:GLN:HG2	2.48	0.48
1:a:223:THR:HG22	2:b:322:SER:HA	1.96	0.48
2:t:49:VAL:HG11	2:t:241:ARG:HG2	1.95	0.48
2:d:7:ILE:HG21	2:d:151:LEU:HD22	1.95	0.48
1:q:398:MET:HG2	2:r:345:ILE:HD11	1.96	0.48
2:l:290:THR:HG23	2:l:293:MET:HE2	1.95	0.48
1:c:234:VAL:HG21	1:c:302:MET:SD	2.54	0.48
1:c:439:THR:HG22	2:b:391:ARG:CG	2.44	0.48
1:q:141:VAL:HG22	1:q:172:TYR:HA	1.96	0.48
2:d:286:VAL:N	2:d:287:PRO:HD2	2.29	0.48
1:w:90:GLU:HB3	1:w:121:ARG:HD3	1.96	0.47
2:n:289:LEU:HD23	2:n:365:VAL:HG23	1.96	0.47
2:n:345:ILE:HG22	2:n:345:ILE:O	2.13	0.47
2:f:232:ALA:O	2:f:236:VAL:HG23	2.14	0.47
1:e:296:PHE:HB3	1:e:341:ILE:HD11	1.95	0.47
2:f:120:VAL:HG11	2:f:155:VAL:HG12	1.95	0.47
1:k:88:HIS:HA	1:e:283:HIS:CG	2.49	0.47
2:l:86:ARG:HA	2:f:281:TYR:CD2	2.50	0.47
2:h:179:VAL:HG21	1:i:258:ASN:O	2.14	0.47
1:c:31:GLN:HE21	1:c:37:PRO:HG3	1.78	0.47
2:j:9:GLY:HA3	2:j:66:MET:HE3	1.95	0.47
1:w:296:PHE:CZ	1:w:351:PHE:HE2	2.31	0.47
1:q:398:MET:HG2	2:r:345:ILE:CD1	2.45	0.47
1:g:182:VAL:HG12	2:h:256:ASN:HD21	1.79	0.47
2:j:6:HIS:HE2	2:j:8:GLN:HB3	1.79	0.47
2:j:290:THR:HG23	2:j:293:MET:HE2	1.96	0.47
1:w:208:ALA:HB2	1:w:304:LYS:HB2	1.97	0.47
1:k:89:PRO:HD3	1:e:283:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:398:MET:HG2	2:h:345:ILE:CD1	2.44	0.47
2:f:330:MET:HE3	2:f:349:ILE:CG2	2.40	0.47
1:w:234:VAL:HG21	1:w:302:MET:SD	2.55	0.47
1:w:398:MET:HG2	2:x:345:ILE:CD1	2.45	0.47
1:m:408:TYR:CG	1:m:418:PHE:HZ	2.32	0.47
1:k:398:MET:HG2	2:l:345:ILE:CD1	2.45	0.47
2:l:286:VAL:N	2:l:287:PRO:HD2	2.30	0.47
2:h:286:VAL:N	2:h:287:PRO:HD2	2.29	0.47
1:e:398:MET:HE3	2:f:345:ILE:HD11	1.97	0.47
2:b:42:LEU:HD13	2:b:356:ILE:HD11	1.97	0.47
2:b:145:SER:OG	2:b:188:SER:HB3	2.13	0.47
1:w:296:PHE:CE1	1:w:377:MET:SD	3.08	0.47
2:r:6:HIS:HE2	2:r:8:GLN:HB3	1.80	0.47
1:k:188:ILE:HD12	1:k:395:PHE:CG	2.49	0.47
2:b:289:LEU:HD23	2:b:365:VAL:HG23	1.97	0.47
1:s:274:PRO:HG3	1:s:374:ALA:HA	1.97	0.47
2:t:395:LEU:O	2:t:398:TYR:N	2.47	0.47
1:a:2:ARG:HA	1:a:133:GLN:CG	2.45	0.47
2:d:179:VAL:HG23	2:d:180:VAL:HG13	1.96	0.47
1:u:223:THR:HG22	2:v:322:SER:HA	1.96	0.47
2:r:345:ILE:O	2:r:345:ILE:HG22	2.15	0.47
2:f:48:ASN:O	2:f:62:ARG:NH2	2.40	0.47
1:a:183:GLU:O	1:a:184:PRO:C	2.58	0.47
2:r:289:LEU:HD23	2:r:365:VAL:HG23	1.97	0.46
1:o:70:LEU:HD12	1:o:99:ALA:HB2	1.98	0.46
2:h:237:THR:O	2:h:241:ARG:NH1	2.48	0.46
2:b:286:VAL:N	2:b:287:PRO:HD2	2.31	0.46
2:d:60:VAL:HG11	2:d:86:ARG:HB2	1.98	0.46
1:g:180:ALA:HB3	1:g:183:GLU:HG3	1.98	0.46
2:h:330:MET:HE3	2:h:349:ILE:CG2	2.42	0.46
1:i:265:ILE:CG2	1:i:265:ILE:O	2.64	0.46
2:x:238:CYS:SG	2:x:354:CYS:SG	3.04	0.46
2:t:286:VAL:N	2:t:287:PRO:HD2	2.30	0.46
2:r:286:VAL:N	2:r:287:PRO:HD2	2.31	0.46
1:e:321:GLY:HA3	1:e:372:MET:O	2.15	0.46
2:f:251:ARG:O	2:f:255:VAL:N	2.48	0.46
1:c:283:HIS:HA	1:i:62:VAL:HG21	1.97	0.46
1:c:409:VAL:HA	1:c:413:MET:O	2.15	0.46
2:b:105:HIS:CE1	2:b:150:LEU:HD13	2.50	0.46
2:v:178:THR:HB	2:v:181:GLU:HG3	1.96	0.46
1:s:286:LEU:HD13	1:s:371:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:21:TRP:HA	2:p:24:ILE:HG22	1.97	0.46
1:m:118:CYS:SG	1:m:153:LEU:HD21	2.55	0.46
1:g:141:VAL:HG22	1:g:172:TYR:HA	1.95	0.46
1:e:276:ILE:CD1	1:e:286:LEU:HD21	2.45	0.46
2:f:237:THR:CG2	2:f:250:LEU:HD21	2.46	0.46
2:f:286:VAL:N	2:f:287:PRO:HD2	2.31	0.46
1:c:346:TRP:CD1	2:b:391:ARG:HD3	2.49	0.46
1:a:68:LEU:HD11	1:a:114:ILE:CG2	2.45	0.46
2:d:281:TYR:CE2	2:j:87:PRO:CD	2.98	0.46
2:v:248:SER:HA	2:v:252:LYS:HD3	1.96	0.46
2:v:345:ILE:HG22	2:v:345:ILE:O	2.16	0.46
1:s:206:ASN:O	1:s:207:GLU:C	2.58	0.46
1:s:430:LYS:O	1:s:433:GLU:N	2.49	0.46
2:r:201:VAL:O	2:r:301:CYS:SG	2.71	0.46
1:g:241:SER:HA	1:g:356:ASN:HD21	1.80	0.46
1:c:106:GLY:O	1:c:111:GLY:HA3	2.15	0.46
1:c:290:GLU:O	1:c:293:ASN:N	2.49	0.46
1:c:290:GLU:O	1:c:291:ILE:C	2.59	0.46
2:b:60:VAL:HG11	2:b:86:ARG:HB2	1.98	0.46
2:d:249:ASP:OD1	2:d:249:ASP:C	2.58	0.46
2:x:345:ILE:HG22	2:x:345:ILE:O	2.16	0.46
1:u:62:VAL:HG21	1:o:283:HIS:HA	1.98	0.46
2:r:60:VAL:HG21	2:l:281:TYR:HA	1.98	0.46
2:r:87:PRO:HD3	2:l:281:TYR:CE1	2.51	0.46
2:l:248:SER:HA	2:l:252:LYS:HD3	1.98	0.46
1:c:348:PRO:HD2	2:b:388:MET:HE3	1.97	0.46
1:s:90:GLU:HB3	1:s:121:ARG:HD3	1.97	0.46
1:m:401:LYS:HG3	2:n:344:TRP:CD1	2.51	0.46
1:k:256:GLN:HG2	2:j:397:TRP:CH2	2.51	0.46
2:h:248:SER:HA	2:h:252:LYS:HD3	1.98	0.46
1:e:346:TRP:O	2:d:388:MET:HA	2.16	0.46
2:f:6:HIS:O	2:f:63:ALA:HA	2.16	0.46
1:c:137:VAL:HG11	1:c:154:LEU:HD21	1.97	0.46
2:b:237:THR:CG2	2:b:250:LEU:HD21	2.46	0.46
2:b:396:HIS:O	2:b:400:GLY:N	2.44	0.46
1:w:349:THR:HG21	2:v:182:PRO:HG3	1.97	0.46
2:x:48:ASN:O	2:x:62:ARG:NH2	2.38	0.46
2:l:330:MET:HE3	2:l:349:ILE:CG2	2.42	0.46
2:f:237:THR:O	2:f:241:ARG:NH1	2.49	0.46
2:f:345:ILE:HG22	2:f:345:ILE:O	2.16	0.46
1:c:171:ILE:HA	1:c:204:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:167:LEU:HD22	1:i:200:VAL:HB	1.97	0.46
1:w:349:THR:CG2	2:v:384:GLN:HB3	2.47	0.45
2:x:237:THR:CG2	2:x:250:LEU:HD21	2.47	0.45
1:m:49:PHE:O	1:m:52:PHE:N	2.48	0.45
1:m:167:LEU:HD22	1:m:200:VAL:HB	1.97	0.45
2:d:6:HIS:ND1	2:d:134:GLN:NE2	2.63	0.45
2:d:267:MET:HE1	2:d:305:PRO:HG3	1.98	0.45
1:w:241:SER:HA	1:w:356:ASN:HD21	1.81	0.45
2:b:263:LEU:HD11	2:b:425:TYR:CD2	2.52	0.45
2:b:322:SER:O	2:b:325:GLU:N	2.49	0.45
1:w:314:ALA:HB2	2:v:394:PHE:HZ	1.81	0.45
2:r:237:THR:CG2	2:r:250:LEU:HD21	2.46	0.45
1:k:102:ASN:HB3	1:k:105:ARG:HG3	1.96	0.45
1:c:276:ILE:HD13	1:c:286:LEU:HD21	1.98	0.45
1:a:141:VAL:HG22	1:a:172:TYR:HA	1.98	0.45
2:j:334:GLN:HE22	2:j:347:ASN:H	1.64	0.45
1:u:256:GLN:O	1:u:260:VAL:HG13	2.15	0.45
2:r:87:PRO:HD3	2:l:281:TYR:CD1	2.51	0.45
2:r:334:GLN:HE22	2:r:347:ASN:H	1.64	0.45
2:n:237:THR:CG2	2:n:250:LEU:HD21	2.46	0.45
1:c:398:MET:C	1:c:400:ALA:H	2.24	0.45
1:c:439:THR:HG22	2:b:391:ARG:HD2	1.98	0.45
1:e:68:LEU:HD11	1:e:114:ILE:CG2	2.46	0.45
1:c:2:ARG:HA	1:c:133:GLN:CG	2.47	0.45
1:i:350:GLY:O	1:i:351:PHE:HB2	2.17	0.45
2:j:286:VAL:N	2:j:287:PRO:HD2	2.31	0.45
1:w:141:VAL:HG22	1:w:172:TYR:HA	1.97	0.45
1:u:405:VAL:HG12	1:u:409:VAL:HG23	1.98	0.45
1:q:206:ASN:HD21	3:q:501:GTP:HN22	1.63	0.45
1:m:21:TRP:CZ2	1:m:65:ALA:HB2	2.52	0.45
2:n:86:ARG:HA	2:h:281:TYR:CD2	2.52	0.45
2:n:121:ARG:O	2:n:125:GLU:HG2	2.16	0.45
1:g:137:VAL:HG11	1:g:154:LEU:HD21	1.99	0.45
1:e:398:MET:CG	2:f:345:ILE:HD11	2.45	0.45
1:c:177:VAL:HG13	2:d:327:ASP:HB3	1.98	0.45
1:a:35:GLN:HA	1:a:59:GLY:O	2.17	0.45
1:a:208:ALA:HB2	1:a:304:LYS:HB2	1.97	0.45
2:d:135:ILE:HB	2:d:166:THR:HG22	1.98	0.45
1:w:216:ASN:HD22	1:w:275:ILE:HB	1.82	0.45
2:x:330:MET:HE3	2:x:349:ILE:CG2	2.43	0.45
2:x:334:GLN:HE22	2:x:347:ASN:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:276:ILE:HD13	1:m:286:LEU:HD21	1.98	0.45
1:c:256:GLN:O	1:c:260:VAL:HG13	2.17	0.45
2:v:237:THR:CG2	2:v:250:LEU:HD21	2.47	0.45
1:c:188:ILE:HG23	1:c:425:LEU:HD12	1.98	0.45
1:w:256:GLN:HG2	2:v:397:TRP:CZ3	2.52	0.45
2:x:289:LEU:HD23	2:x:365:VAL:HG23	1.98	0.45
1:u:265:ILE:CG2	1:u:265:ILE:O	2.64	0.45
1:k:158:SER:HA	1:k:166:LYS:HE2	1.99	0.45
1:a:102:ASN:HB3	1:a:105:ARG:HG3	1.99	0.45
2:b:330:MET:HE3	2:b:349:ILE:CG2	2.42	0.45
1:i:274:PRO:HG3	1:i:374:ALA:HA	1.98	0.45
2:x:286:VAL:N	2:x:287:PRO:HD2	2.31	0.45
1:m:182:VAL:HG12	2:n:256:ASN:HD21	1.81	0.45
1:g:276:ILE:HD13	1:g:286:LEU:HD21	1.98	0.45
1:e:223:THR:HG22	2:f:322:SER:HA	1.99	0.45
1:e:224:TYR:CG	3:e:501:GTP:C6	3.05	0.45
1:i:1:MET:N	1:i:130:THR:O	2.50	0.45
1:i:68:LEU:HD23	1:i:153:LEU:HD11	1.99	0.45
1:w:329:ASN:ND2	2:v:175:VAL:HG22	2.32	0.44
2:v:238:CYS:SG	2:v:354:CYS:SG	3.15	0.44
2:v:286:VAL:N	2:v:287:PRO:HD2	2.32	0.44
2:t:143:THR:N	5:t:502:GDP:O3B	2.47	0.44
1:q:103:PHE:CD2	1:q:413:MET:HE1	2.52	0.44
1:o:398:MET:C	1:o:400:ALA:H	2.25	0.44
1:k:398:MET:HG2	2:l:345:ILE:HD11	1.99	0.44
1:g:68:LEU:HD11	1:g:114:ILE:CG2	2.47	0.44
1:g:208:ALA:HB2	1:g:304:LYS:HB2	1.99	0.44
2:f:289:LEU:HD23	2:f:365:VAL:HG23	1.99	0.44
2:f:334:GLN:HE22	2:f:347:ASN:N	2.15	0.44
1:a:70:LEU:HD12	1:a:99:ALA:HB2	1.99	0.44
1:s:188:ILE:CG1	1:s:425:LEU:HD12	2.47	0.44
1:c:398:MET:HG2	2:d:345:ILE:HD13	1.99	0.44
2:d:323:THR:HG22	2:d:353:ILE:HG13	1.99	0.44
1:u:216:ASN:HD22	1:u:275:ILE:HB	1.82	0.44
2:t:342:VAL:CG1	2:t:348:ASN:HD21	2.31	0.44
1:k:398:MET:C	1:k:400:ALA:H	2.25	0.44
1:e:348:PRO:HG3	2:d:384:GLN:O	2.16	0.44
1:a:141:VAL:O	1:a:147:SER:OG	2.36	0.44
1:w:68:LEU:HD11	1:w:114:ILE:CG2	2.48	0.44
1:s:167:LEU:HD22	1:s:200:VAL:HB	1.98	0.44
2:r:237:THR:O	2:r:241:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:191:THR:O	1:g:195:LEU:N	2.50	0.44
1:c:68:LEU:HD21	1:c:149:LEU:HD21	1.99	0.44
1:w:256:GLN:O	2:v:397:TRP:CZ2	2.70	0.44
1:w:346:TRP:O	2:v:388:MET:HA	2.16	0.44
2:x:238:CYS:O	2:x:241:ARG:N	2.49	0.44
1:q:136:LEU:HD22	1:q:169:PHE:HE1	1.83	0.44
1:m:398:MET:HG2	2:n:345:ILE:CD1	2.47	0.44
2:f:60:VAL:HG11	2:f:86:ARG:HB2	1.99	0.44
1:w:14:ILE:HG21	1:w:74:VAL:HG12	2.00	0.44
1:w:223:THR:HG22	2:x:322:SER:HA	1.99	0.44
2:x:60:VAL:HG11	2:x:86:ARG:HB2	2.00	0.44
2:v:330:MET:HE3	2:v:349:ILE:CG2	2.44	0.44
2:t:345:ILE:O	2:t:345:ILE:HG22	2.17	0.44
2:n:178:THR:HB	2:n:181:GLU:HG3	1.99	0.44
2:n:311:LEU:HD22	2:n:425:TYR:CD1	2.53	0.44
1:g:90:GLU:HB3	1:g:121:ARG:HD3	2.00	0.44
2:f:36:TYR:CD1	2:f:44:LEU:HD21	2.52	0.44
1:a:316:SER:OG	1:a:378:ILE:HB	2.16	0.44
2:d:6:HIS:HE2	2:d:8:GLN:HB3	1.83	0.44
2:d:178:THR:HB	2:d:181:GLU:HG3	2.00	0.44
1:w:155:GLU:HG2	1:w:197:HIS:CD2	2.53	0.44
1:q:68:LEU:HD11	1:q:114:ILE:CG2	2.48	0.44
1:k:136:LEU:HD22	1:k:169:PHE:HE1	1.82	0.44
2:l:237:THR:CG2	2:l:250:LEU:HD21	2.47	0.44
1:a:136:LEU:HD23	1:a:167:LEU:HB2	2.00	0.44
1:w:343:PHE:CZ	1:w:351:PHE:CZ	3.06	0.44
1:q:276:ILE:HD13	1:q:286:LEU:HD21	1.99	0.44
2:p:179:VAL:HG23	2:p:180:VAL:HG13	1.99	0.44
1:g:188:ILE:HG23	1:g:425:LEU:CD1	2.48	0.44
1:e:2:ARG:HA	1:e:133:GLN:CG	2.47	0.44
2:d:237:THR:CG2	2:d:250:LEU:HD21	2.48	0.44
2:d:281:TYR:CD2	2:j:87:PRO:CD	3.00	0.44
1:w:136:LEU:HD22	1:w:169:PHE:HE1	1.83	0.44
1:u:305:CYS:SG	1:u:387:VAL:HG21	2.58	0.44
2:n:68:LEU:HD23	2:n:112:LEU:HD22	1.99	0.44
2:b:3:GLU:HG2	2:b:62:ARG:NH2	2.33	0.44
1:q:88:HIS:ND1	1:k:283:HIS:HB2	2.33	0.43
1:e:181:VAL:H	2:f:256:ASN:HD22	1.63	0.43
1:e:406:HIS:CE1	1:e:407:TRP:CE2	3.06	0.43
2:b:344:TRP:CD1	2:b:345:ILE:HG12	2.53	0.43
1:q:171:ILE:HA	1:q:204:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:265:ILE:HG21	1:g:313:MET:HE1	2.01	0.43
1:e:216:ASN:HD22	1:e:275:ILE:HB	1.84	0.43
1:w:171:ILE:HA	1:w:204:LEU:O	2.18	0.43
2:t:60:VAL:HG21	2:n:281:TYR:HA	2.00	0.43
1:m:180:ALA:HB3	1:m:183:GLU:HG3	2.00	0.43
2:n:28:HIS:NE2	2:n:241:ARG:HD2	2.33	0.43
2:h:178:THR:HB	2:h:181:GLU:HG3	2.00	0.43
1:u:68:LEU:HD11	1:u:114:ILE:CG2	2.49	0.43
1:k:68:LEU:HD11	1:k:114:ILE:CG2	2.47	0.43
1:c:188:ILE:HD12	1:c:395:PHE:CB	2.49	0.43
1:c:292:THR:HG21	1:c:331:SER:HB3	1.99	0.43
1:a:14:ILE:HG21	1:a:74:VAL:HG12	2.00	0.43
1:a:398:MET:C	1:a:400:ALA:N	2.76	0.43
2:d:396:HIS:CE1	2:d:397:TRP:CZ2	3.06	0.43
2:n:318:ARG:HB3	2:n:357:PRO:HA	2.00	0.43
1:c:141:VAL:HG22	1:c:172:TYR:HA	2.00	0.43
1:u:269:LEU:HD21	1:u:305:CYS:SG	2.59	0.43
1:q:351:PHE:N	2:p:179:VAL:HG12	2.34	0.43
1:o:1:MET:N	1:o:130:THR:O	2.52	0.43
2:p:289:LEU:HD23	2:p:365:VAL:HG23	1.99	0.43
2:l:61:PRO:HD2	2:l:84:LEU:O	2.19	0.43
1:e:136:LEU:HD22	1:e:169:PHE:HE1	1.82	0.43
2:d:307:HIS:O	2:d:426:GLN:NE2	2.51	0.43
1:w:180:ALA:HB3	1:w:183:GLU:HG3	2.00	0.43
1:m:9:VAL:HA	1:m:68:LEU:O	2.19	0.43
1:m:103:PHE:CD2	1:m:413:MET:HE1	2.53	0.43
1:k:14:ILE:HG21	1:k:74:VAL:HG12	2.00	0.43
1:e:188:ILE:HG23	1:e:425:LEU:HD12	2.00	0.43
1:c:68:LEU:HD11	1:c:114:ILE:CG2	2.49	0.43
1:c:248:LEU:HD23	1:c:353:VAL:HG23	2.01	0.43
1:a:265:ILE:O	1:a:265:ILE:CG2	2.67	0.43
2:d:232:ALA:O	2:d:236:VAL:HG23	2.19	0.43
1:q:14:ILE:HG21	1:q:74:VAL:HG12	2.00	0.43
1:m:265:ILE:CG2	1:m:380:ASN:HD21	2.31	0.43
1:c:136:LEU:HD22	1:c:169:PHE:HE1	1.84	0.43
2:b:6:HIS:HB2	2:b:134:GLN:HE21	1.83	0.43
2:b:322:SER:O	2:b:323:THR:C	2.62	0.43
2:x:102:ALA:HB1	2:x:401:GLU:HB2	2.01	0.43
1:m:14:ILE:HG21	1:m:74:VAL:HG12	2.00	0.43
1:e:170:THR:HG21	1:e:194:LEU:HD11	2.00	0.43
1:e:269:LEU:HD21	1:e:305:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:269:LEU:HD21	1:c:305:CYS:SG	2.59	0.43
2:b:6:HIS:HE2	2:b:8:GLN:HB3	1.83	0.43
1:w:88:HIS:HA	1:q:283:HIS:CG	2.53	0.43
1:u:70:LEU:HD21	1:u:149:LEU:HD22	2.00	0.43
1:o:248:LEU:HD23	1:o:353:VAL:HG23	2.01	0.43
1:k:137:VAL:HG11	1:k:154:LEU:HD21	2.00	0.43
1:g:88:HIS:ND1	1:g:89:PRO:HD2	2.34	0.43
1:c:401:LYS:HG3	2:d:344:TRP:CG	2.54	0.43
2:d:120:VAL:HG11	2:d:155:VAL:HG12	2.01	0.43
2:d:290:THR:HG23	2:d:293:MET:HE2	2.00	0.43
1:w:439:THR:HG22	2:v:391:ARG:CG	2.49	0.42
1:u:90:GLU:HB3	1:u:121:ARG:HD3	2.00	0.42
2:v:201:VAL:O	2:v:301:CYS:SG	2.76	0.42
1:q:180:ALA:HB3	1:q:183:GLU:HG3	2.01	0.42
2:n:64:ILE:HD13	2:n:120:VAL:HG22	2.01	0.42
1:c:348:PRO:HD2	2:b:388:MET:CE	2.49	0.42
2:d:281:TYR:HA	2:j:60:VAL:HG21	2.01	0.42
2:v:263:LEU:HD11	2:v:425:TYR:CD2	2.54	0.42
1:s:321:GLY:O	1:s:323:VAL:N	2.50	0.42
1:q:208:ALA:HB2	1:q:304:LYS:HB2	2.00	0.42
1:q:408:TYR:CG	1:q:418:PHE:HZ	2.37	0.42
2:p:178:THR:HB	2:p:181:GLU:HG3	2.02	0.42
1:k:305:CYS:SG	1:k:387:VAL:HG21	2.59	0.42
2:h:67:ASP:O	2:h:92:PHE:HA	2.19	0.42
1:a:9:VAL:HA	1:a:68:LEU:O	2.19	0.42
2:p:137:HIS:O	2:p:168:SER:HA	2.20	0.42
2:n:279:GLN:O	2:n:280:GLN:C	2.62	0.42
1:k:439:THR:HG22	2:j:391:ARG:HD2	2.00	0.42
1:g:171:ILE:HA	1:g:204:LEU:O	2.19	0.42
2:f:3:GLU:HG2	2:f:62:ARG:NH2	2.34	0.42
2:v:7:ILE:HG21	2:v:151:LEU:HD22	2.01	0.42
2:n:248:SER:HA	2:n:252:LYS:HD3	2.01	0.42
1:k:180:ALA:HB3	1:k:183:GLU:HG3	2.02	0.42
1:g:265:ILE:O	1:g:265:ILE:CG2	2.68	0.42
1:e:141:VAL:O	1:e:147:SER:OG	2.38	0.42
2:f:135:ILE:HB	2:f:166:THR:HG22	2.01	0.42
1:c:329:ASN:HD21	2:b:175:VAL:HG22	1.84	0.42
2:b:7:ILE:HG21	2:b:151:LEU:HD22	2.02	0.42
2:d:281:TYR:CD2	2:j:87:PRO:HD2	2.54	0.42
1:u:276:ILE:HD13	1:u:286:LEU:HD21	2.00	0.42
1:o:155:GLU:HG2	1:o:197:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:405:VAL:HG12	1:m:409:VAL:HG23	2.01	0.42
2:n:52:ASN:OD1	2:n:62:ARG:NH2	2.52	0.42
1:k:265:ILE:O	1:k:265:ILE:CG2	2.68	0.42
2:h:237:THR:CG2	2:h:250:LEU:HD21	2.48	0.42
2:b:135:ILE:HB	2:b:166:THR:HG22	2.02	0.42
2:d:42:LEU:HD13	2:d:356:ILE:HD11	2.01	0.42
1:u:137:VAL:HG11	1:u:154:LEU:HD21	2.01	0.42
1:k:90:GLU:HB3	1:k:121:ARG:HD3	2.01	0.42
2:h:60:VAL:HG21	2:b:281:TYR:HA	2.01	0.42
2:f:217:LEU:HD12	2:f:217:LEU:N	2.35	0.42
1:i:103:PHE:CD2	1:i:413:MET:HE1	2.54	0.42
1:w:102:ASN:HB3	1:w:105:ARG:HG3	2.02	0.42
1:u:170:THR:HG21	1:u:194:LEU:HD11	2.02	0.42
1:m:88:HIS:O	1:m:89:PRO:C	2.62	0.42
1:g:14:ILE:HG21	1:g:74:VAL:HG12	2.01	0.42
1:e:255:PHE:HB3	1:e:259:LEU:HD12	2.01	0.42
1:c:292:THR:HG21	1:c:331:SER:HB2	2.02	0.42
1:a:409:VAL:HA	1:a:413:MET:O	2.20	0.42
2:j:201:VAL:HG23	2:j:301:CYS:SG	2.59	0.42
2:x:135:ILE:HB	2:x:166:THR:HG22	2.00	0.42
1:u:14:ILE:HG21	1:u:74:VAL:HG12	2.02	0.42
1:u:188:ILE:HD12	1:u:395:PHE:CD1	2.55	0.42
1:g:136:LEU:HD22	1:g:169:PHE:HE1	1.84	0.42
1:c:102:ASN:OD1	1:c:104:ALA:HB3	2.19	0.42
1:c:145:THR:H	3:c:501:GTP:PB	2.42	0.42
2:x:7:ILE:HG21	2:x:151:LEU:HD22	2.01	0.42
1:u:155:GLU:HG2	1:u:197:HIS:CD2	2.55	0.42
2:p:91:VAL:HG11	2:p:116:VAL:HG22	2.02	0.42
1:e:68:LEU:HD21	1:e:149:LEU:HD21	2.01	0.42
1:e:402:ARG:C	1:e:405:VAL:HG23	2.44	0.42
1:a:385:ALA:O	1:a:388:PHE:N	2.53	0.42
1:i:70:LEU:HD12	1:i:99:ALA:HB2	2.01	0.42
2:j:267:MET:HE1	2:j:305:PRO:HG3	2.02	0.42
2:n:135:ILE:HB	2:n:166:THR:HG22	2.00	0.42
2:h:1:MET:HG2	2:h:128:ASP:HB2	2.02	0.42
2:h:384:GLN:OE1	1:i:349:THR:HG23	2.20	0.42
1:e:90:GLU:HB3	1:e:121:ARG:HD3	2.02	0.42
1:c:207:GLU:O	1:c:210:TYR:HB2	2.20	0.42
1:c:413:MET:HE2	1:c:417:GLU:HG2	2.01	0.42
2:x:268:ILE:HA	2:x:367:PHE:O	2.19	0.41
1:u:171:ILE:HA	1:u:204:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:216:ASN:HD22	1:q:275:ILE:HB	1.84	0.41
1:q:405:VAL:HG12	1:q:409:VAL:HG23	2.02	0.41
1:k:70:LEU:HD21	1:k:149:LEU:HD22	2.02	0.41
2:l:1:MET:HG2	2:l:128:ASP:HB2	2.03	0.41
1:a:292:THR:HG22	1:a:319:TYR:OH	2.20	0.41
2:b:249:ASP:OD1	2:b:249:ASP:C	2.62	0.41
1:u:349:THR:HG23	2:t:384:GLN:OE1	2.20	0.41
2:r:55:THR:HG23	2:l:283:ALA:HA	2.02	0.41
1:o:276:ILE:CD1	1:o:286:LEU:HD21	2.50	0.41
2:p:7:ILE:O	2:p:135:ILE:HA	2.20	0.41
2:p:102:ALA:HB1	2:p:401:GLU:HB2	2.02	0.41
1:m:6:SER:O	1:m:65:ALA:HA	2.20	0.41
1:m:14:ILE:HG23	1:m:67:PHE:HD2	1.85	0.41
1:k:296:PHE:HB3	1:k:341:ILE:HD11	2.01	0.41
2:l:6:HIS:O	2:l:63:ALA:HA	2.20	0.41
2:l:105:HIS:O	2:l:150:LEU:HD22	2.21	0.41
1:g:70:LEU:HD21	1:g:149:LEU:HD22	2.02	0.41
1:e:292:THR:HG22	1:e:319:TYR:OH	2.21	0.41
1:a:9:VAL:HG12	1:a:145:THR:HG22	2.02	0.41
1:a:311:LYS:HA	1:a:342:GLN:O	2.20	0.41
1:u:136:LEU:HD22	1:u:169:PHE:HE1	1.85	0.41
1:s:430:LYS:O	1:s:431:ASP:C	2.62	0.41
1:o:261:PRO:HA	2:n:394:PHE:CD1	2.56	0.41
2:n:238:CYS:HG	2:n:354:CYS:HG	1.67	0.41
1:k:276:ILE:HD13	1:k:286:LEU:HD21	2.01	0.41
1:c:319:TYR:HB3	1:c:323:VAL:HG21	2.02	0.41
1:a:93:ILE:HD11	1:a:121:ARG:HG3	2.02	0.41
1:w:137:VAL:HG11	1:w:154:LEU:HD21	2.02	0.41
2:t:323:THR:HG22	2:t:353:ILE:HG13	2.02	0.41
1:o:21:TRP:CZ2	1:o:65:ALA:HB2	2.55	0.41
1:m:70:LEU:HD21	1:m:149:LEU:HD22	2.01	0.41
2:l:68:LEU:HD23	2:l:112:LEU:HD22	2.02	0.41
2:h:391:ARG:CG	1:i:439:THR:HG22	2.51	0.41
1:c:4:VAL:CG1	1:c:136:LEU:HG	2.51	0.41
1:c:102:ASN:HD21	1:c:408:TYR:HA	1.83	0.41
1:a:21:TRP:CZ2	1:a:65:ALA:HB2	2.55	0.41
2:b:179:VAL:HG23	2:b:180:VAL:HG13	2.01	0.41
2:b:268:ILE:HA	2:b:367:PHE:O	2.21	0.41
2:d:13:GLY:HA3	2:d:136:THR:O	2.21	0.41
2:v:60:VAL:HG11	2:v:86:ARG:HB2	2.02	0.41
1:s:248:LEU:HD23	1:s:353:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:395:LEU:O	2:t:396:HIS:C	2.63	0.41
2:r:248:SER:HA	2:r:252:LYS:HD3	2.02	0.41
1:g:188:ILE:HD12	1:g:425:LEU:HD12	2.03	0.41
2:h:135:ILE:HB	2:h:166:THR:HG22	2.03	0.41
2:f:27:GLU:OE2	2:f:241:ARG:NH2	2.53	0.41
2:b:68:LEU:HD23	2:b:112:LEU:HD22	2.02	0.41
2:b:100:ASN:OD1	2:b:100:ASN:C	2.64	0.41
2:d:318:ARG:HB2	2:d:364:ALA:HB3	2.03	0.41
1:u:180:ALA:HB3	1:u:183:GLU:HG3	2.01	0.41
1:s:21:TRP:CZ2	1:s:65:ALA:HB2	2.56	0.41
1:s:398:MET:HE3	2:t:345:ILE:HD11	2.02	0.41
1:q:6:SER:O	1:q:65:ALA:HA	2.20	0.41
1:q:329:ASN:ND2	2:p:175:VAL:HG22	2.35	0.41
1:q:348:PRO:HD2	2:p:388:MET:HE3	2.01	0.41
2:r:1:MET:HG2	2:r:128:ASP:HB2	2.01	0.41
2:n:317:PHE:HB3	2:n:321:MET:SD	2.61	0.41
1:g:70:LEU:HD12	1:g:99:ALA:HB2	2.03	0.41
1:w:276:ILE:HD13	1:w:286:LEU:HD21	2.01	0.41
2:t:87:PRO:CD	2:n:281:TYR:CD2	3.04	0.41
2:t:318:ARG:HB3	2:t:357:PRO:HA	2.02	0.41
1:m:1:MET:N	1:m:130:THR:O	2.54	0.41
1:a:14:ILE:HG23	1:a:67:PHE:HD2	1.85	0.41
1:a:30:ILE:HD13	1:a:53:PHE:CD1	2.56	0.41
2:b:156:ARG:NH1	2:b:195:ASN:O	2.53	0.41
1:i:261:PRO:HD2	1:i:265:ILE:HG22	2.02	0.41
2:p:6:HIS:HE2	2:p:8:GLN:HB3	1.86	0.41
1:m:70:LEU:HD12	1:m:99:ALA:HB2	2.02	0.41
2:n:406:MET:O	2:n:409:THR:OG1	2.28	0.41
2:h:48:ASN:O	2:h:62:ARG:NH2	2.38	0.41
1:a:291:ILE:HG23	1:a:375:VAL:HG12	2.03	0.41
2:b:120:VAL:HG11	2:b:155:VAL:HG12	2.02	0.41
2:d:113:ILE:O	2:d:116:VAL:N	2.53	0.41
1:i:103:PHE:CE2	1:i:413:MET:HE1	2.56	0.41
1:i:256:GLN:O	1:i:260:VAL:HG13	2.21	0.41
2:x:263:LEU:HD11	2:x:425:TYR:CD2	2.56	0.41
1:u:88:HIS:ND1	1:o:283:HIS:CB	2.84	0.41
1:u:208:ALA:HB2	1:u:304:LYS:HB2	2.03	0.41
1:q:14:ILE:HG23	1:q:67:PHE:HD2	1.86	0.41
1:q:70:LEU:HD12	1:q:99:ALA:HB2	2.03	0.41
1:o:352:LYS:NZ	2:n:99:ASN:HD21	2.19	0.41
1:e:306:ASP:HB2	1:e:309:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:36:TYR:CE1	2:f:44:LEU:HG	2.55	0.41
1:c:14:ILE:HG21	1:c:74:VAL:HG12	2.02	0.41
1:c:311:LYS:HA	1:c:342:GLN:O	2.21	0.41
2:b:5:VAL:HG22	2:b:62:ARG:CD	2.51	0.41
2:b:102:ALA:HB1	2:b:401:GLU:HB2	2.02	0.41
2:d:5:VAL:O	2:d:133:PHE:HA	2.21	0.41
1:u:398:MET:C	1:u:400:ALA:H	2.28	0.41
2:t:342:VAL:HG12	2:t:348:ASN:HD21	1.85	0.41
1:q:70:LEU:HD21	1:q:149:LEU:HD22	2.02	0.41
2:r:268:ILE:HA	2:r:367:PHE:O	2.21	0.41
1:m:88:HIS:HA	1:g:283:HIS:CG	2.55	0.41
1:m:409:VAL:HA	1:m:413:MET:O	2.21	0.41
1:c:158:SER:HA	1:c:166:LYS:HE2	2.03	0.41
1:c:346:TRP:O	2:b:388:MET:HG2	2.21	0.41
1:a:181:VAL:H	2:b:256:ASN:HD22	1.68	0.41
2:r:330:MET:HE3	2:r:349:ILE:CG2	2.41	0.40
1:o:237:SER:HA	1:o:320:ARG:HD2	2.03	0.40
2:n:3:GLU:HG2	2:n:62:ARG:NH2	2.36	0.40
2:h:102:ALA:HB1	2:h:401:GLU:HB2	2.03	0.40
2:f:334:GLN:HE22	2:f:347:ASN:H	1.69	0.40
1:c:188:ILE:HG23	1:c:425:LEU:CD1	2.51	0.40
1:a:145:THR:O	1:a:149:LEU:N	2.54	0.40
1:w:255:PHE:HB3	1:w:259:LEU:HD12	2.02	0.40
2:x:248:SER:HA	2:x:252:LYS:HD3	2.02	0.40
1:u:188:ILE:HG12	1:u:425:LEU:CD1	2.52	0.40
1:q:439:THR:HG22	2:p:391:ARG:CG	2.51	0.40
2:p:267:MET:HE1	2:p:305:PRO:HG3	2.03	0.40
1:m:208:ALA:HB2	1:m:304:LYS:HB2	2.03	0.40
1:k:103:PHE:CD2	1:k:413:MET:HE1	2.56	0.40
1:a:17:GLY:O	1:a:18:ASN:C	2.63	0.40
1:a:402:ARG:O	1:a:405:VAL:HG23	2.21	0.40
2:d:397:TRP:O	2:d:401:GLU:HG2	2.20	0.40
1:q:305:CYS:SG	1:q:387:VAL:CG2	3.09	0.40
1:m:223:THR:HG22	2:n:322:SER:HA	2.03	0.40
1:g:305:CYS:SG	1:g:387:VAL:HG21	2.61	0.40
1:e:398:MET:HG2	2:f:345:ILE:CD1	2.46	0.40
2:f:263:LEU:HD11	2:f:425:TYR:CD2	2.57	0.40
1:c:2:ARG:HB3	1:c:242:LEU:HB3	2.03	0.40
1:c:102:ASN:HD21	1:c:408:TYR:CA	2.35	0.40
2:b:345:ILE:O	2:b:345:ILE:HG22	2.20	0.40
2:j:49:VAL:HG11	2:j:241:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:62:VAL:HG21	1:q:283:HIS:HA	2.04	0.40
2:v:105:HIS:O	2:v:150:LEU:HD22	2.22	0.40
2:t:86:ARG:HA	2:n:281:TYR:CD1	2.57	0.40
1:q:137:VAL:HG11	1:q:154:LEU:HD21	2.04	0.40
1:o:273:ALA:HB3	1:o:274:PRO:HD3	2.04	0.40
1:k:305:CYS:SG	1:k:387:VAL:CG2	3.09	0.40
1:g:248:LEU:HD12	1:g:248:LEU:HA	1.95	0.40
1:e:137:VAL:HG11	1:e:154:LEU:HD21	2.03	0.40
1:a:248:LEU:HD12	1:a:248:LEU:HA	1.96	0.40
1:i:398:MET:HE3	2:j:345:ILE:HD11	2.04	0.40
2:v:120:VAL:HG11	2:v:155:VAL:HG12	2.03	0.40
2:t:5:VAL:HG22	2:t:62:ARG:CD	2.52	0.40
1:m:136:LEU:HD22	1:m:169:PHE:HE1	1.87	0.40
2:n:421:GLU:O	2:n:424:GLN:HB3	2.21	0.40
1:k:170:THR:HG21	1:k:194:LEU:HD11	2.03	0.40
2:l:334:GLN:HE22	2:l:347:ASN:H	1.69	0.40
1:g:73:THR:OG1	2:h:2:ARG:NH2	2.54	0.40
2:b:318:ARG:HB3	2:b:357:PRO:HA	2.03	0.40
2:d:36:TYR:CE1	2:d:44:LEU:HG	2.56	0.40
2:d:238:CYS:SG	2:d:318:ARG:NE	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	438/449 (98%)	390 (89%)	45 (10%)	3 (1%)	18	55
1	c	438/449 (98%)	405 (92%)	30 (7%)	3 (1%)	18	55
1	e	438/449 (98%)	403 (92%)	34 (8%)	1 (0%)	43	77
1	g	438/449 (98%)	413 (94%)	25 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	438/449 (98%)	410 (94%)	24 (6%)	4 (1%)	14	49
1	k	438/449 (98%)	413 (94%)	25 (6%)	0	100	100
1	m	438/449 (98%)	393 (90%)	44 (10%)	1 (0%)	43	77
1	o	438/449 (98%)	405 (92%)	31 (7%)	2 (0%)	24	63
1	q	438/449 (98%)	414 (94%)	24 (6%)	0	100	100
1	s	438/449 (98%)	374 (85%)	60 (14%)	4 (1%)	14	49
1	u	438/449 (98%)	407 (93%)	31 (7%)	0	100	100
1	w	438/449 (98%)	418 (95%)	20 (5%)	0	100	100
2	b	428/443 (97%)	393 (92%)	35 (8%)	0	100	100
2	d	438/443 (99%)	407 (93%)	30 (7%)	1 (0%)	43	77
2	f	428/443 (97%)	398 (93%)	28 (6%)	2 (0%)	24	63
2	h	428/443 (97%)	405 (95%)	23 (5%)	0	100	100
2	j	428/443 (97%)	401 (94%)	27 (6%)	0	100	100
2	l	428/443 (97%)	410 (96%)	18 (4%)	0	100	100
2	n	438/443 (99%)	403 (92%)	34 (8%)	1 (0%)	43	77
2	p	424/443 (96%)	397 (94%)	27 (6%)	0	100	100
2	r	428/443 (97%)	409 (96%)	19 (4%)	0	100	100
2	t	428/443 (97%)	387 (90%)	39 (9%)	2 (0%)	24	63
2	v	428/443 (97%)	406 (95%)	22 (5%)	0	100	100
2	x	428/443 (97%)	407 (95%)	21 (5%)	0	100	100
All	All	10408/10704 (97%)	9668 (93%)	716 (7%)	24 (0%)	44	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	n	432	GLU
1	a	403	ALA
1	s	322	ASP
1	c	266	HIS
1	c	291	ILE
1	o	38	SER
1	m	403	ALA
1	e	266	HIS
1	a	240	ALA
1	i	38	SER

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Mol	Chain	Res	Type
1	i	282	TYR
1	i	403	ALA
1	s	206	ASN
2	t	143	THR
1	o	399	TYR
1	a	399	TYR
1	i	351	PHE
2	f	275	SER
2	f	280	GLN
1	c	399	TYR
1	s	265	ILE
1	s	261	PRO
2	d	434	GLY
2	t	175	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	369/376 (98%)	361 (98%)	8 (2%)	45	64
1	c	368/376 (98%)	355 (96%)	13 (4%)	32	53
1	e	368/376 (98%)	359 (98%)	9 (2%)	43	63
1	g	370/376 (98%)	359 (97%)	11 (3%)	36	57
1	i	368/376 (98%)	356 (97%)	12 (3%)	33	55
1	k	368/376 (98%)	355 (96%)	13 (4%)	32	53
1	m	369/376 (98%)	356 (96%)	13 (4%)	32	53
1	o	367/376 (98%)	356 (97%)	11 (3%)	36	57
1	q	367/376 (98%)	356 (97%)	11 (3%)	36	57
1	s	369/376 (98%)	357 (97%)	12 (3%)	33	55
1	u	369/376 (98%)	358 (97%)	11 (3%)	36	57
1	w	368/376 (98%)	355 (96%)	13 (4%)	32	53
2	b	364/376 (97%)	356 (98%)	8 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	363/376 (96%)	358 (99%)	5 (1%)	59	71
2	f	364/376 (97%)	362 (100%)	2 (0%)	81	81
2	h	365/376 (97%)	361 (99%)	4 (1%)	65	74
2	j	365/376 (97%)	362 (99%)	3 (1%)	73	77
2	l	365/376 (97%)	363 (100%)	2 (0%)	81	81
2	n	364/376 (97%)	361 (99%)	3 (1%)	73	77
2	p	363/376 (96%)	357 (98%)	6 (2%)	53	67
2	r	364/376 (97%)	361 (99%)	3 (1%)	73	77
2	t	365/376 (97%)	362 (99%)	3 (1%)	73	77
2	v	365/376 (97%)	364 (100%)	1 (0%)	86	84
2	x	365/376 (97%)	363 (100%)	2 (0%)	81	81
All	All	8792/9024 (97%)	8613 (98%)	179 (2%)	48	65

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	w	102	ASN
1	w	137	VAL
1	w	140	SER
1	w	202	VAL
1	w	227	LEU
1	w	231	ILE
1	w	235	ILE
1	w	254	GLU
1	w	260	VAL
1	w	291	ILE
1	w	305	CYS
1	w	329	ASN
1	w	332	ILE
2	x	365	VAL
2	x	368	VAL
1	u	137	VAL
1	u	140	SER
1	u	202	VAL
1	u	227	LEU
1	u	231	ILE
1	u	235	ILE
1	u	254	GLU

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Mol	Chain	Res	Type
1	u	260	VAL
1	u	291	ILE
1	u	305	CYS
1	u	332	ILE
2	v	368	VAL
1	s	137	VAL
1	s	140	SER
1	s	174	SER
1	s	188	ILE
1	s	227	LEU
1	s	235	ILE
1	s	254	GLU
1	s	260	VAL
1	s	305	CYS
1	s	373	ARG
1	s	381	SER
1	s	413	MET
2	t	274	THR
2	t	365	VAL
2	t	420	SER
1	q	137	VAL
1	q	140	SER
1	q	202	VAL
1	q	227	LEU
1	q	231	ILE
1	q	235	ILE
1	q	254	GLU
1	q	260	VAL
1	q	291	ILE
1	q	305	CYS
1	q	332	ILE
2	r	31	ASP
2	r	365	VAL
2	r	368	VAL
1	o	137	VAL
1	o	174	SER
1	o	188	ILE
1	o	227	LEU
1	o	235	ILE
1	o	250	VAL
1	o	254	GLU
1	o	260	VAL

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Mol	Chain	Res	Type
1	o	305	CYS
1	o	332	ILE
1	o	337	THR
2	p	31	ASP
2	p	197	ASP
2	p	274	THR
2	p	292	GLN
2	p	322	SER
2	p	328	GLU
1	m	27	GLU
1	m	137	VAL
1	m	140	SER
1	m	141	VAL
1	m	227	LEU
1	m	231	ILE
1	m	235	ILE
1	m	254	GLU
1	m	260	VAL
1	m	265	ILE
1	m	291	ILE
1	m	305	CYS
1	m	332	ILE
2	n	31	ASP
2	n	53	GLU
2	n	368	VAL
1	k	137	VAL
1	k	140	SER
1	k	174	SER
1	k	202	VAL
1	k	227	LEU
1	k	231	ILE
1	k	235	ILE
1	k	254	GLU
1	k	260	VAL
1	k	291	ILE
1	k	305	CYS
1	k	332	ILE
1	k	362	VAL
2	l	31	ASP
2	l	368	VAL
1	g	137	VAL
1	g	140	SER

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Mol	Chain	Res	Type
1	g	202	VAL
1	g	227	LEU
1	g	231	ILE
1	g	235	ILE
1	g	254	GLU
1	g	260	VAL
1	g	291	ILE
1	g	305	CYS
1	g	332	ILE
2	h	31	ASP
2	h	274	THR
2	h	365	VAL
2	h	368	VAL
1	e	137	VAL
1	e	140	SER
1	e	202	VAL
1	e	254	GLU
1	e	260	VAL
1	e	305	CYS
1	e	329	ASN
1	e	332	ILE
1	e	438	GLU
2	f	274	THR
2	f	368	VAL
1	c	119	LEU
1	c	137	VAL
1	c	140	SER
1	c	174	SER
1	c	202	VAL
1	c	227	LEU
1	c	231	ILE
1	c	235	ILE
1	c	260	VAL
1	c	300	ASN
1	c	305	CYS
1	c	331	SER
1	c	332	ILE
1	a	137	VAL
1	a	140	SER
1	a	202	VAL
1	a	254	GLU
1	a	260	VAL

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Mol	Chain	Res	Type
1	a	291	ILE
1	a	305	CYS
1	a	332	ILE
2	b	135	ILE
2	b	203	ASP
2	b	222	TYR
2	b	249	ASP
2	b	274	THR
2	b	355	ASP
2	b	365	VAL
2	b	368	VAL
2	d	12	CYS
2	d	113	ILE
2	d	135	ILE
2	d	368	VAL
2	d	427	ASP
1	i	137	VAL
1	i	140	SER
1	i	174	SER
1	i	231	ILE
1	i	235	ILE
1	i	254	GLU
1	i	260	VAL
1	i	265	ILE
1	i	305	CYS
1	i	329	ASN
1	i	332	ILE
1	i	438	GLU
2	j	31	ASP
2	j	197	ASP
2	j	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (228) such sidechains are listed below:

Mol	Chain	Res	Type
1	w	15	GLN
1	w	91	GLN
1	w	192	HIS
1	w	206	ASN
1	w	216	ASN
1	w	293	ASN
1	w	342	GLN

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Mol	Chain	Res	Type
1	w	356	ASN
2	x	14	ASN
2	x	134	GLN
2	x	226	ASN
2	x	247	ASN
2	x	256	ASN
2	x	292	GLN
2	x	298	ASN
2	x	348	ASN
2	x	375	GLN
2	x	423	GLN
1	u	15	GLN
1	u	91	GLN
1	u	192	HIS
1	u	206	ASN
1	u	216	ASN
1	u	258	ASN
1	u	293	ASN
1	u	342	GLN
1	u	356	ASN
1	u	380	ASN
2	v	15	GLN
2	v	131	GLN
2	v	134	GLN
2	v	226	ASN
2	v	256	ASN
2	v	292	GLN
2	v	298	ASN
2	v	348	ASN
1	s	91	GLN
1	s	102	ASN
1	s	258	ASN
1	s	356	ASN
1	s	380	ASN
1	s	393	HIS
2	t	100	ASN
2	t	190	HIS
2	t	204	ASN
2	t	226	ASN
2	t	247	ASN
2	t	256	ASN
2	t	292	GLN

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Mol	Chain	Res	Type
2	t	298	ASN
2	t	348	ASN
2	t	375	GLN
1	q	15	GLN
1	q	85	GLN
1	q	133	GLN
1	q	206	ASN
1	q	216	ASN
1	q	258	ASN
1	q	285	GLN
1	q	293	ASN
1	q	309	HIS
1	q	342	GLN
1	q	356	ASN
1	q	380	ASN
2	r	15	GLN
2	r	134	GLN
2	r	226	ASN
2	r	247	ASN
2	r	256	ASN
2	r	292	GLN
2	r	298	ASN
2	r	348	ASN
2	r	423	GLN
1	o	15	GLN
1	o	50	ASN
1	o	85	GLN
1	o	102	ASN
1	o	107	HIS
1	o	192	HIS
1	o	216	ASN
1	o	258	ASN
1	o	293	ASN
1	o	342	GLN
1	o	356	ASN
1	o	393	HIS
2	p	99	ASN
2	p	131	GLN
2	p	134	GLN
2	p	195	ASN
2	p	204	ASN
2	p	226	ASN

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Mol	Chain	Res	Type
2	p	247	ASN
2	p	375	GLN
1	m	15	GLN
1	m	61	HIS
1	m	85	GLN
1	m	107	HIS
1	m	206	ASN
1	m	258	ASN
1	m	285	GLN
1	m	293	ASN
1	m	342	GLN
1	m	356	ASN
1	m	380	ASN
2	n	99	ASN
2	n	131	GLN
2	n	134	GLN
2	n	226	ASN
2	n	245	GLN
2	n	247	ASN
2	n	256	ASN
2	n	292	GLN
2	n	298	ASN
2	n	348	ASN
2	n	414	ASN
1	k	15	GLN
1	k	258	ASN
1	k	293	ASN
1	k	309	HIS
1	k	342	GLN
2	l	134	GLN
2	l	226	ASN
2	l	245	GLN
2	l	247	ASN
2	l	256	ASN
2	l	280	GLN
2	l	292	GLN
2	l	298	ASN
2	l	348	ASN
2	l	375	GLN
2	l	423	GLN
1	g	15	GLN
1	g	85	GLN

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Mol	Chain	Res	Type
1	g	258	ASN
1	g	283	HIS
1	g	293	ASN
1	g	309	HIS
1	g	342	GLN
1	g	356	ASN
2	h	14	ASN
2	h	99	ASN
2	h	134	GLN
2	h	226	ASN
2	h	247	ASN
2	h	256	ASN
2	h	292	GLN
2	h	298	ASN
2	h	348	ASN
2	h	396	HIS
2	h	426	GLN
1	e	15	GLN
1	e	61	HIS
1	e	85	GLN
1	e	88	HIS
1	e	91	GLN
1	e	206	ASN
1	e	216	ASN
1	e	256	GLN
1	e	285	GLN
1	e	293	ASN
1	e	309	HIS
1	e	342	GLN
1	e	380	ASN
2	f	8	GLN
2	f	15	GLN
2	f	105	HIS
2	f	134	GLN
2	f	226	ASN
2	f	247	ASN
2	f	256	ASN
2	f	292	GLN
2	f	329	GLN
2	f	348	ASN
1	c	31	GLN
1	c	85	GLN

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Mol	Chain	Res	Type
1	c	88	HIS
1	c	293	ASN
1	c	342	GLN
1	a	15	GLN
1	a	85	GLN
1	a	88	HIS
1	a	192	HIS
1	a	197	HIS
1	a	206	ASN
1	a	258	ASN
1	a	283	HIS
1	a	285	GLN
1	a	293	ASN
1	a	342	GLN
1	a	393	HIS
2	b	14	ASN
2	b	99	ASN
2	b	105	HIS
2	b	134	GLN
2	b	226	ASN
2	b	247	ASN
2	b	256	ASN
2	b	292	GLN
2	b	298	ASN
2	b	329	GLN
2	b	348	ASN
2	d	14	ASN
2	d	99	ASN
2	d	134	GLN
2	d	226	ASN
2	d	256	ASN
2	d	298	ASN
2	d	329	GLN
2	d	348	ASN
2	d	426	GLN
1	i	15	GLN
1	i	85	GLN
1	i	192	HIS
1	i	258	ASN
1	i	293	ASN
1	i	309	HIS
1	i	342	GLN

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Mol	Chain	Res	Type
1	i	380	ASN
2	j	99	ASN
2	j	105	HIS
2	j	204	ASN
2	j	226	ASN
2	j	247	ASN
2	j	256	ASN
2	j	280	GLN
2	j	292	GLN
2	j	298	ASN
2	j	414	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 12 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GDP	f	501	-	29,30,30	1.23	5 (17%)	45,47,47	1.99	8 (17%)
5	GDP	b	501	-	29,30,30	1.32	4 (13%)	45,47,47	1.90	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	r	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	6 (13%)
3	GTP	g	501	4	33,34,34	0.54	0	50,54,54	0.57	0
3	GTP	i	501	4	33,34,34	0.51	0	50,54,54	0.54	0
3	GTP	s	501	4	33,34,34	0.52	0	50,54,54	0.59	0
5	GDP	n	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.80	7 (15%)
3	GTP	o	501	4	33,34,34	0.54	0	50,54,54	0.57	0
5	GDP	l	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.79	7 (15%)
3	GTP	a	501	4	33,34,34	0.59	0	50,54,54	0.54	0
5	GDP	j	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	6 (13%)
3	GTP	k	501	4	33,34,34	0.54	0	50,54,54	0.54	0
3	GTP	m	501	4	33,34,34	0.51	0	50,54,54	0.60	0
3	GTP	w	501	4	33,34,34	0.55	0	50,54,54	0.56	0
3	GTP	e	501	4	33,34,34	0.55	0	50,54,54	0.59	0
5	GDP	x	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	8 (17%)
5	GDP	p	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.83	8 (17%)
5	GDP	t	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.94	8 (17%)
5	GDP	h	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.84	7 (15%)
3	GTP	c	501	4	33,34,34	0.67	1 (3%)	50,54,54	0.62	0
3	GTP	u	501	4	33,34,34	0.52	0	50,54,54	0.56	0
3	GTP	q	501	4	33,34,34	0.53	0	50,54,54	0.57	0
5	GDP	v	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	f	501	-	-	4/16/32/32	0/3/3/3
5	GDP	b	501	-	-	4/16/32/32	0/3/3/3
5	GDP	r	501	-	-	4/16/32/32	0/3/3/3
3	GTP	g	501	4	-	3/22/38/38	0/3/3/3
3	GTP	i	501	4	-	6/22/38/38	0/3/3/3
3	GTP	s	501	4	-	3/22/38/38	0/3/3/3
5	GDP	n	501	-	-	4/16/32/32	0/3/3/3
3	GTP	o	501	4	-	4/22/38/38	0/3/3/3
5	GDP	l	501	-	-	3/16/32/32	0/3/3/3
3	GTP	a	501	4	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	j	501	-	-	7/16/32/32	0/3/3/3
3	GTP	k	501	4	-	3/22/38/38	0/3/3/3
3	GTP	m	501	4	-	4/22/38/38	0/3/3/3
3	GTP	w	501	4	-	5/22/38/38	0/3/3/3
3	GTP	e	501	4	-	3/22/38/38	0/3/3/3
5	GDP	x	502	-	-	5/16/32/32	0/3/3/3
5	GDP	p	501	-	-	1/16/32/32	0/3/3/3
5	GDP	t	502	-	-	4/16/32/32	0/3/3/3
5	GDP	h	501	-	-	4/16/32/32	0/3/3/3
3	GTP	c	501	4	-	5/22/38/38	0/3/3/3
3	GTP	u	501	4	-	3/22/38/38	0/3/3/3
3	GTP	q	501	4	-	5/22/38/38	0/3/3/3
5	GDP	v	501	-	-	4/16/32/32	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	b	501	GDP	PA-O3A	3.50	1.63	1.59
5	p	501	GDP	C5-C4	3.31	1.47	1.38
5	j	501	GDP	C5-C4	3.29	1.47	1.38
5	h	501	GDP	C5-C4	3.27	1.47	1.38
5	r	501	GDP	C5-C4	3.22	1.47	1.38
5	v	501	GDP	C5-C4	3.18	1.47	1.38
5	n	501	GDP	C5-C4	3.12	1.47	1.38
5	x	502	GDP	C5-C4	3.11	1.47	1.38
5	l	501	GDP	C5-C4	3.07	1.47	1.38
5	f	501	GDP	C5-C4	3.06	1.47	1.38
5	b	501	GDP	C5-C4	3.04	1.47	1.38
5	t	502	GDP	C5-C4	2.98	1.46	1.38
5	b	501	GDP	C6-N1	-2.46	1.34	1.38
5	t	502	GDP	C6-N1	-2.44	1.34	1.38
5	n	501	GDP	C5-N7	-2.43	1.34	1.39
5	t	502	GDP	C5-N7	-2.42	1.34	1.39
5	j	501	GDP	C5-N7	-2.29	1.34	1.39
5	l	501	GDP	C5-N7	-2.28	1.34	1.39
5	f	501	GDP	C6-N1	-2.27	1.34	1.38
5	l	501	GDP	C6-N1	-2.27	1.34	1.38
5	f	501	GDP	PA-O3A	2.27	1.62	1.59
5	n	501	GDP	C6-N1	-2.27	1.34	1.38
5	v	501	GDP	C5-N7	-2.23	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	v	501	GDP	C6-N1	-2.21	1.34	1.38
5	r	501	GDP	C6-N1	-2.19	1.34	1.38
5	h	501	GDP	C5-N7	-2.19	1.34	1.39
5	p	501	GDP	C5-N7	-2.18	1.34	1.39
5	j	501	GDP	C6-N1	-2.16	1.34	1.38
5	h	501	GDP	C6-N1	-2.16	1.34	1.38
5	x	502	GDP	C5-N7	-2.14	1.34	1.39
5	r	501	GDP	C5-N7	-2.12	1.34	1.39
5	b	501	GDP	C5-N7	-2.11	1.34	1.39
5	f	501	GDP	C5-N7	-2.09	1.34	1.39
3	c	501	GTP	PA-O3A	2.06	1.61	1.59
5	l	501	GDP	PA-O3A	2.05	1.61	1.59
5	x	502	GDP	C6-N1	-2.03	1.35	1.38
5	p	501	GDP	C6-N1	-2.03	1.35	1.38
5	f	501	GDP	C2-N3	2.03	1.38	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	501	GDP	C5-C4-N3	-6.83	117.52	128.39
5	b	501	GDP	C5-C4-N3	-6.59	117.90	128.39
5	t	502	GDP	C5-C4-N3	-6.58	117.92	128.39
5	h	501	GDP	C5-C4-N3	-6.23	118.47	128.39
5	p	501	GDP	C5-C4-N3	-6.22	118.49	128.39
5	v	501	GDP	C5-C4-N3	-6.12	118.66	128.39
5	j	501	GDP	C5-C4-N3	-6.10	118.68	128.39
5	r	501	GDP	C5-C4-N3	-6.07	118.72	128.39
5	l	501	GDP	C5-C4-N3	-6.03	118.80	128.39
5	f	501	GDP	C2-N3-C4	6.00	122.64	112.30
5	n	501	GDP	C5-C4-N3	-5.96	118.90	128.39
5	x	502	GDP	C5-C4-N3	-5.95	118.92	128.39
5	t	502	GDP	C2-N3-C4	5.74	122.19	112.30
5	b	501	GDP	C2-N3-C4	5.58	121.91	112.30
5	h	501	GDP	C2-N3-C4	5.42	121.63	112.30
5	x	502	GDP	C2-N3-C4	5.36	121.53	112.30
5	p	501	GDP	C2-N3-C4	5.34	121.49	112.30
5	l	501	GDP	C2-N3-C4	5.34	121.49	112.30
5	n	501	GDP	C2-N3-C4	5.33	121.49	112.30
5	r	501	GDP	C2-N3-C4	5.33	121.48	112.30
5	j	501	GDP	C2-N3-C4	5.29	121.42	112.30
5	v	501	GDP	C2-N3-C4	5.27	121.38	112.30
5	f	501	GDP	N9-C4-N3	5.24	136.43	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	t	502	GDP	N9-C4-N3	5.06	136.08	125.95
5	b	501	GDP	N9-C4-N3	4.71	135.37	125.95
5	x	502	GDP	N9-C4-N3	4.61	135.17	125.95
5	p	501	GDP	N9-C4-N3	4.58	135.11	125.95
5	r	501	GDP	N9-C4-N3	4.51	134.97	125.95
5	h	501	GDP	N9-C4-N3	4.49	134.93	125.95
5	v	501	GDP	N9-C4-N3	4.46	134.88	125.95
5	l	501	GDP	N9-C4-N3	4.46	134.86	125.95
5	n	501	GDP	N9-C4-N3	4.40	134.75	125.95
5	j	501	GDP	N9-C4-N3	4.25	134.46	125.95
5	b	501	GDP	C6-C5-N7	3.62	136.88	130.29
5	f	501	GDP	C6-C5-N7	3.49	136.65	130.29
5	r	501	GDP	C6-C5-N7	3.39	136.46	130.29
5	h	501	GDP	C6-C5-N7	3.37	136.42	130.29
5	l	501	GDP	C6-C5-N7	3.33	136.36	130.29
5	p	501	GDP	C6-C5-N7	3.31	136.31	130.29
5	j	501	GDP	C6-C5-N7	3.31	136.31	130.29
5	x	502	GDP	C6-C5-N7	3.30	136.29	130.29
5	v	501	GDP	C6-C5-N7	3.28	136.26	130.29
5	b	501	GDP	C4-C5-N7	-3.19	105.61	110.67
5	n	501	GDP	C6-C5-N7	3.04	135.83	130.29
5	t	502	GDP	C6-C5-N7	2.97	135.69	130.29
5	t	502	GDP	O6-C6-C5	-2.82	119.09	126.53
5	f	501	GDP	C4-C5-N7	-2.81	106.22	110.67
5	j	501	GDP	C4-C5-N7	-2.75	106.32	110.67
5	h	501	GDP	C4-C5-N7	-2.74	106.32	110.67
5	n	501	GDP	O6-C6-C5	-2.70	119.40	126.53
5	p	501	GDP	C4-C5-N7	-2.68	106.42	110.67
5	t	502	GDP	C3'-C2'-C1'	2.62	106.43	101.46
5	x	502	GDP	O6-C6-C5	-2.53	119.85	126.53
5	r	501	GDP	C4-C5-N7	-2.52	106.68	110.67
5	v	501	GDP	C3'-C2'-C1'	2.50	106.19	101.46
5	l	501	GDP	C4-C5-N7	-2.47	106.76	110.67
5	v	501	GDP	C4-C5-N7	-2.46	106.77	110.67
5	t	502	GDP	C5-C6-N1	2.44	119.47	113.25
5	h	501	GDP	C3'-C2'-C1'	2.41	106.02	101.46
5	p	501	GDP	C3'-C2'-C1'	2.40	106.00	101.46
5	b	501	GDP	C8-N7-C5	2.38	108.50	104.26
5	v	501	GDP	O6-C6-C5	-2.38	120.26	126.53
5	n	501	GDP	C3'-C2'-C1'	2.34	105.88	101.46
5	l	501	GDP	O6-C6-C5	-2.34	120.37	126.53
5	f	501	GDP	C5-C6-N1	2.30	119.11	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	501	GDP	O6-C6-C5	-2.30	120.45	126.53
5	j	501	GDP	O6-C6-C5	-2.28	120.51	126.53
5	h	501	GDP	O6-C6-C5	-2.27	120.55	126.53
5	x	502	GDP	C4-C5-N7	-2.24	107.12	110.67
5	r	501	GDP	O6-C6-C5	-2.23	120.63	126.53
5	f	501	GDP	C8-N7-C5	2.23	108.23	104.26
5	p	501	GDP	O6-C6-C5	-2.16	120.84	126.53
5	x	502	GDP	C5-C6-N1	2.12	118.64	113.25
5	n	501	GDP	C4-C5-N7	-2.10	107.33	110.67
5	t	502	GDP	C4-C5-N7	-2.06	107.40	110.67
5	b	501	GDP	O6-C6-C5	-2.05	121.13	126.53
5	b	501	GDP	C5-C6-N1	2.03	118.42	113.25
5	l	501	GDP	C5-C6-N1	2.02	118.40	113.25
5	x	502	GDP	C2'-C3'-C4'	2.01	106.49	102.61
5	p	501	GDP	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	w	501	GTP	C5'-O5'-PA-O3A
3	w	501	GTP	C5'-O5'-PA-O2A
3	u	501	GTP	C5'-O5'-PA-O3A
3	u	501	GTP	C5'-O5'-PA-O2A
3	s	501	GTP	C5'-O5'-PA-O3A
3	s	501	GTP	C5'-O5'-PA-O2A
3	q	501	GTP	C5'-O5'-PA-O3A
3	q	501	GTP	C5'-O5'-PA-O2A
3	o	501	GTP	C5'-O5'-PA-O3A
3	o	501	GTP	C5'-O5'-PA-O1A
3	o	501	GTP	C5'-O5'-PA-O2A
3	m	501	GTP	C5'-O5'-PA-O3A
3	m	501	GTP	C5'-O5'-PA-O2A
3	k	501	GTP	C5'-O5'-PA-O3A
3	k	501	GTP	C5'-O5'-PA-O2A
3	g	501	GTP	C5'-O5'-PA-O3A
3	g	501	GTP	C5'-O5'-PA-O2A
3	e	501	GTP	C5'-O5'-PA-O3A
3	e	501	GTP	C5'-O5'-PA-O2A
3	c	501	GTP	PB-O3B-PG-O2G
3	c	501	GTP	C5'-O5'-PA-O3A
3	c	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	a	501	GTP	C5'-O5'-PA-O3A
3	a	501	GTP	C5'-O5'-PA-O2A
3	i	501	GTP	C5'-O5'-PA-O3A
3	i	501	GTP	C5'-O5'-PA-O1A
3	i	501	GTP	C5'-O5'-PA-O2A
5	x	502	GDP	C5'-O5'-PA-O2A
5	t	502	GDP	C5'-O5'-PA-O3A
5	t	502	GDP	C5'-O5'-PA-O1A
5	t	502	GDP	C5'-O5'-PA-O2A
5	j	501	GDP	C5'-O5'-PA-O2A
5	h	501	GDP	O4'-C4'-C5'-O5'
5	r	501	GDP	O4'-C4'-C5'-O5'
5	n	501	GDP	O4'-C4'-C5'-O5'
5	h	501	GDP	C3'-C4'-C5'-O5'
5	f	501	GDP	O4'-C4'-C5'-O5'
5	r	501	GDP	C3'-C4'-C5'-O5'
5	n	501	GDP	C3'-C4'-C5'-O5'
5	v	501	GDP	O4'-C4'-C5'-O5'
5	l	501	GDP	O4'-C4'-C5'-O5'
5	f	501	GDP	C3'-C4'-C5'-O5'
5	l	501	GDP	C3'-C4'-C5'-O5'
5	x	502	GDP	O4'-C4'-C5'-O5'
5	x	502	GDP	C3'-C4'-C5'-O5'
5	v	501	GDP	C3'-C4'-C5'-O5'
3	a	501	GTP	C4'-C5'-O5'-PA
5	x	502	GDP	PB-O3A-PA-O1A
5	r	501	GDP	PB-O3A-PA-O1A
5	p	501	GDP	PB-O3A-PA-O1A
5	f	501	GDP	PB-O3A-PA-O1A
5	b	501	GDP	PB-O3A-PA-O1A
5	j	501	GDP	PB-O3A-PA-O1A
3	e	501	GTP	C4'-C5'-O5'-PA
5	x	502	GDP	C5'-O5'-PA-O3A
5	j	501	GDP	C5'-O5'-PA-O3A
5	j	501	GDP	C5'-O5'-PA-O1A
3	s	501	GTP	PB-O3A-PA-O2A
3	o	501	GTP	PB-O3A-PA-O2A
3	c	501	GTP	PB-O3A-PA-O2A
5	h	501	GDP	PB-O3A-PA-O1A
3	q	501	GTP	C4'-C5'-O5'-PA
3	k	501	GTP	C4'-C5'-O5'-PA
3	q	501	GTP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	n	501	GDP	PB-O3A-PA-O1A
3	g	501	GTP	C4'-C5'-O5'-PA
3	u	501	GTP	C4'-C5'-O5'-PA
5	b	501	GDP	O4'-C4'-C5'-O5'
5	j	501	GDP	C3'-C4'-C5'-O5'
3	w	501	GTP	PB-O3A-PA-O1A
3	w	501	GTP	PB-O3A-PA-O2A
3	q	501	GTP	PB-O3A-PA-O1A
3	m	501	GTP	PB-O3A-PA-O1A
3	m	501	GTP	PB-O3A-PA-O2A
3	i	501	GTP	PB-O3A-PA-O2A
5	r	501	GDP	PB-O3A-PA-O2A
5	h	501	GDP	PB-O3A-PA-O2A
5	f	501	GDP	PB-O3A-PA-O2A
5	b	501	GDP	PB-O3A-PA-O2A
3	c	501	GTP	PB-O3B-PG-O1G
5	j	501	GDP	O4'-C4'-C5'-O5'
3	w	501	GTP	C4'-C5'-O5'-PA
3	i	501	GTP	C4'-C5'-O5'-PA
3	i	501	GTP	PB-O3A-PA-O1A
5	v	501	GDP	PB-O3A-PA-O1A
5	v	501	GDP	PB-O3A-PA-O2A
5	t	502	GDP	PB-O3A-PA-O2A
5	n	501	GDP	PB-O3A-PA-O2A
5	l	501	GDP	PB-O3A-PA-O2A
5	j	501	GDP	PB-O3A-PA-O2A
5	b	501	GDP	C3'-C4'-C5'-O5'

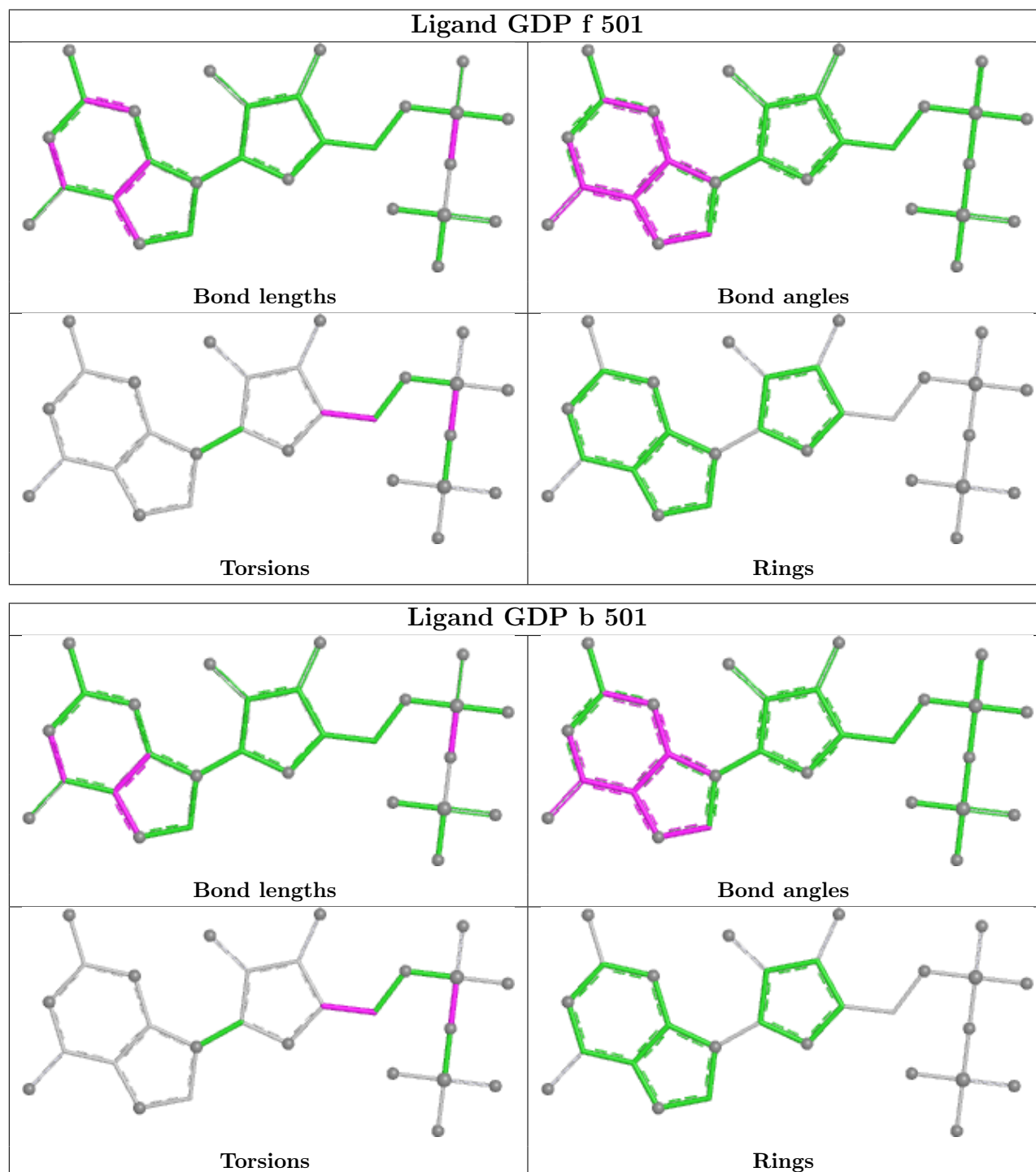
There are no ring outliers.

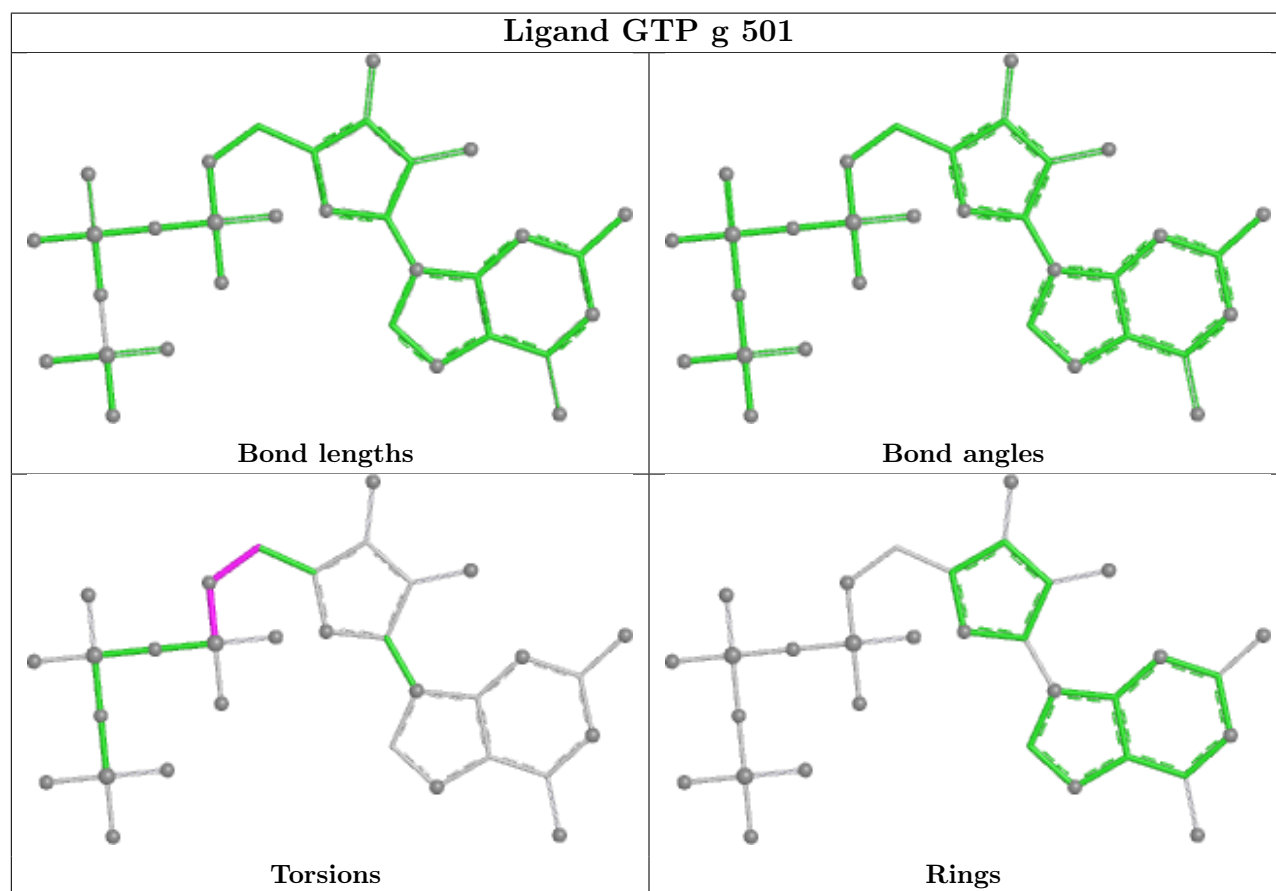
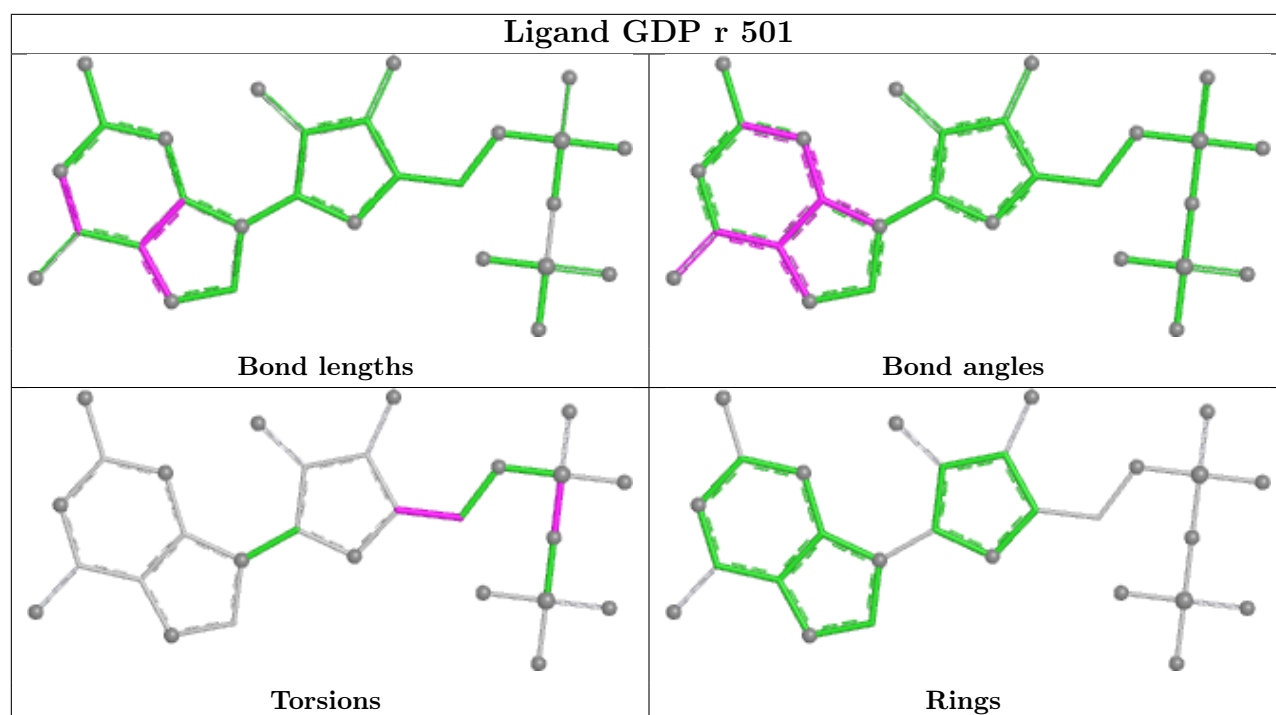
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	w	501	GTP	1	0
3	e	501	GTP	2	0
5	t	502	GDP	1	0
3	c	501	GTP	1	0
3	q	501	GTP	1	0

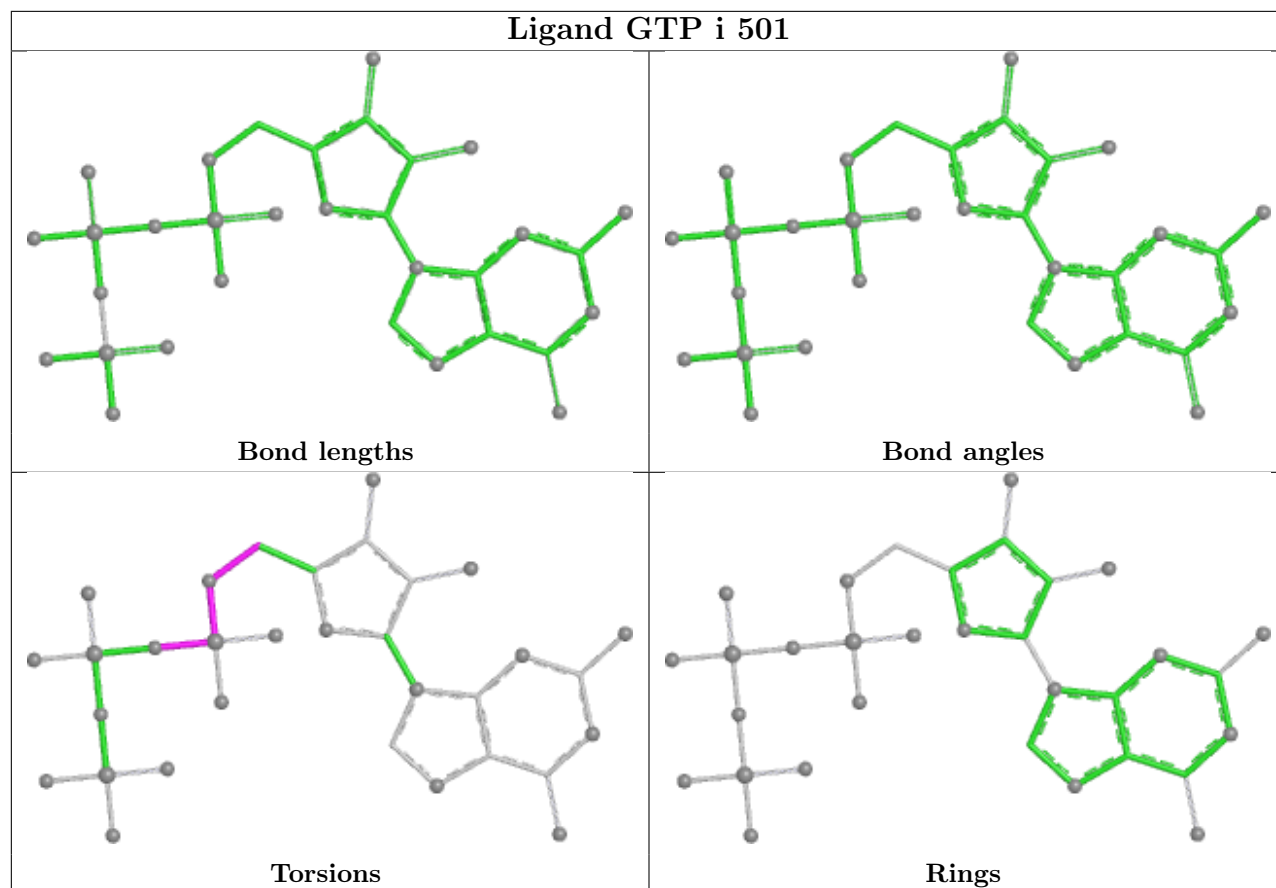
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

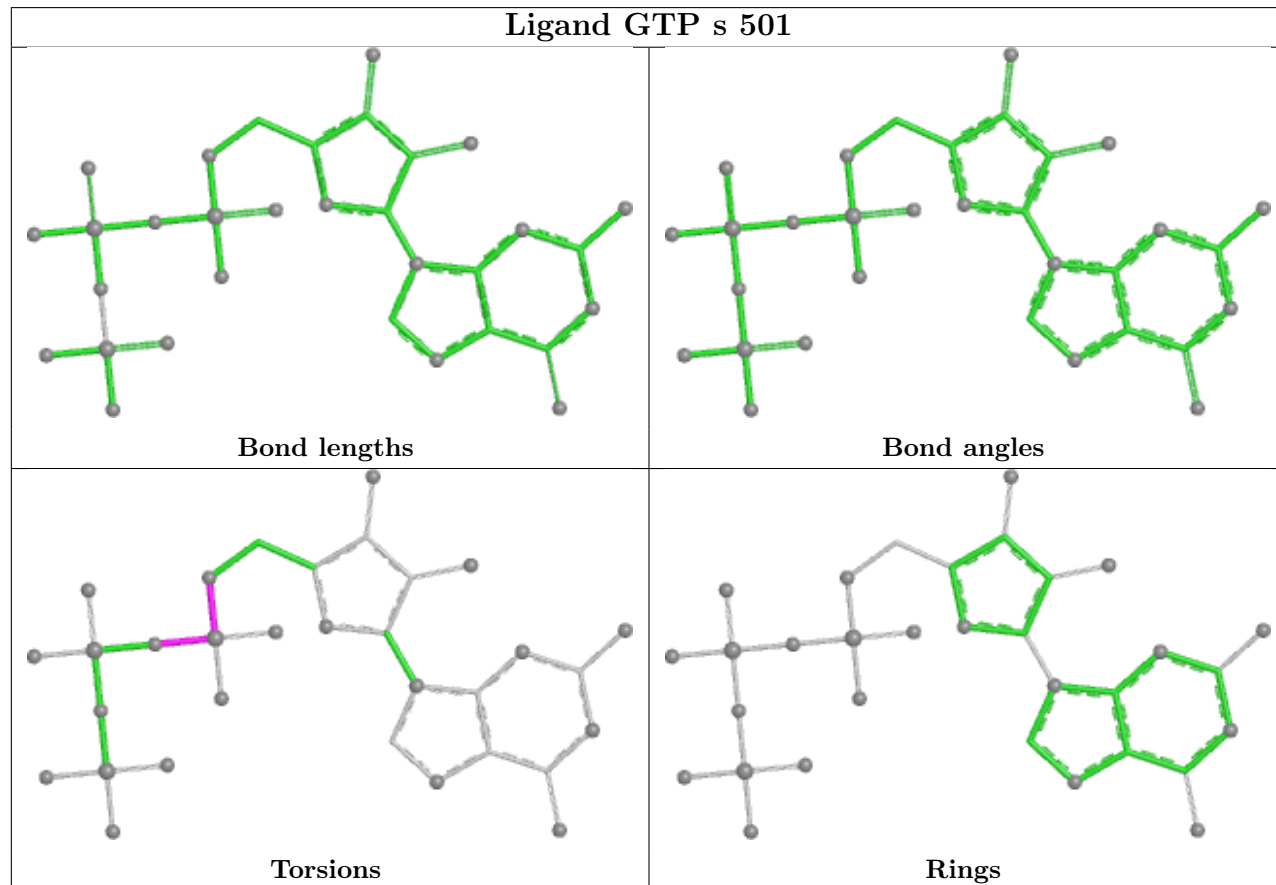


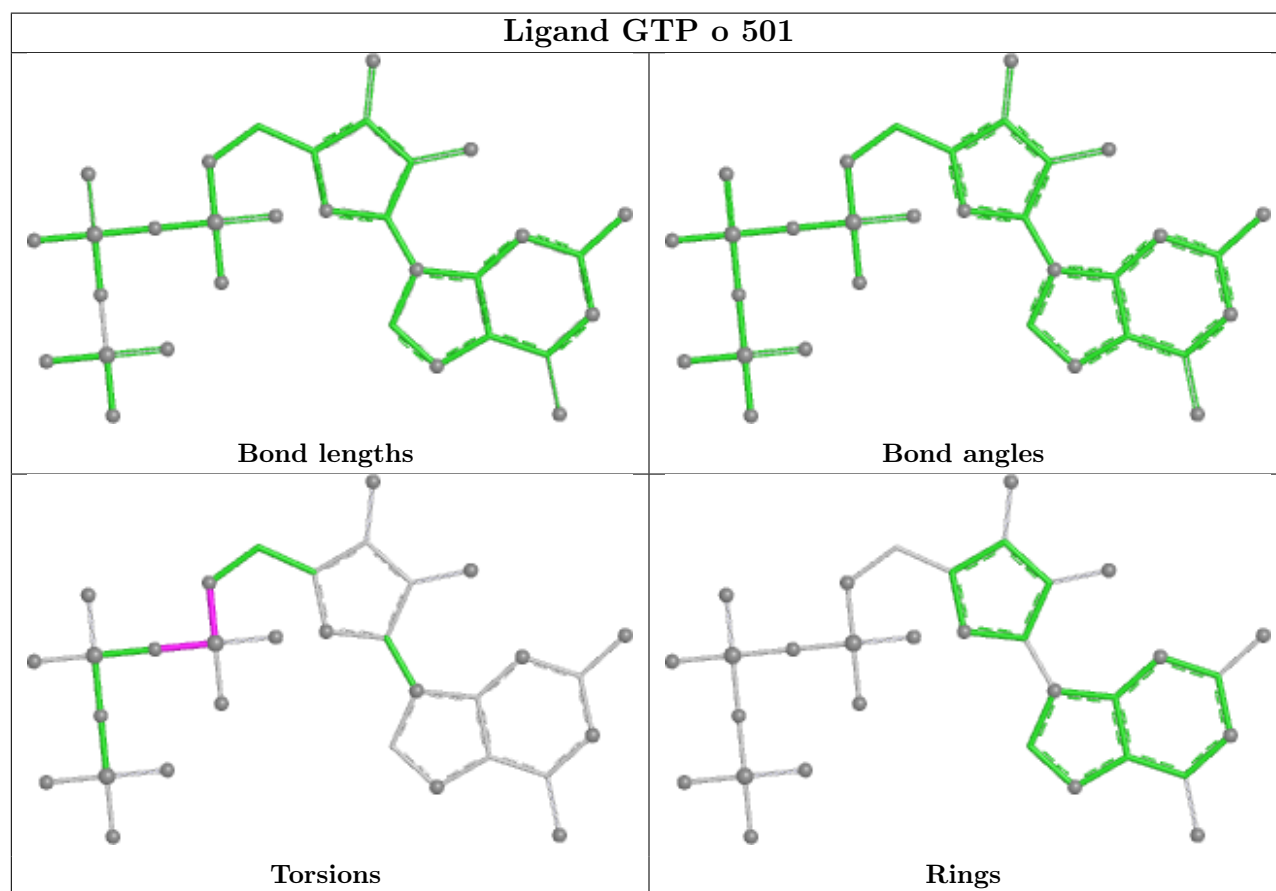
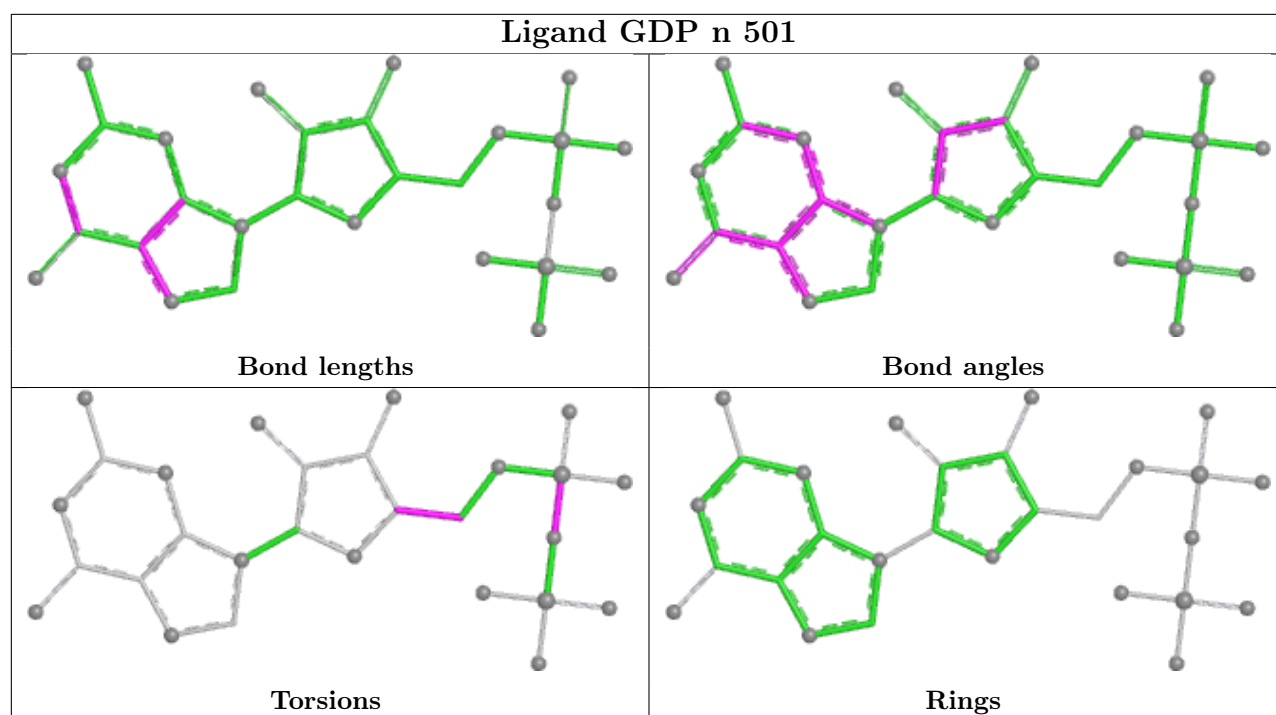


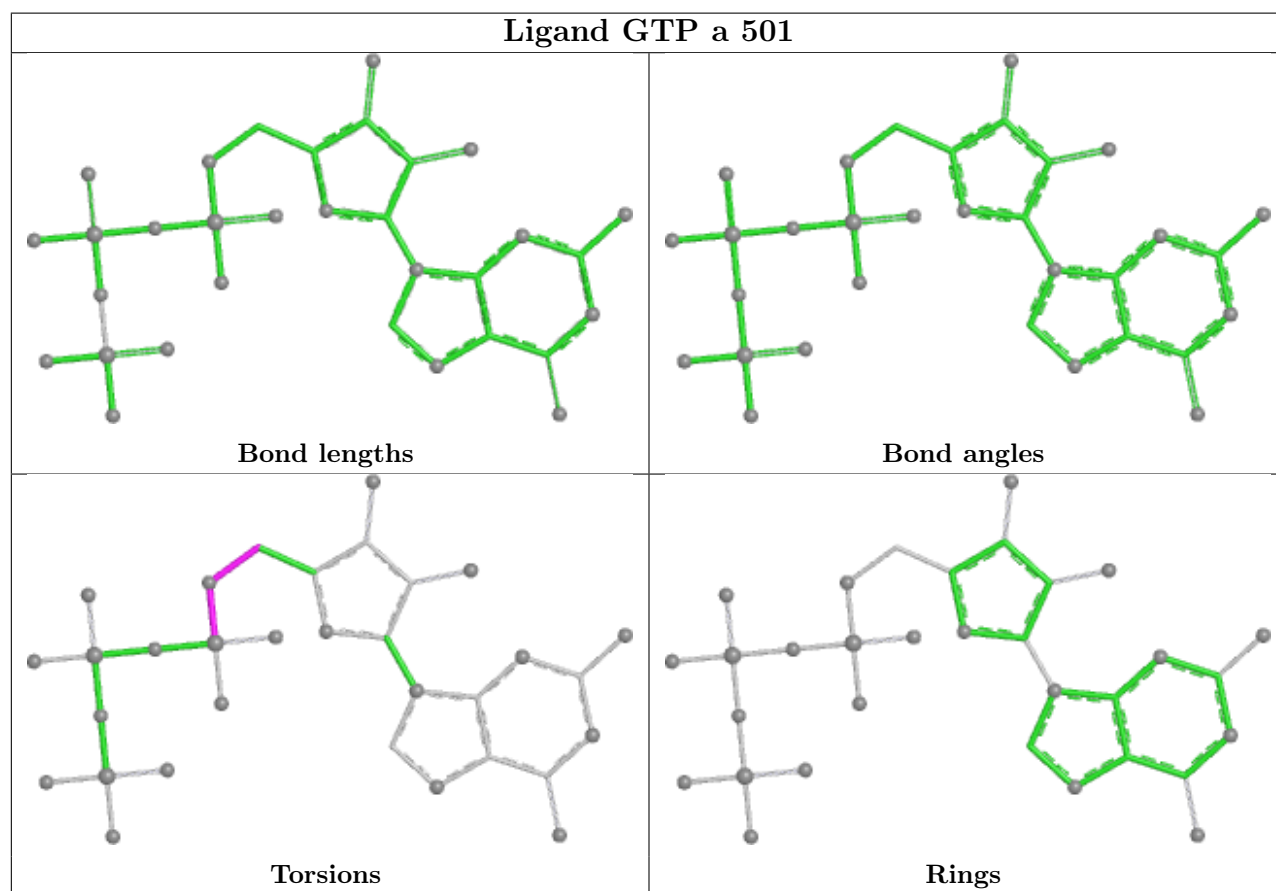
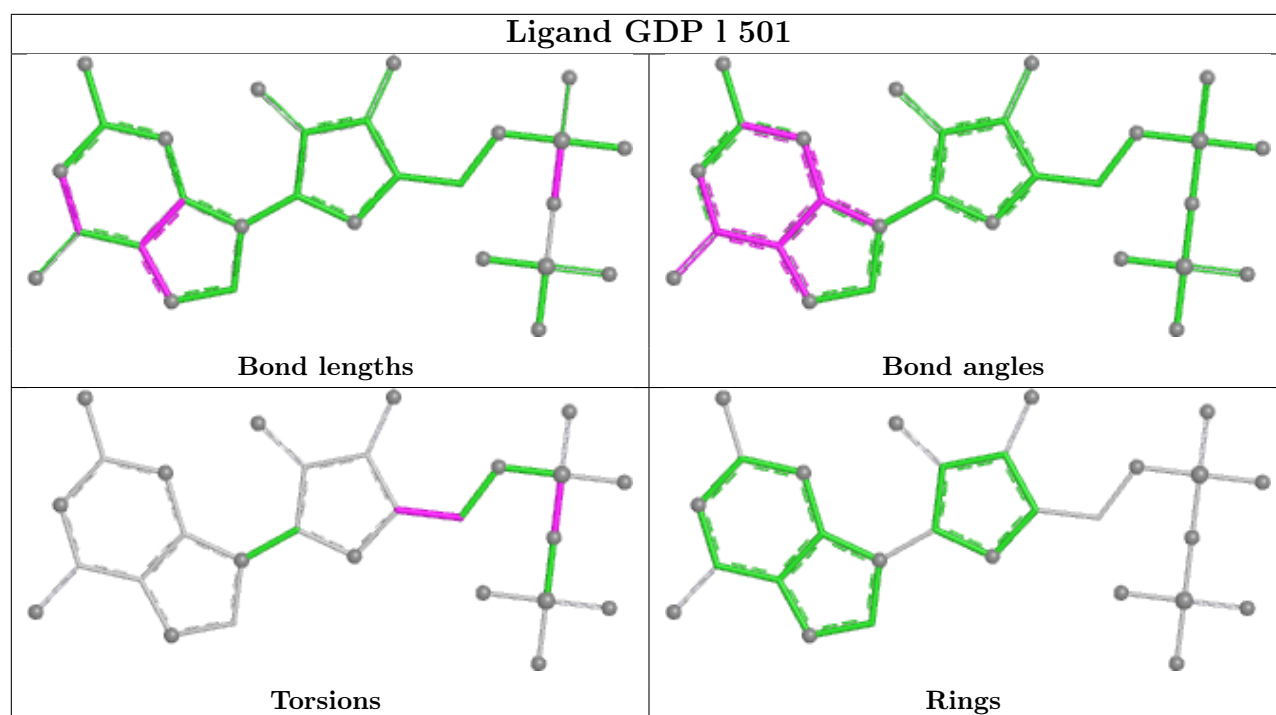
Ligand GTP i 501

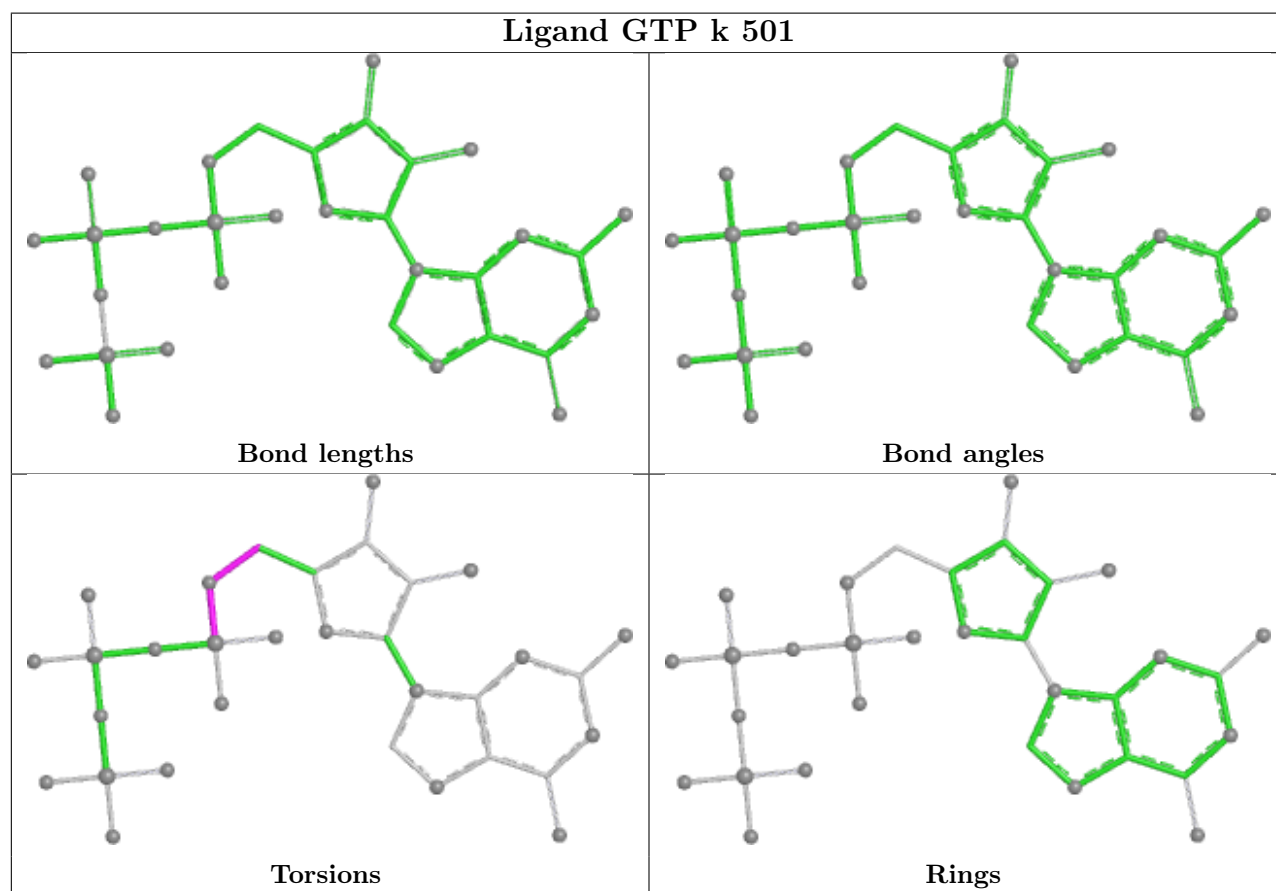
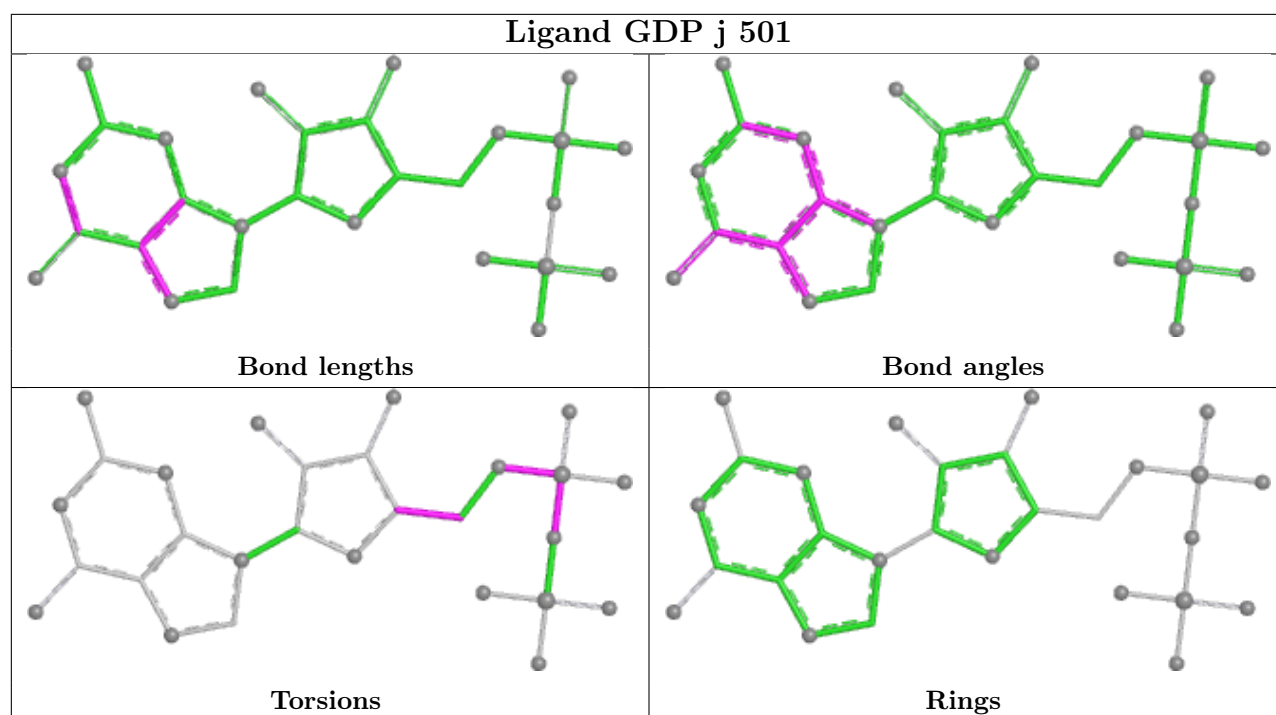


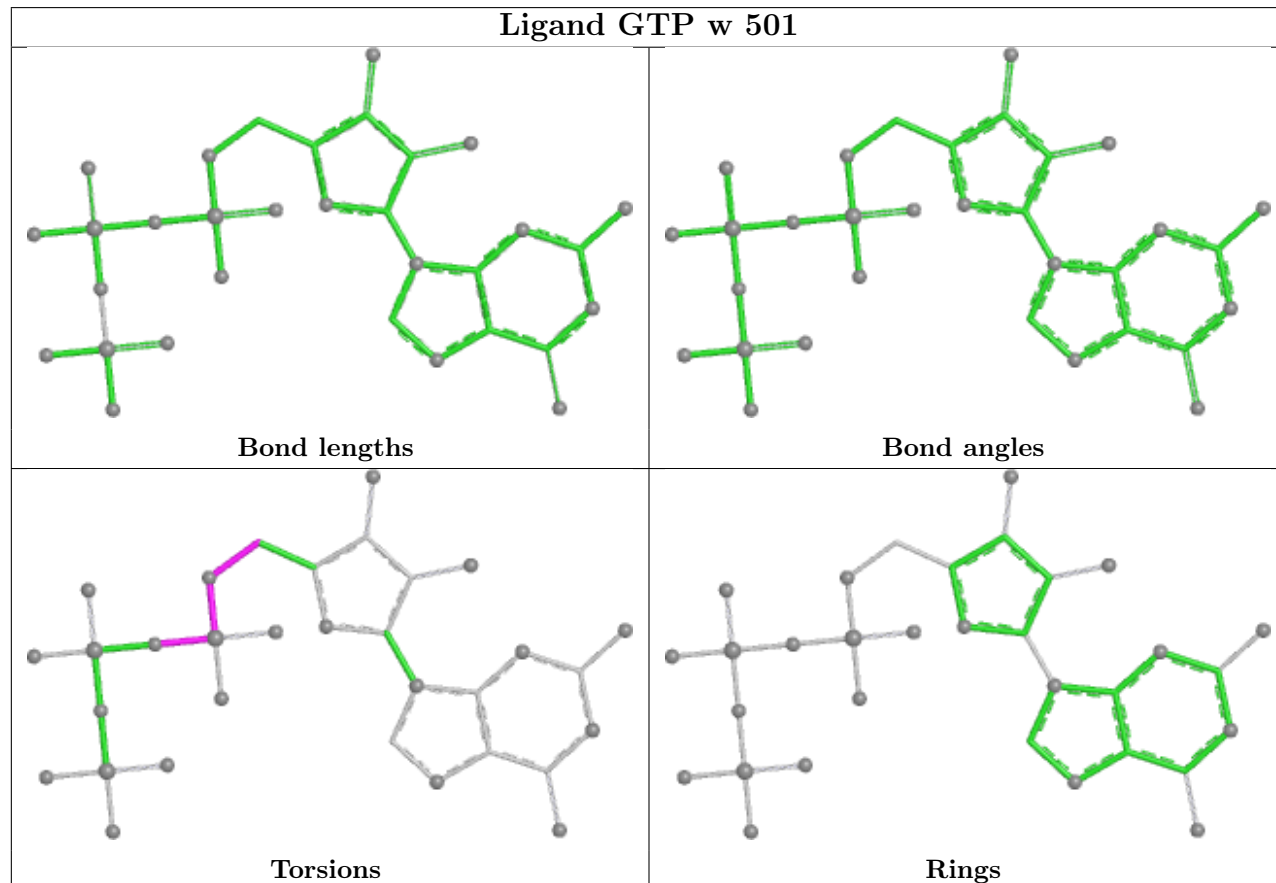
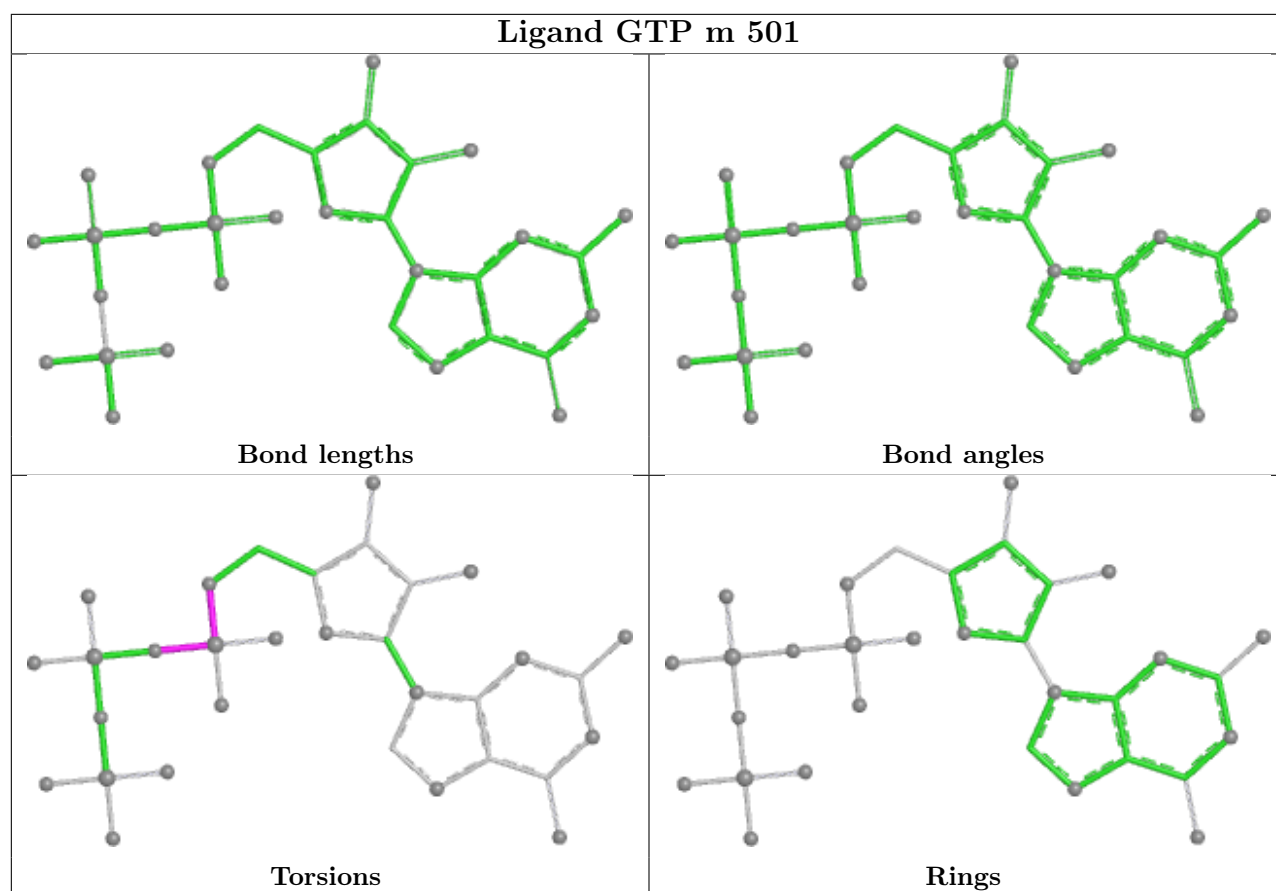
Ligand GTP s 501

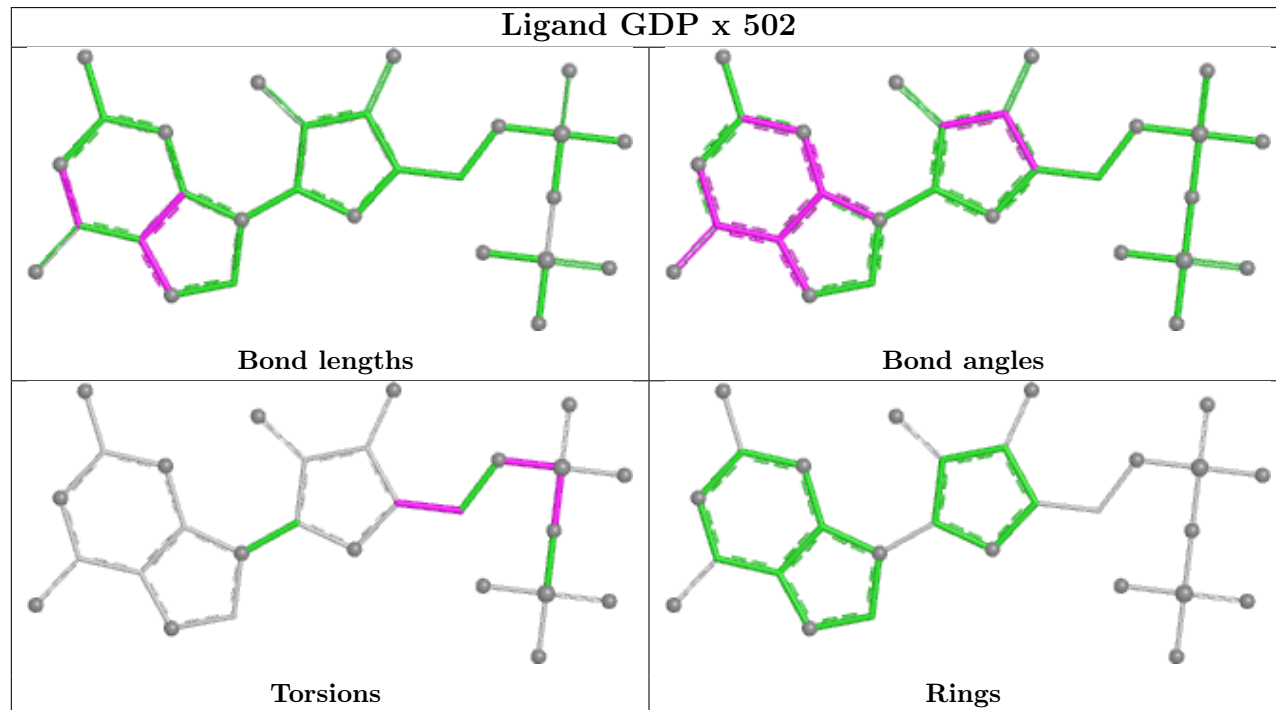
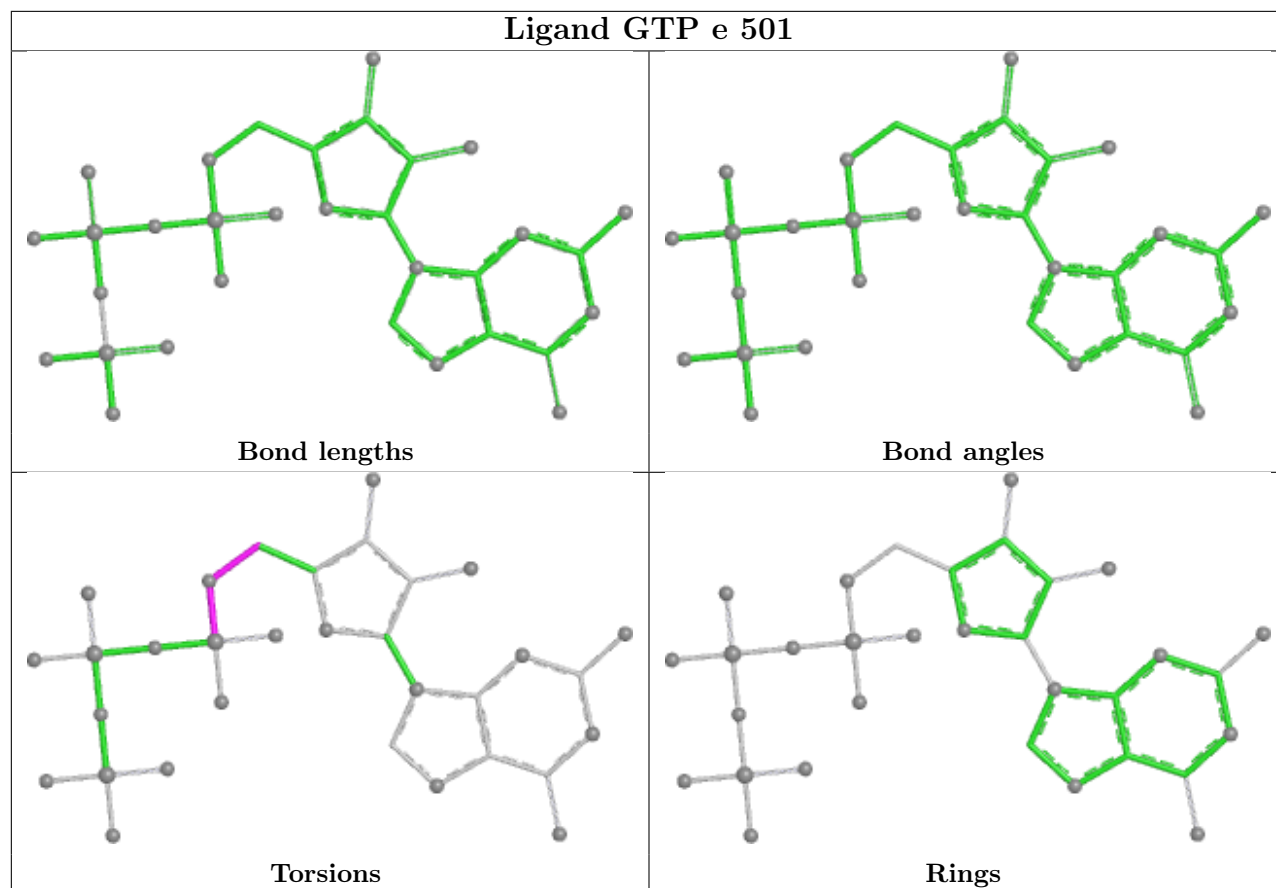


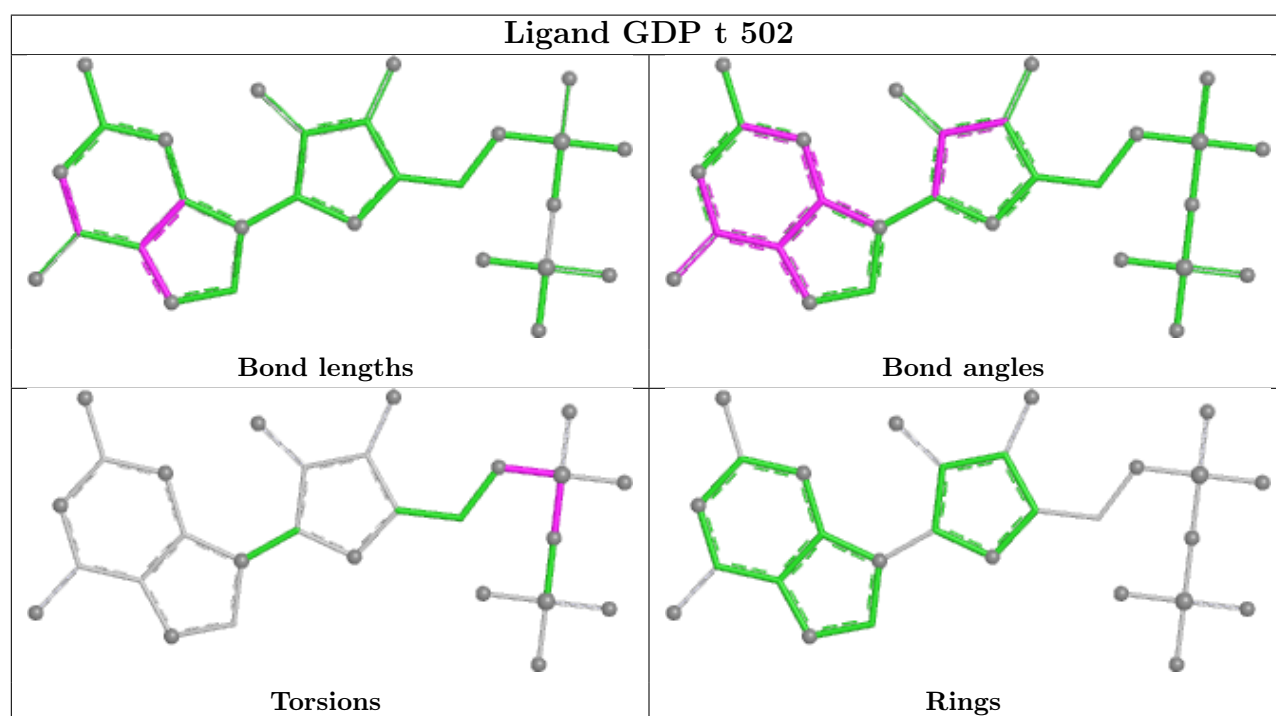
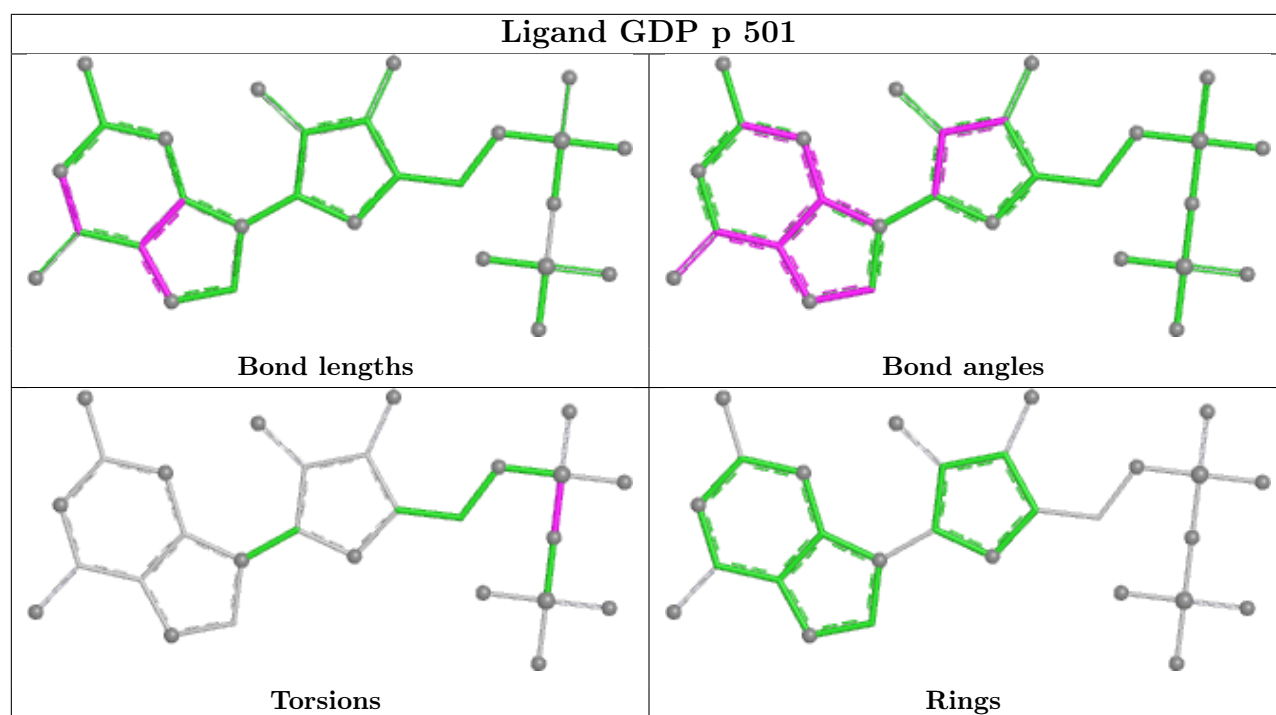


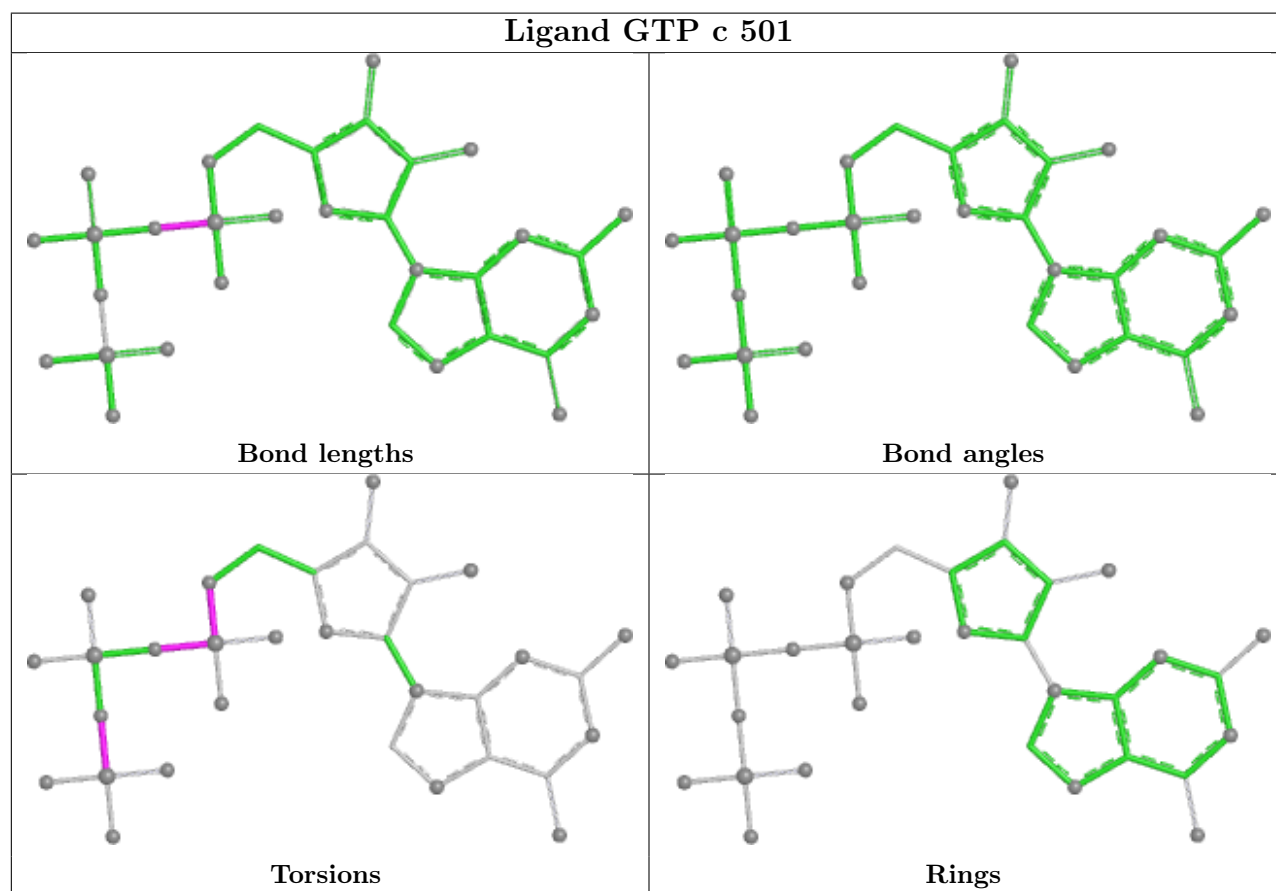
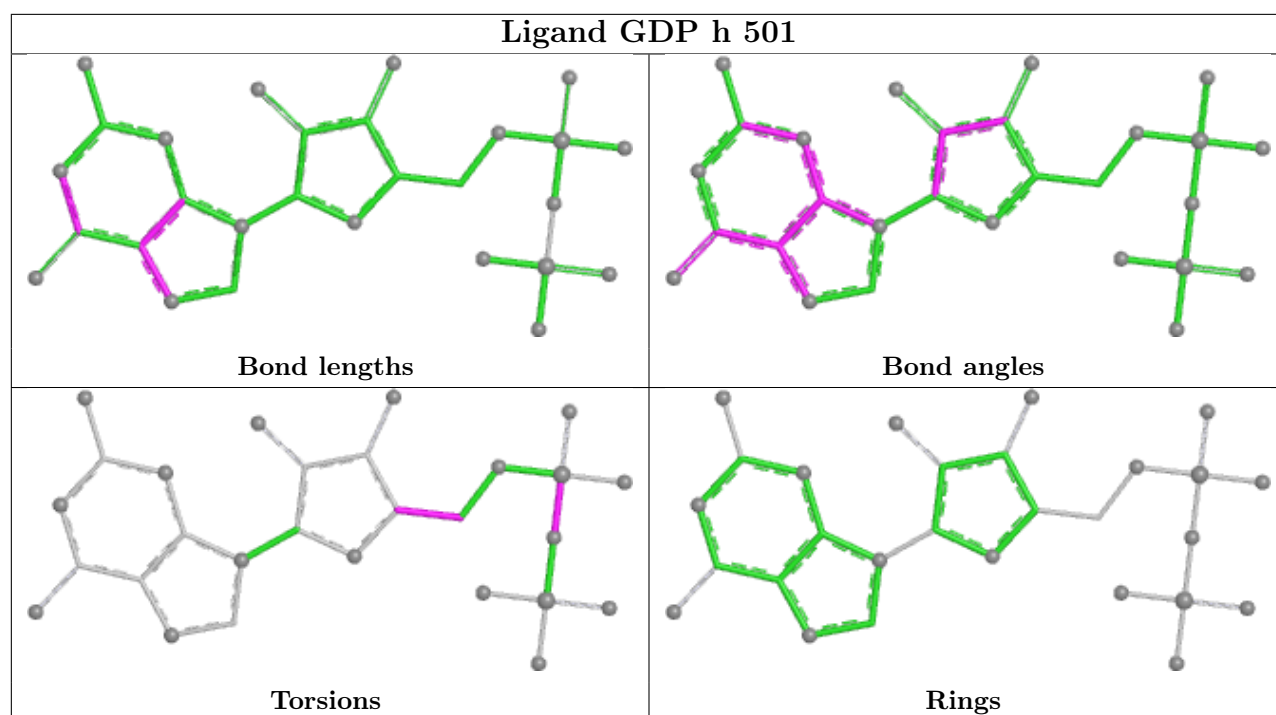




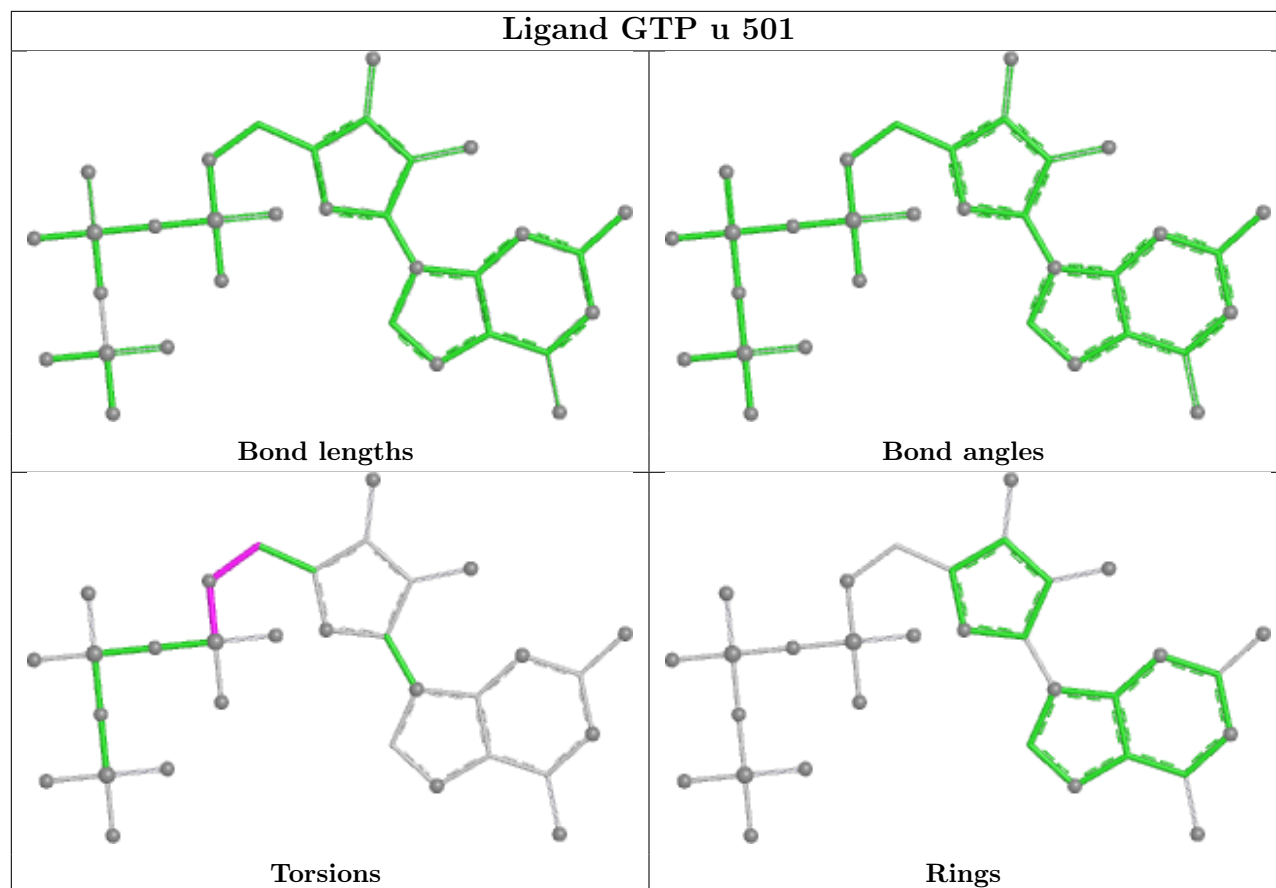




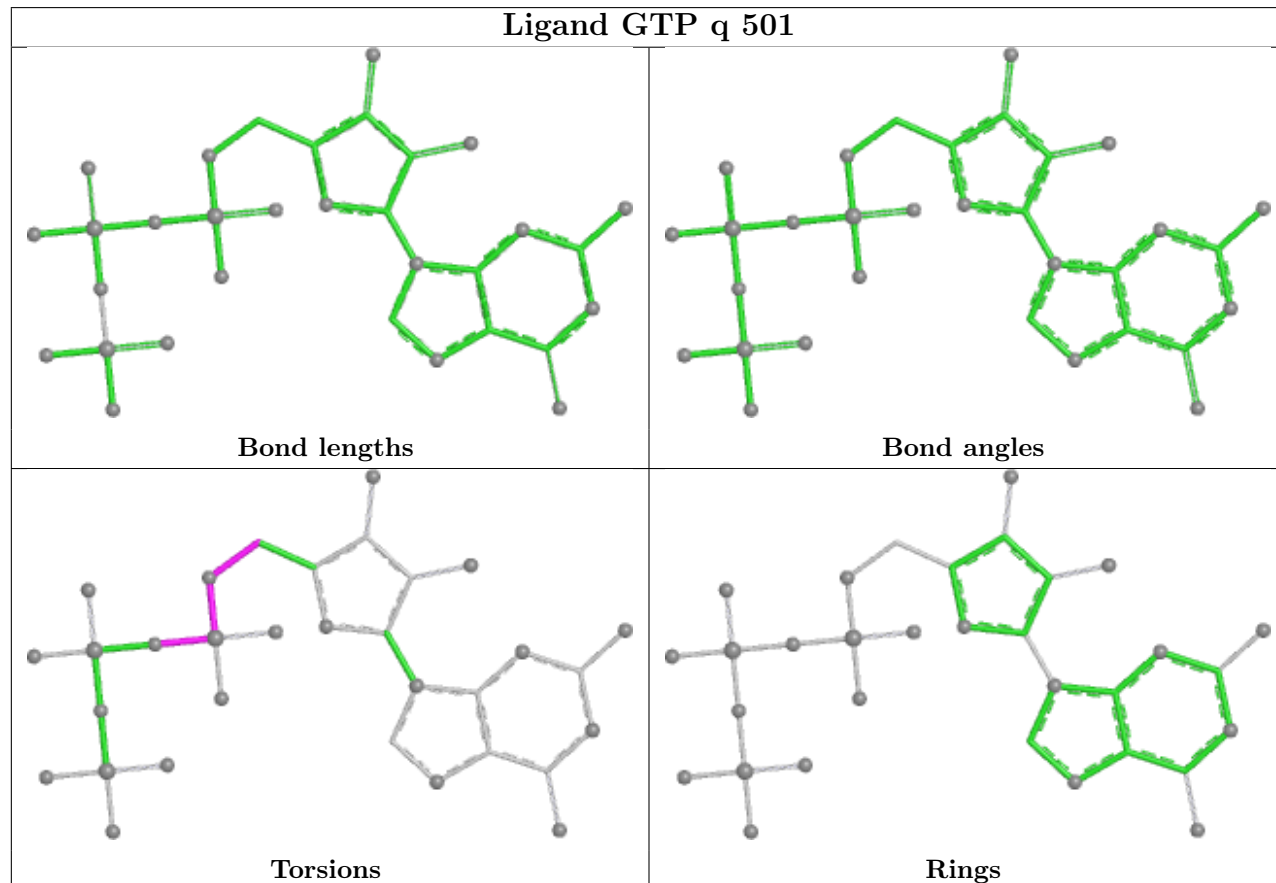


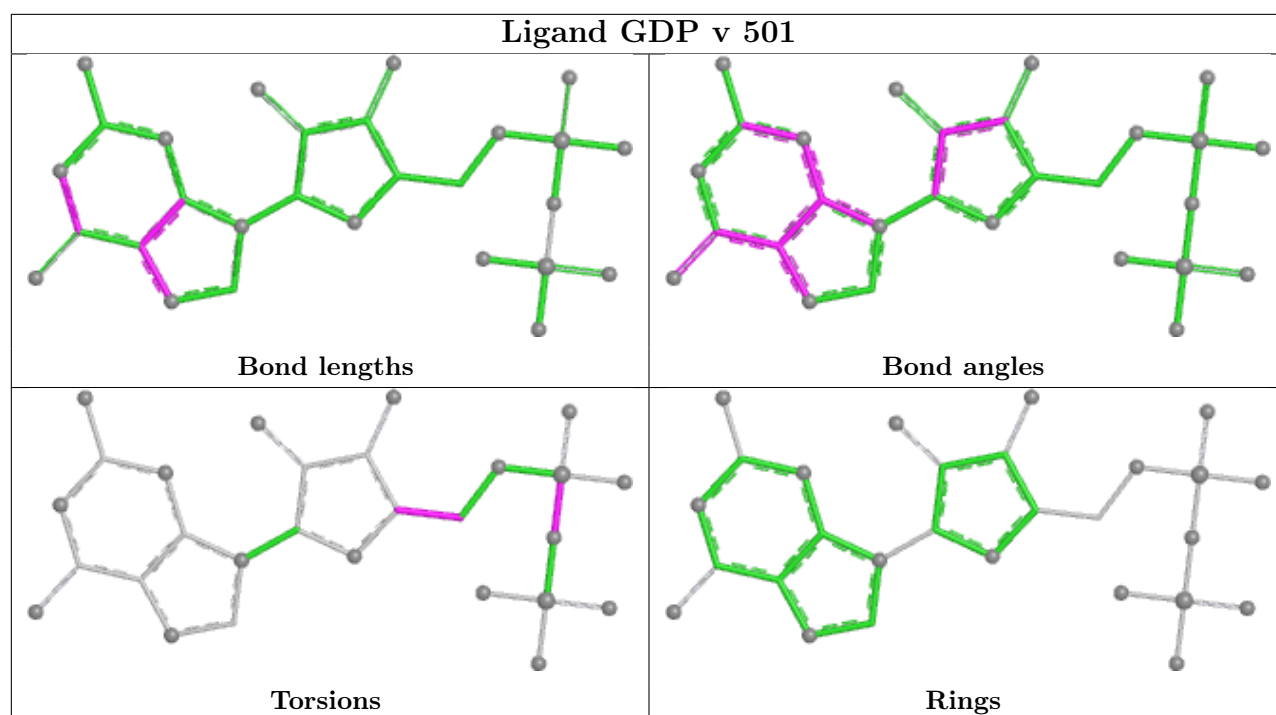


Ligand GTP u 501



Ligand GTP q 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

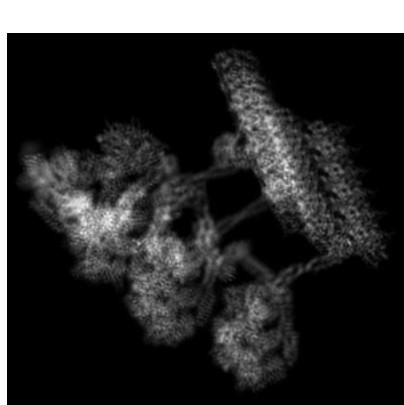
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22677. These allow visual inspection of the internal detail of the map and identification of artifacts.

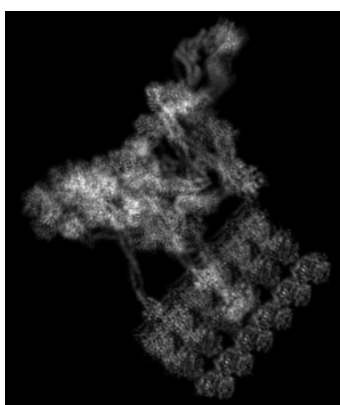
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

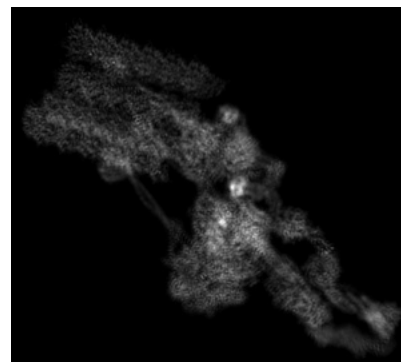
6.1.1 Primary map



X



Y



Z

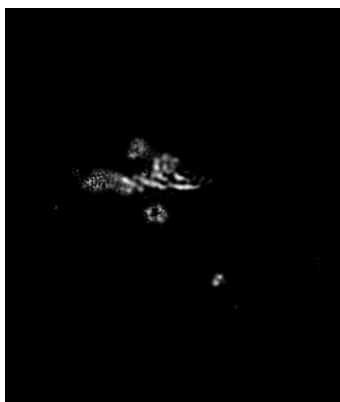
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 199



Y Index: 179



Z Index: 168

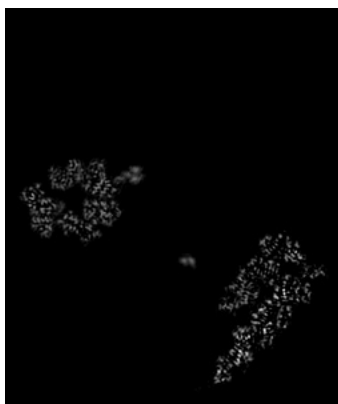
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

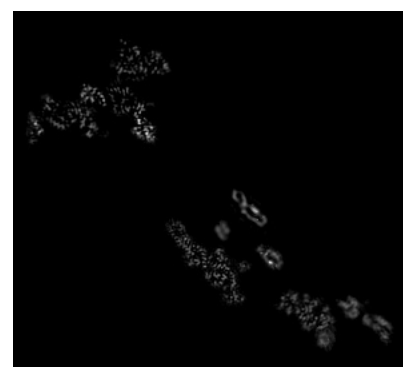
6.3.1 Primary map



X Index: 222



Y Index: 223

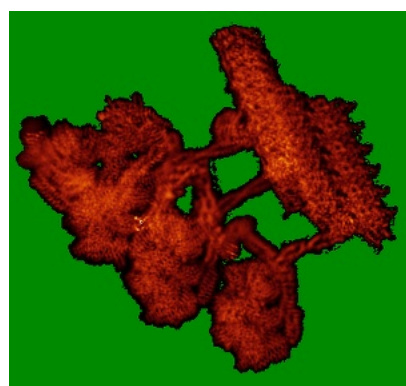


Z Index: 191

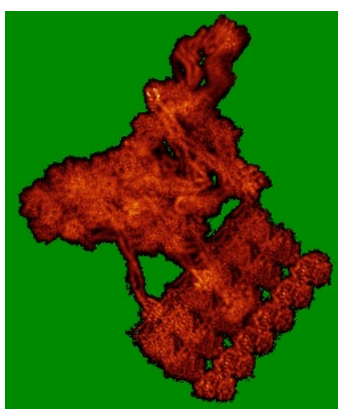
The images above show the largest variance slices of the map in three orthogonal directions.

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

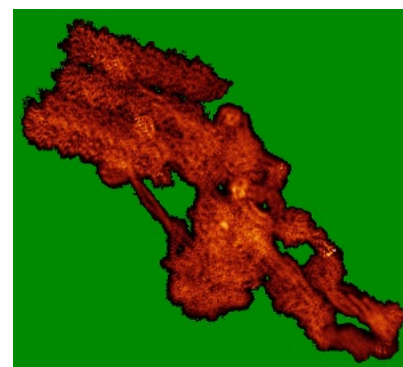
6.4.1 Primary map



X



Y

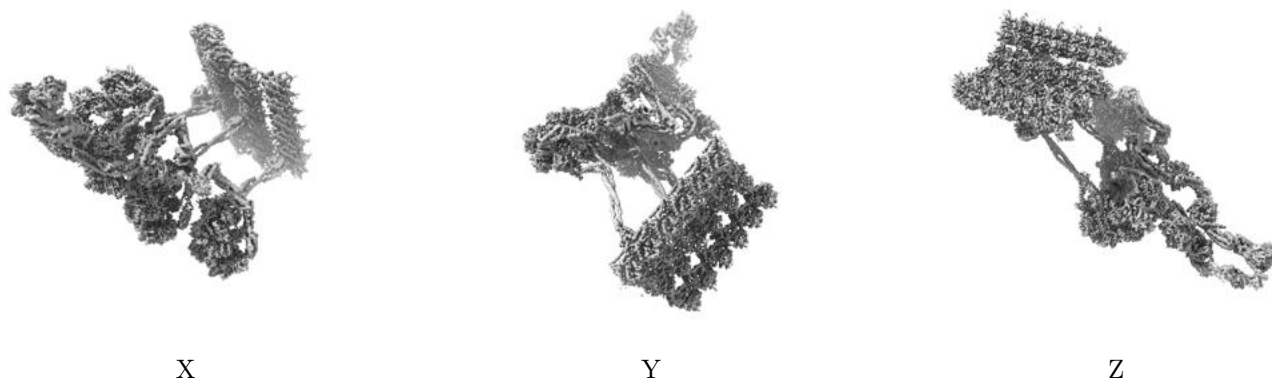


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

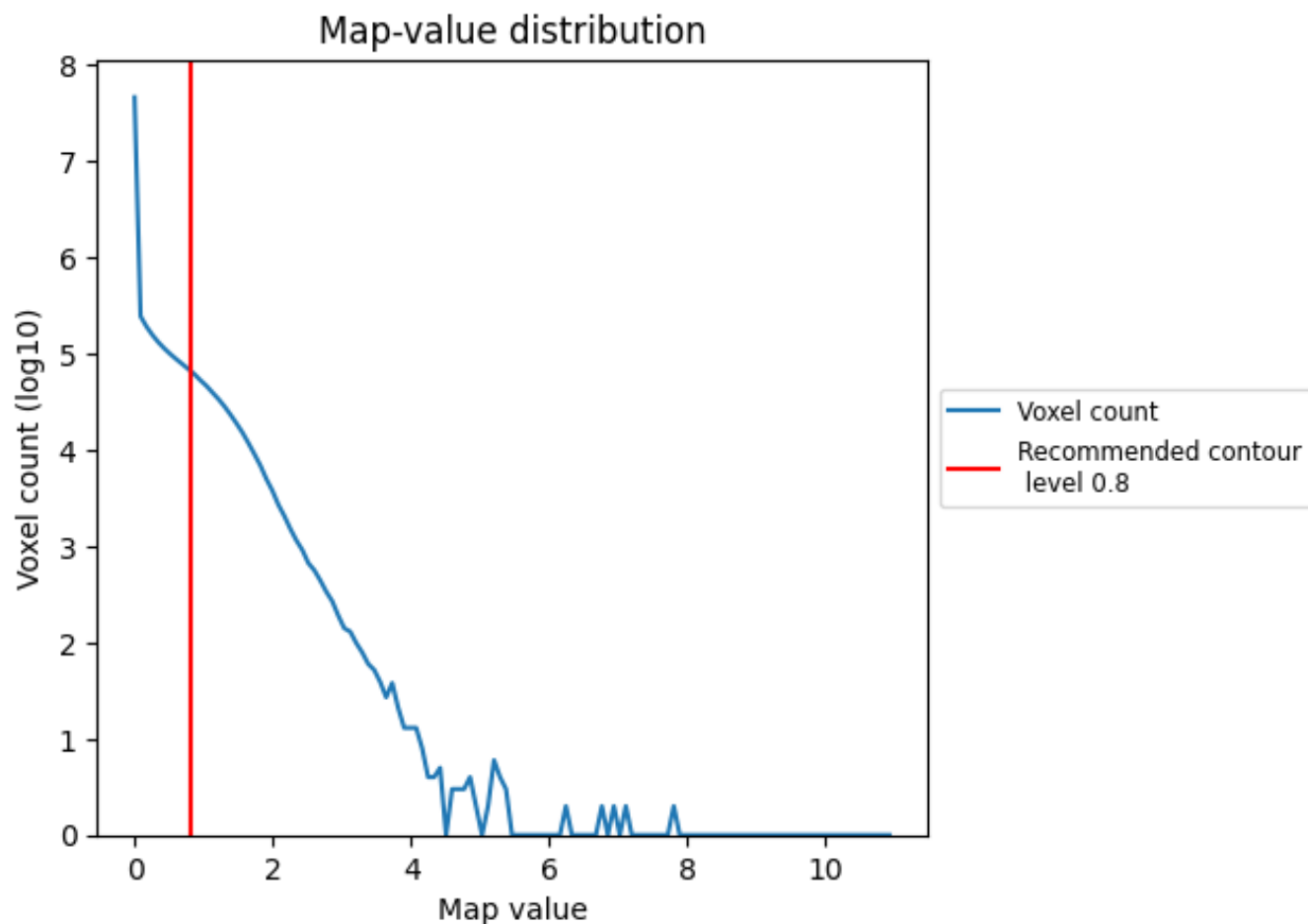
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

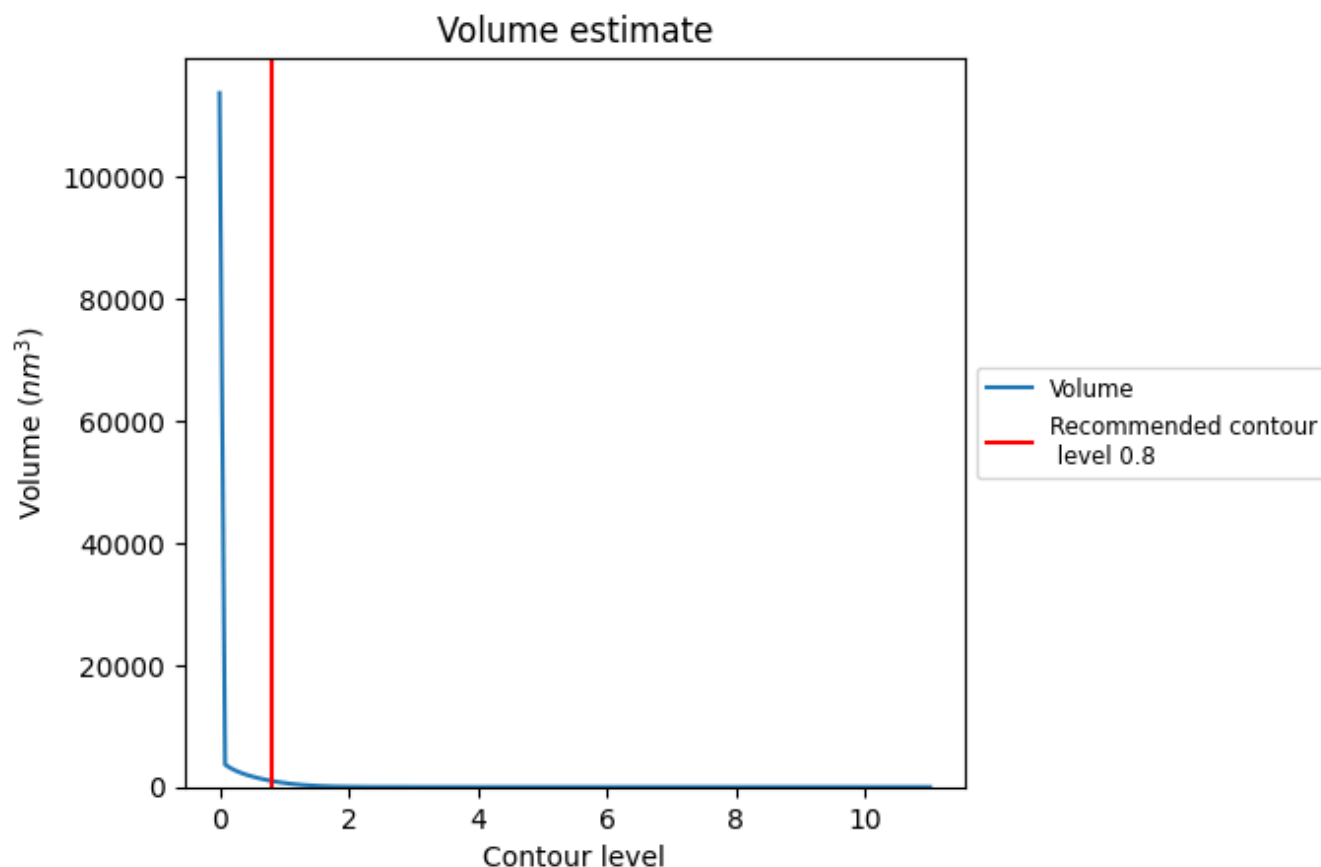
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1003 nm^3 ; this corresponds to an approximate mass of 906 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

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

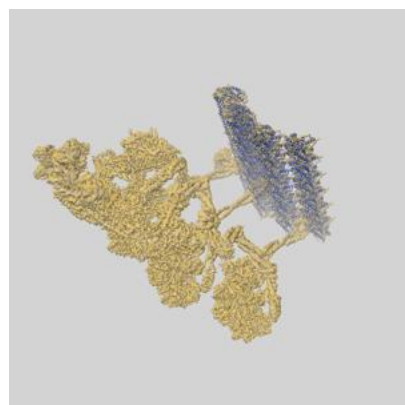
8 Fourier-Shell correlation ⓘ

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

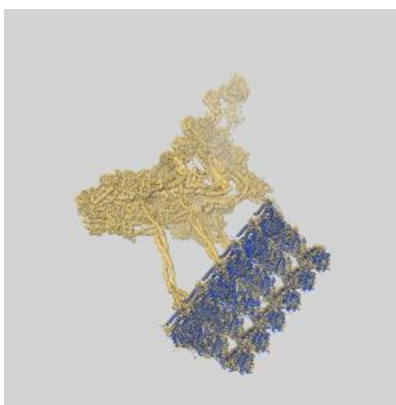
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22677 and PDB model 7N32. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

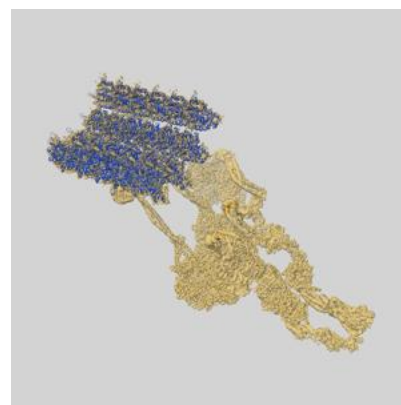
9.1 Map-model overlay [i](#)



X



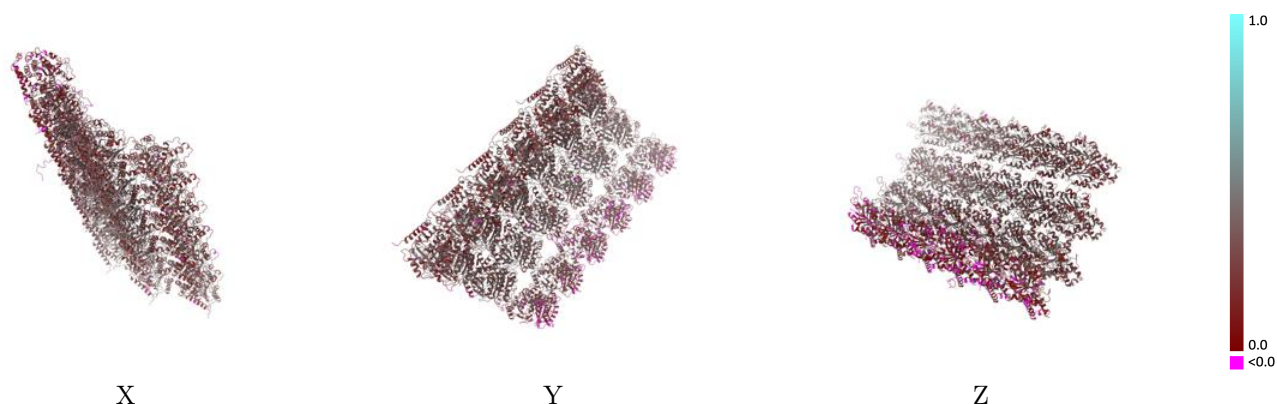
Y



Z

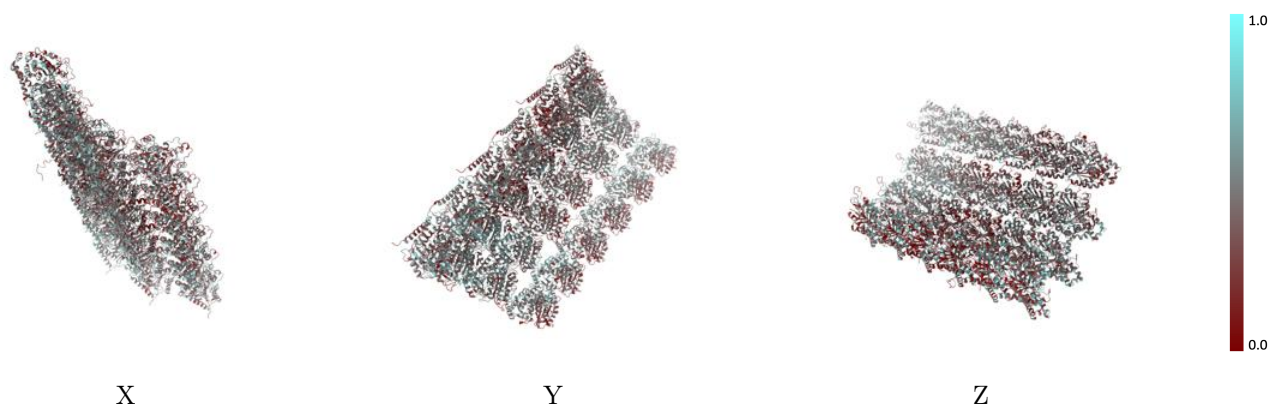
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



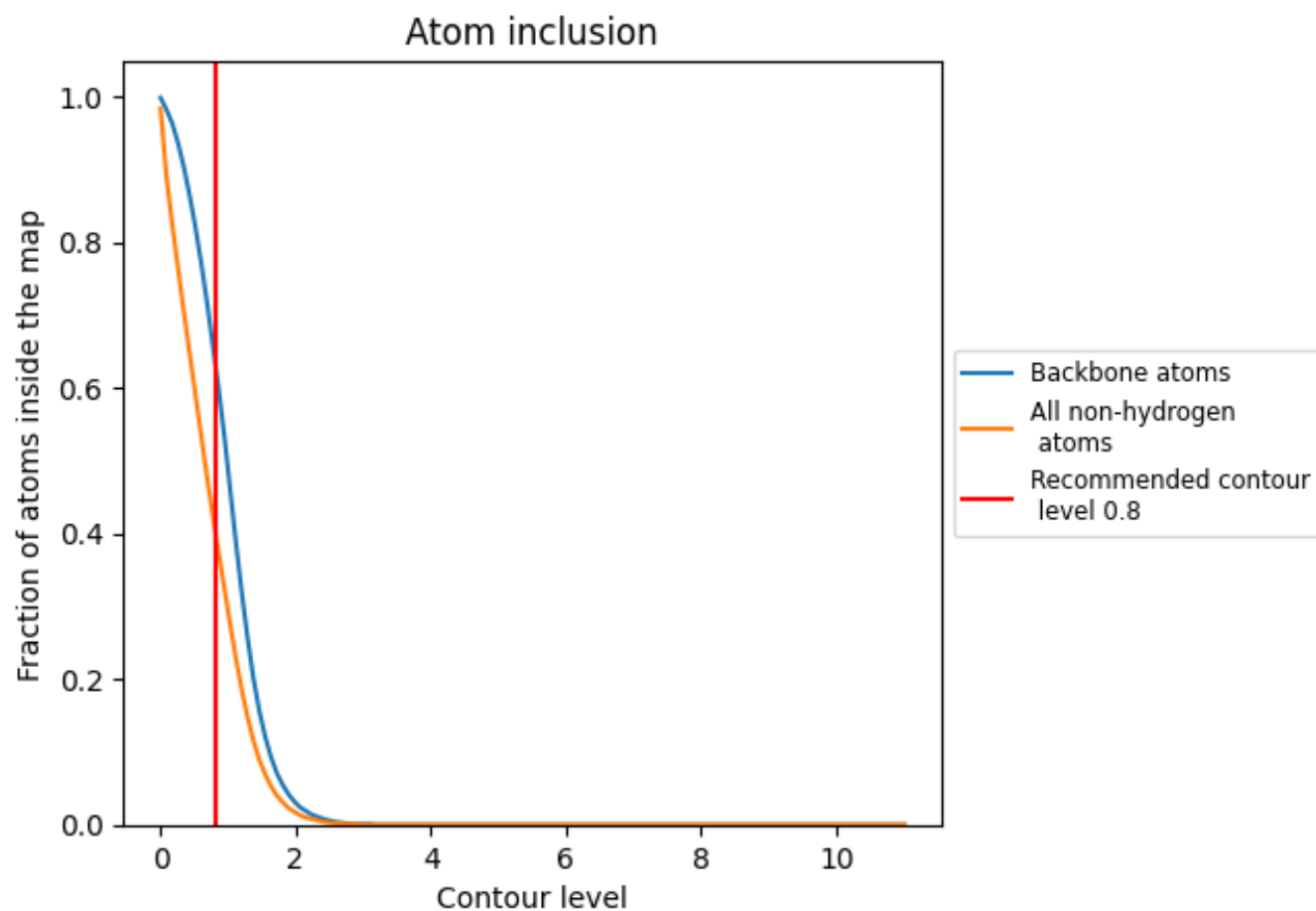
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 41% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4080	 0.2820
a	 0.4070	 0.1760
b	 0.4490	 0.2160
c	 0.3280	 0.1470
d	 0.3560	 0.1580
e	 0.4220	 0.2070
f	 0.4240	 0.2020
g	 0.4560	 0.3130
h	 0.4750	 0.3370
i	 0.3610	 0.3110
j	 0.3550	 0.3090
k	 0.4200	 0.3150
l	 0.4400	 0.3140
m	 0.4440	 0.3000
n	 0.4740	 0.3080
o	 0.3420	 0.3320
p	 0.3820	 0.3570
q	 0.4160	 0.3220
r	 0.4350	 0.3120
s	 0.4300	 0.3040
t	 0.4700	 0.3130
u	 0.3990	 0.2990
v	 0.4090	 0.3090
w	 0.3240	 0.2990
x	 0.3840	 0.3030

