Full wwPDB EM Validation Report ⓘ

Jan 21, 2023 – 08:02 pm GMT

PDB ID	:	8C5C
EMDB ID	:	EMD-16435
Title	:	microtubule decorated with tubulin oligomers in presence of APC C-terminal domain. (here only map corresponding to the 13-pf microtubule is represented)
Authors	:	Serre, L.; Arnal, I.
Deposited on	:	2023-01-06
Resolution	:	5.30 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

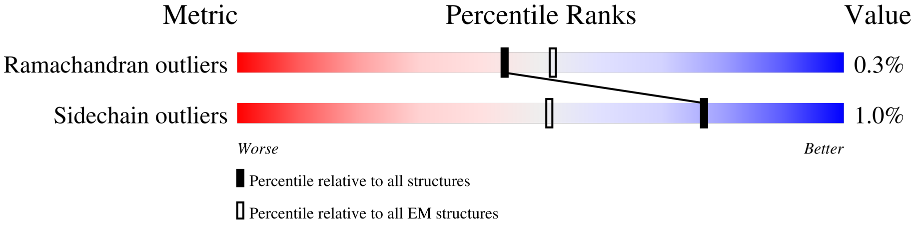
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

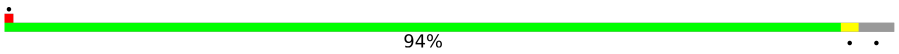
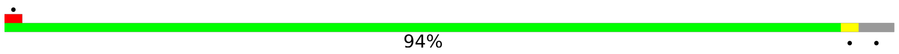
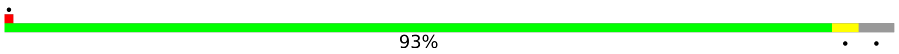
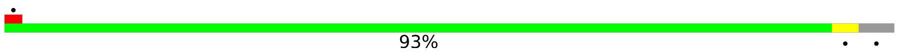
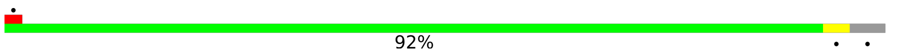
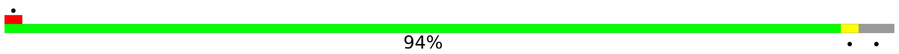
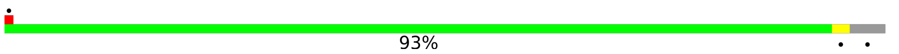
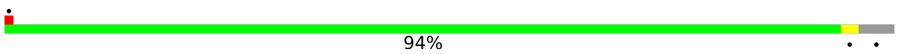
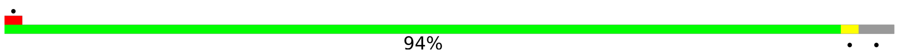
The reported resolution of this entry is 5.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



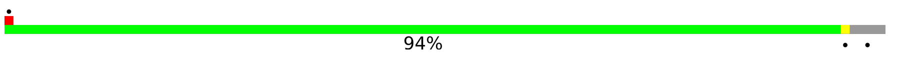
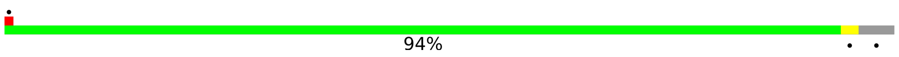
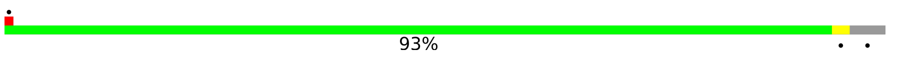
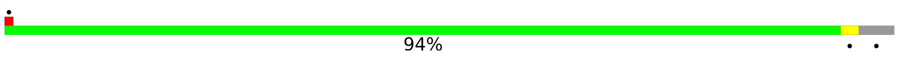
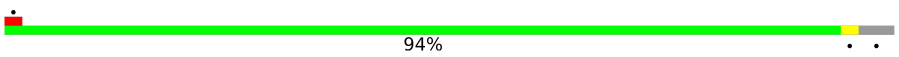
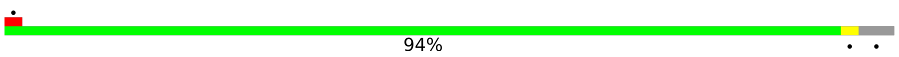
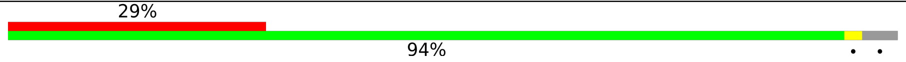
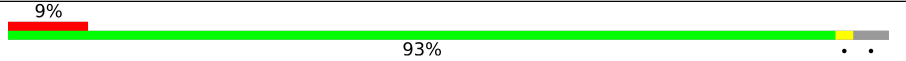
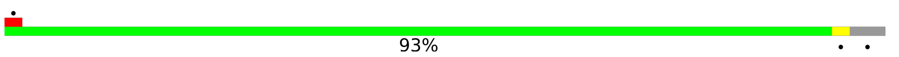
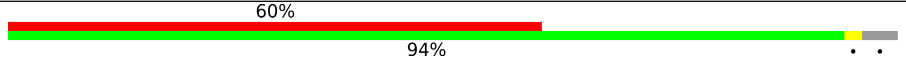
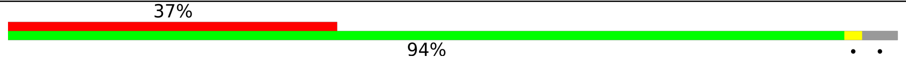
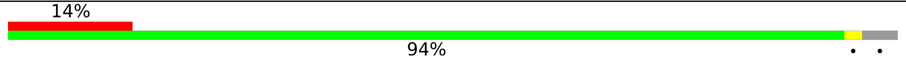
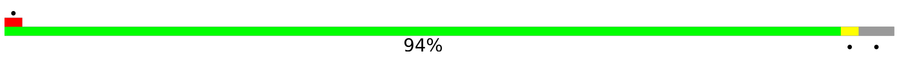
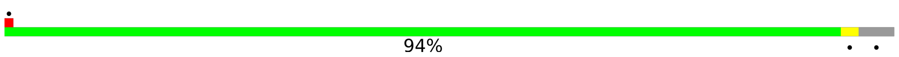
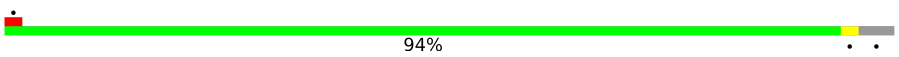
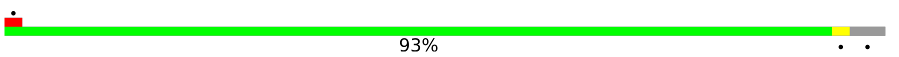
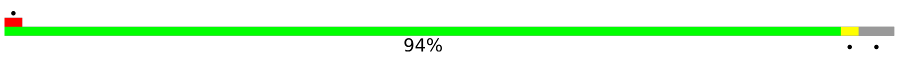
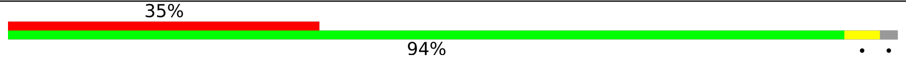
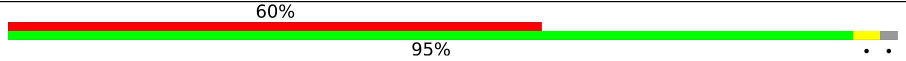
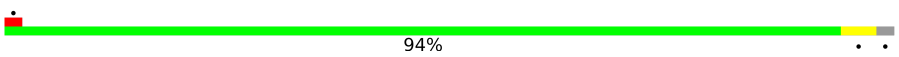
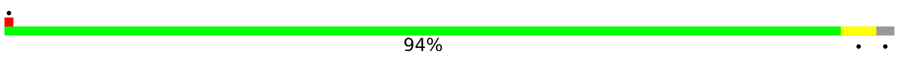
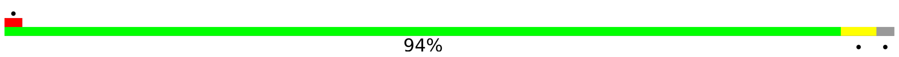
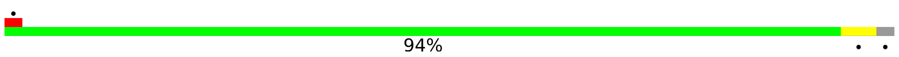
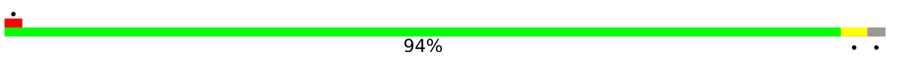
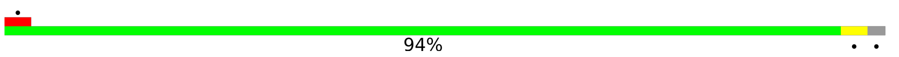
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	446	
1	b	446	
1	c	446	
1	d	446	
1	e	446	
1	f	446	
1	g	446	
1	h	446	
1	i	446	

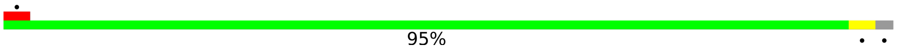
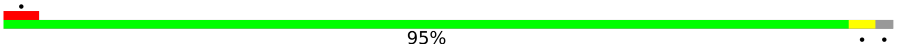
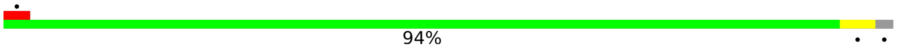
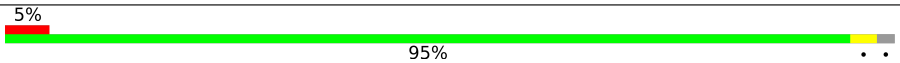
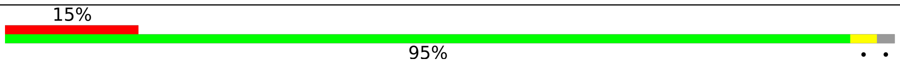
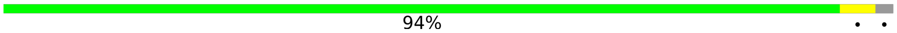
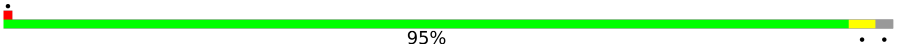
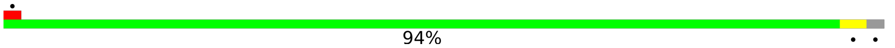
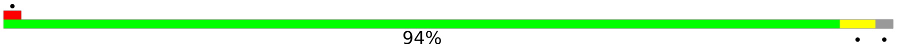
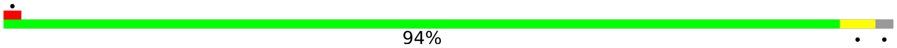
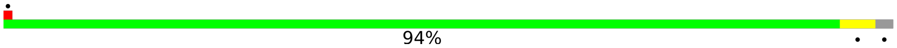
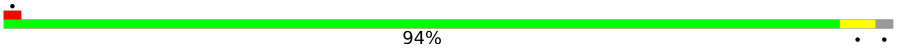
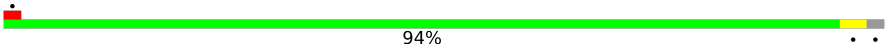
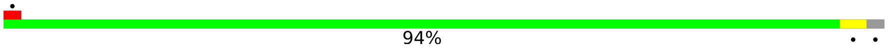
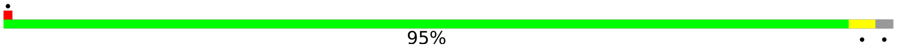
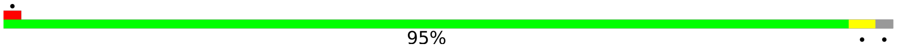
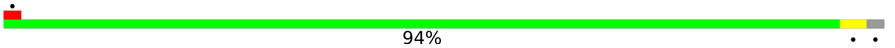
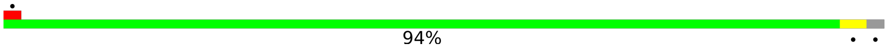
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	j	446	
1	k	446	
1	l	446	
1	m	446	
1	n	446	
1	o	446	
1	p	446	
1	q	446	
1	r	446	
1	s	446	
1	t	446	
1	u	446	
1	v	446	
1	w	446	
1	x	446	
1	y	446	
1	z	446	
2	A	451	
2	B	451	
2	C	451	
2	D	451	
2	E	451	
2	F	451	
2	G	451	
2	H	451	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	451	
2	J	451	
2	K	451	
2	L	451	
2	M	451	
2	N	451	
2	O	451	
2	P	451	
2	Q	451	
2	R	451	
2	S	451	
2	T	451	
2	U	451	
2	V	451	
2	W	451	
2	X	451	
2	Y	451	
2	Z	451	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 178971 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 beta chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	a	429	Total C N O S 3376 2119 578 652 27	0	0
1	b	429	Total C N O S 3376 2119 578 652 27	0	0
1	c	429	Total C N O S 3376 2119 578 652 27	0	0
1	d	429	Total C N O S 3376 2119 578 652 27	0	0
1	e	429	Total C N O S 3376 2119 578 652 27	0	0
1	f	429	Total C N O S 3376 2119 578 652 27	0	0
1	g	429	Total C N O S 3376 2119 578 652 27	0	0
1	h	429	Total C N O S 3376 2119 578 652 27	0	0
1	i	429	Total C N O S 3376 2119 578 652 27	0	0
1	j	429	Total C N O S 3376 2119 578 652 27	0	0
1	k	429	Total C N O S 3376 2119 578 652 27	0	0
1	l	429	Total C N O S 3376 2119 578 652 27	0	0
1	m	429	Total C N O S 3376 2119 578 652 27	0	0
1	n	429	Total C N O S 3376 2119 578 652 27	0	0
1	o	429	Total C N O S 3376 2119 578 652 27	0	0
1	p	429	Total C N O S 3376 2119 578 652 27	0	0
1	q	429	Total C N O S 3376 2119 578 652 27	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	r	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	s	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	t	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	u	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	v	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	w	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	x	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	y	429	Total 3376	C 2119	N 578	O 652	S 27	0	0
1	z	429	Total 3376	C 2119	N 578	O 652	S 27	0	0

- Molecule 2 is a protein called Tubulin alpha-1B chain.

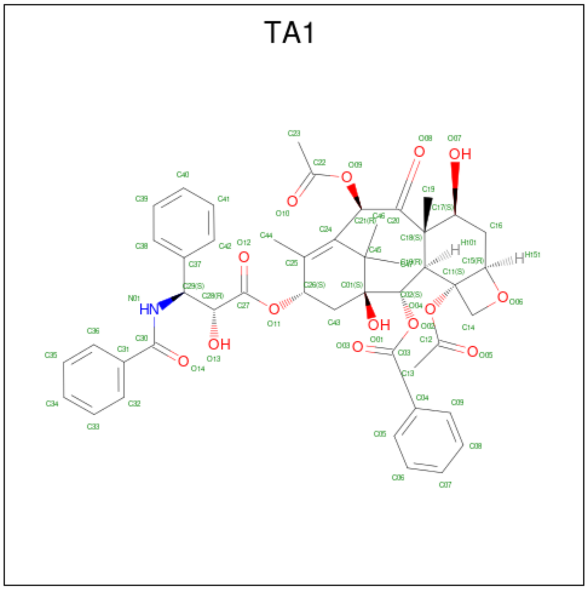
Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	O	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	P	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	Q	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	R	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	S	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	T	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	U	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	V	441	Total 3446	C 2180	N 585	O 659	S 22	0	0
2	W	441	Total 3446	C 2180	N 585	O 659	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf	Trace
2	X	441	Total C N O S 3446 2180 585 659 22	0	0
2	Y	441	Total C N O S 3446 2180 585 659 22	0	0
2	Z	441	Total C N O S 3446 2180 585 659 22	0	0
2	A	441	Total C N O S 3446 2180 585 659 22	0	0
2	B	441	Total C N O S 3446 2180 585 659 22	0	0
2	C	441	Total C N O S 3446 2180 585 659 22	0	0
2	D	441	Total C N O S 3446 2180 585 659 22	0	0
2	E	441	Total C N O S 3446 2180 585 659 22	0	0
2	F	441	Total C N O S 3446 2180 585 659 22	0	0
2	G	441	Total C N O S 3446 2180 585 659 22	0	0
2	H	441	Total C N O S 3446 2180 585 659 22	0	0
2	I	441	Total C N O S 3446 2180 585 659 22	0	0
2	J	441	Total C N O S 3446 2180 585 659 22	0	0
2	K	441	Total C N O S 3446 2180 585 659 22	0	0
2	L	441	Total C N O S 3446 2180 585 659 22	0	0
2	M	441	Total C N O S 3446 2180 585 659 22	0	0

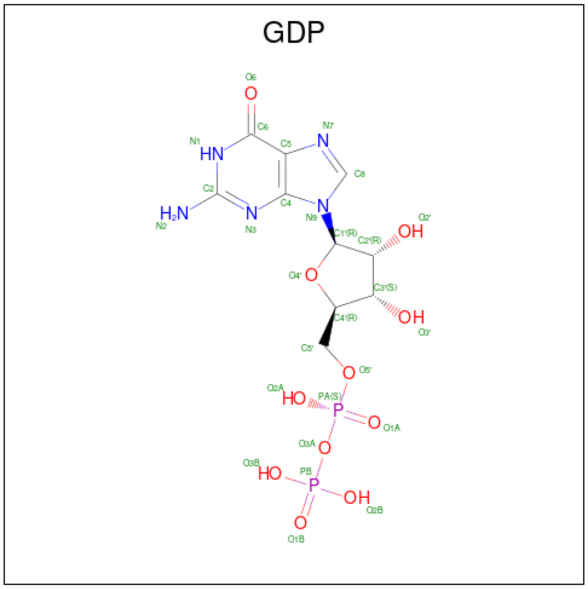
- Molecule 3 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	a	1	Total C N O 62 47 1 14	0
3	b	1	Total C N O 62 47 1 14	0
3	c	1	Total C N O 62 47 1 14	0
3	d	1	Total C N O 62 47 1 14	0
3	e	1	Total C N O 62 47 1 14	0
3	f	1	Total C N O 62 47 1 14	0
3	g	1	Total C N O 62 47 1 14	0
3	h	1	Total C N O 62 47 1 14	0
3	i	1	Total C N O 62 47 1 14	0
3	j	1	Total C N O 62 47 1 14	0
3	k	1	Total C N O 62 47 1 14	0
3	l	1	Total C N O 62 47 1 14	0
3	m	1	Total C N O 62 47 1 14	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

$C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).

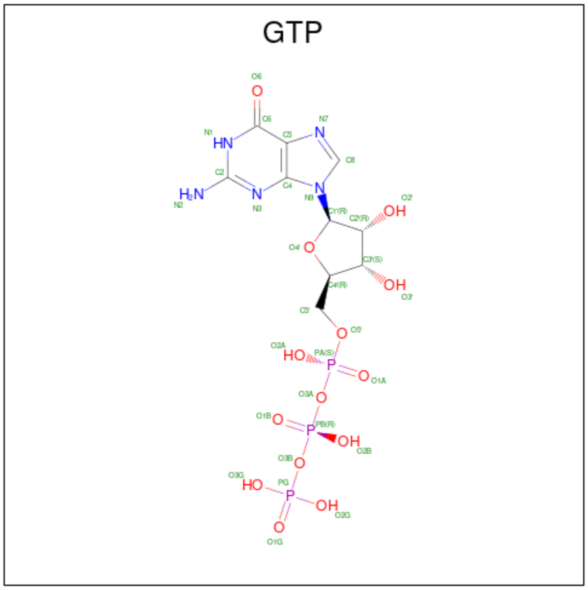


Mol	Chain	Residues	Atoms					AltConf
4	a	1	Total 28	C 10	N 5	O 11	P 2	0
4	b	1	Total 28	C 10	N 5	O 11	P 2	0
4	c	1	Total 28	C 10	N 5	O 11	P 2	0
4	d	1	Total 28	C 10	N 5	O 11	P 2	0
4	e	1	Total 28	C 10	N 5	O 11	P 2	0
4	f	1	Total 28	C 10	N 5	O 11	P 2	0
4	g	1	Total 28	C 10	N 5	O 11	P 2	0
4	h	1	Total 28	C 10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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	N	1	Total Mg 1 1	0
5	O	1	Total Mg 1 1	0
5	P	1	Total Mg 1 1	0
5	Q	1	Total Mg 1 1	0
5	R	1	Total Mg 1 1	0
5	S	1	Total Mg 1 1	0
5	T	1	Total Mg 1 1	0
5	U	1	Total Mg 1 1	0
5	V	1	Total Mg 1 1	0
5	W	1	Total Mg 1 1	0
5	X	1	Total Mg 1 1	0
5	Y	1	Total Mg 1 1	0
5	Z	1	Total Mg 1 1	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



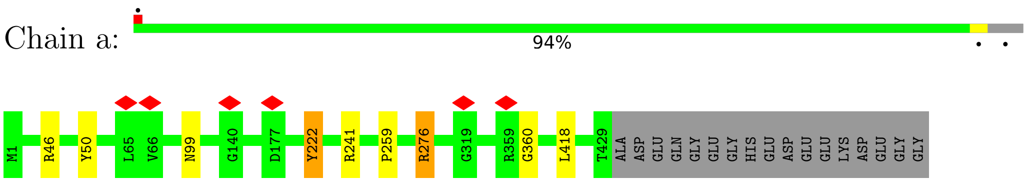
Mol	Chain	Residues	Atoms					AltConf
6	N	1	Total 32	C 10	N 5	O 14	P 3	0
6	O	1	Total 32	C 10	N 5	O 14	P 3	0
6	P	1	Total 32	C 10	N 5	O 14	P 3	0
6	Q	1	Total 32	C 10	N 5	O 14	P 3	0
6	R	1	Total 32	C 10	N 5	O 14	P 3	0
6	S	1	Total 32	C 10	N 5	O 14	P 3	0
6	T	1	Total 32	C 10	N 5	O 14	P 3	0
6	U	1	Total 32	C 10	N 5	O 14	P 3	0
6	V	1	Total 32	C 10	N 5	O 14	P 3	0
6	W	1	Total 32	C 10	N 5	O 14	P 3	0
6	X	1	Total 32	C 10	N 5	O 14	P 3	0
6	Y	1	Total 32	C 10	N 5	O 14	P 3	0
6	Z	1	Total 32	C 10	N 5	O 14	P 3	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

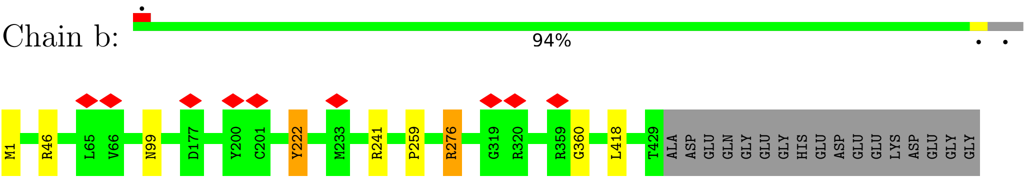
- Molecule 1: Tubulin beta chain

Chain a:



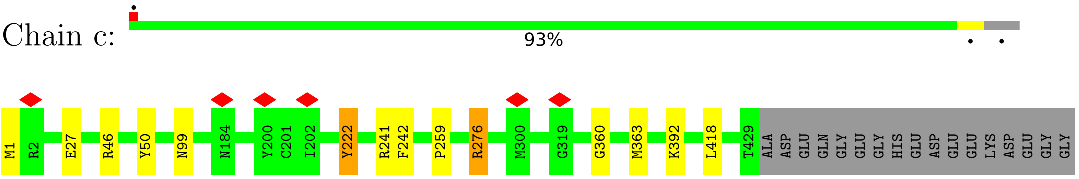
- Molecule 1: Tubulin beta chain

Chain b:



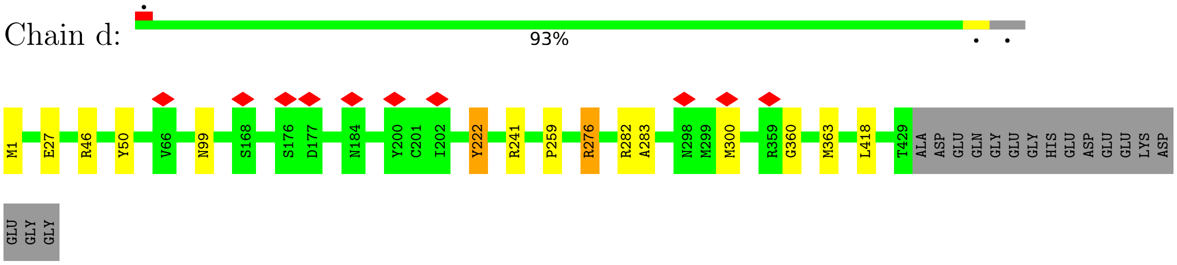
- Molecule 1: Tubulin beta chain

Chain c:



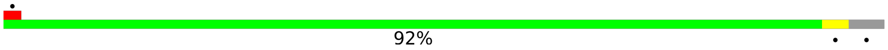
- Molecule 1: Tubulin beta chain

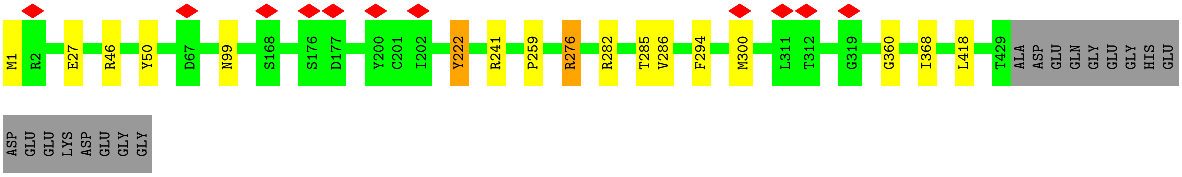
Chain d:



- Molecule 1: Tubulin beta chain

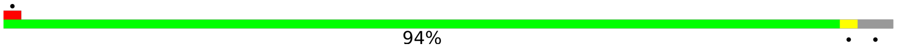
Chain e:





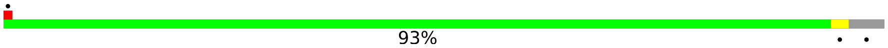
- Molecule 1: Tubulin beta chain

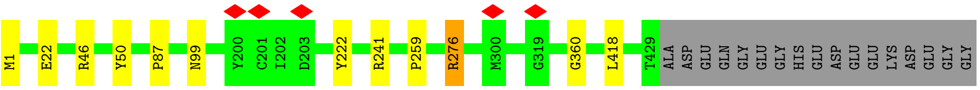
Chain f:



- Molecule 1: Tubulin beta chain

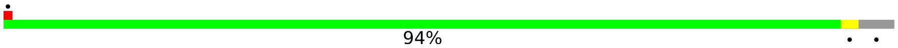
Chain g:

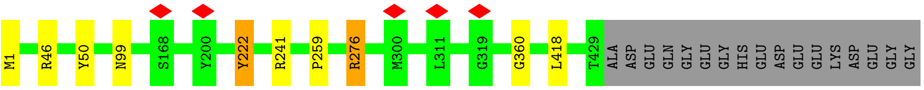




- Molecule 1: Tubulin beta chain

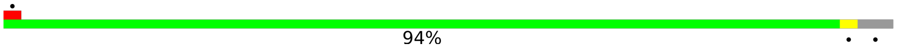
Chain h:

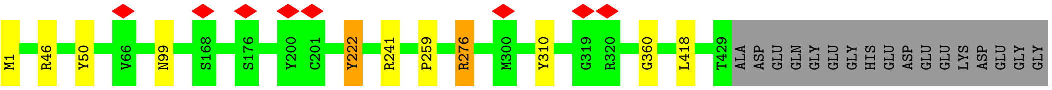




- Molecule 1: Tubulin beta chain

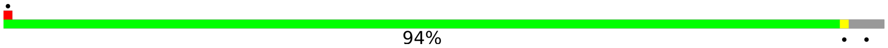
Chain i:

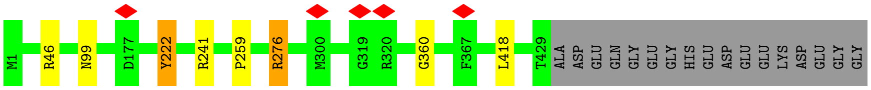




- Molecule 1: Tubulin beta chain

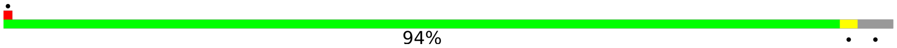
Chain j:

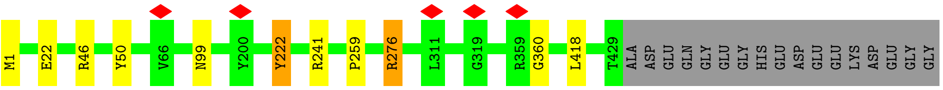




- Molecule 1: Tubulin beta chain

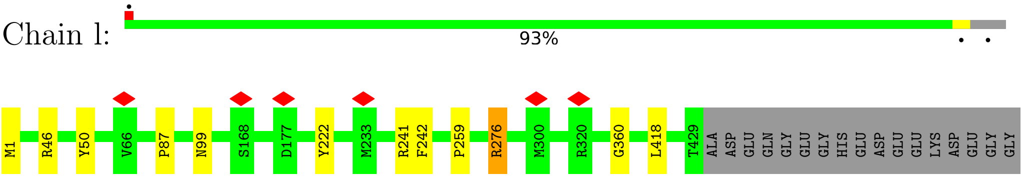
Chain k:





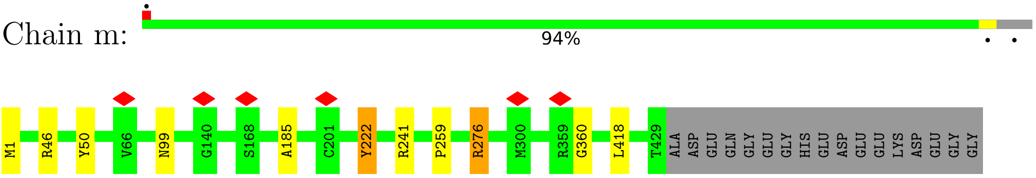
- Molecule 1: Tubulin beta chain

Chain l:



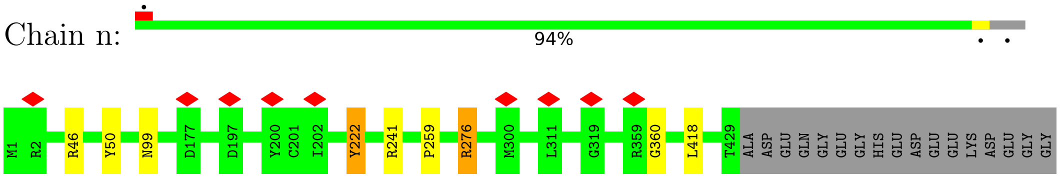
- Molecule 1: Tubulin beta chain

Chain m:



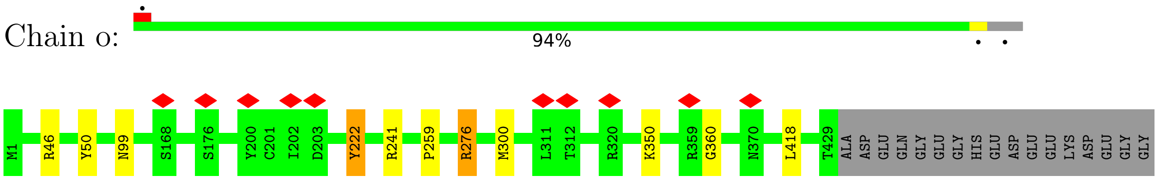
- Molecule 1: Tubulin beta chain

Chain n:



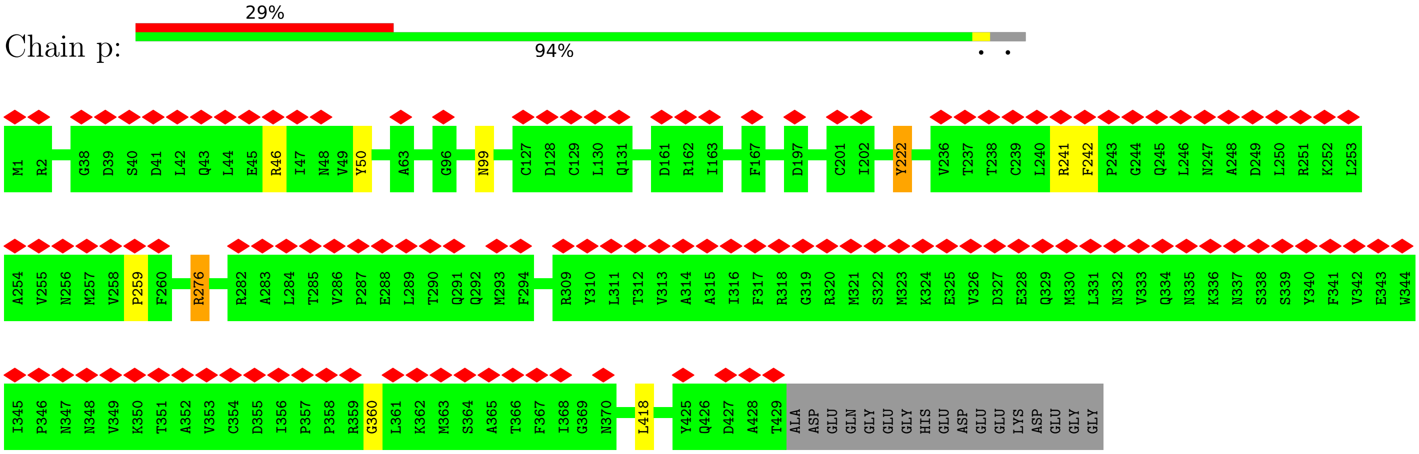
- Molecule 1: Tubulin beta chain

Chain o:



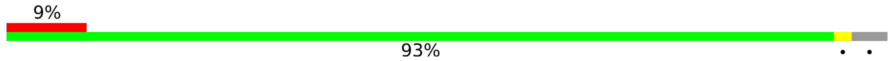
- Molecule 1: Tubulin beta chain

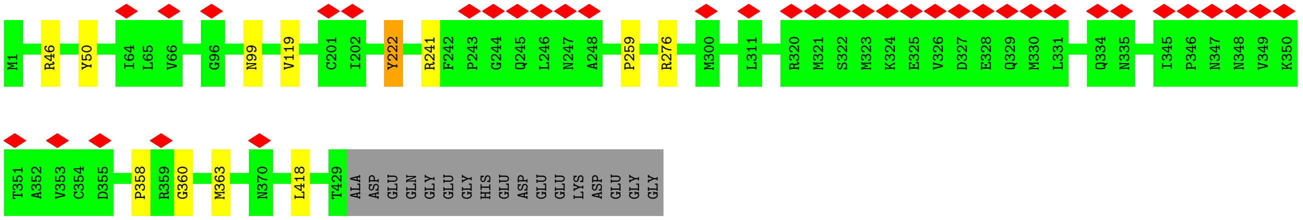
Chain p:



- Molecule 1: Tubulin beta chain

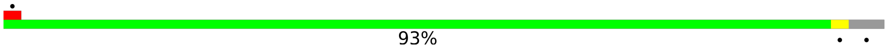
Chain q:

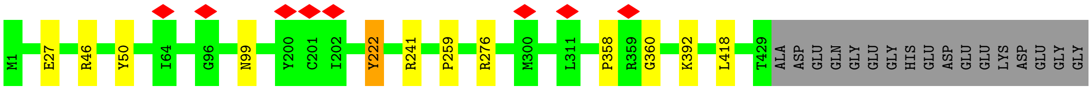




- Molecule 1: Tubulin beta chain

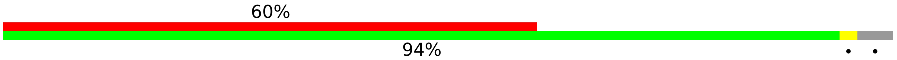
Chain r:

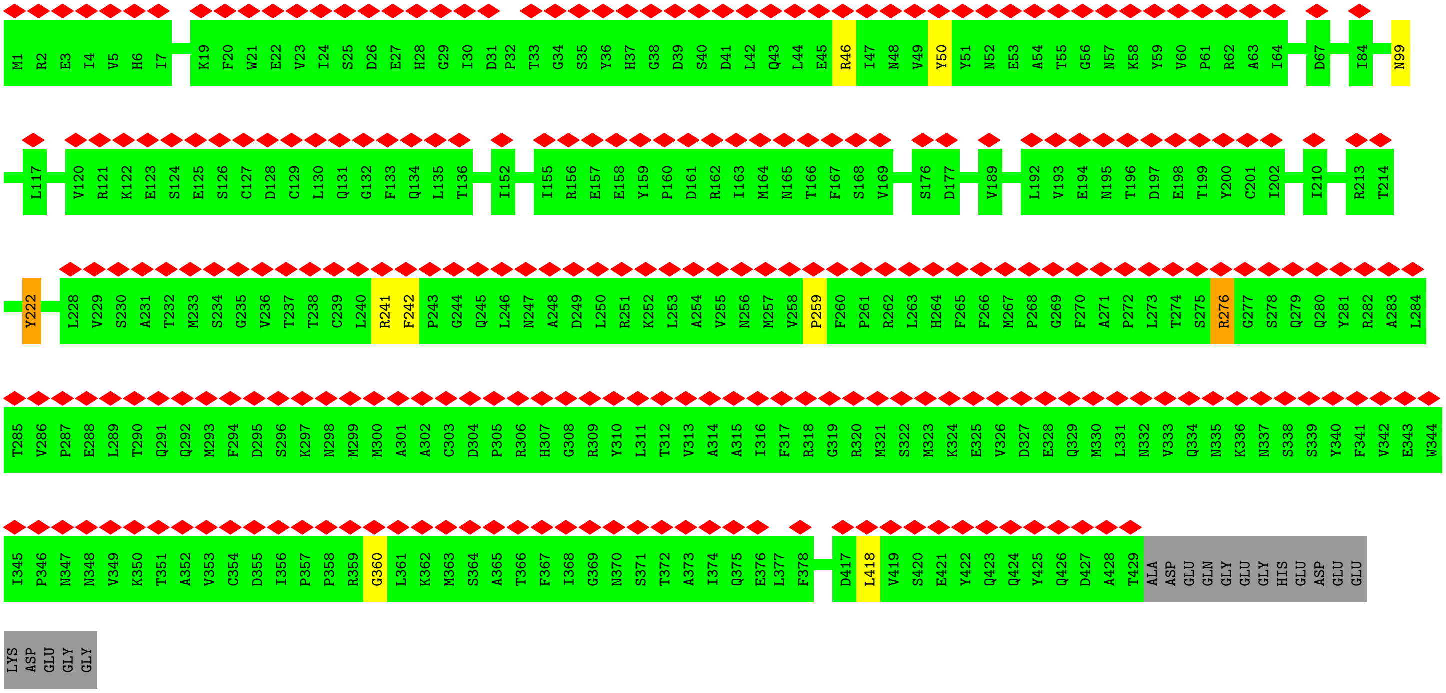




- Molecule 1: Tubulin beta chain

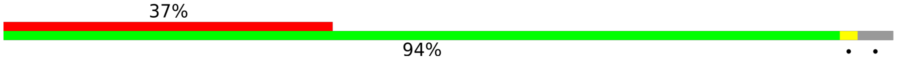
Chain s:

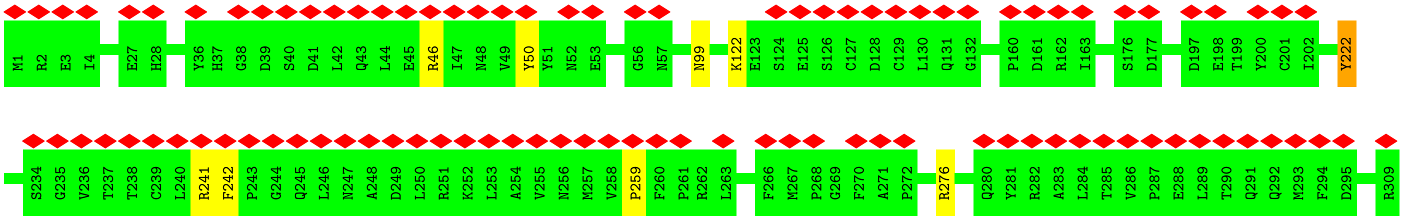


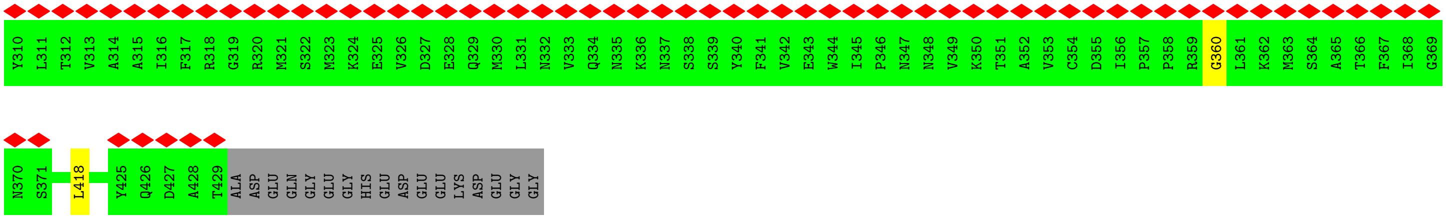


- Molecule 1: Tubulin beta chain

Chain t:

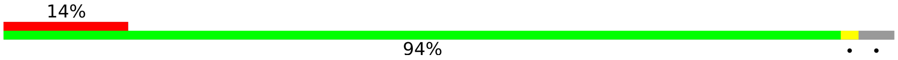


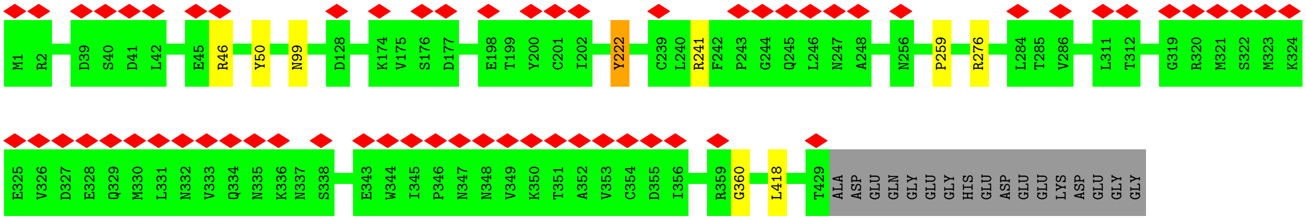




- Molecule 1: Tubulin beta chain

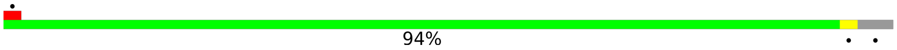
Chain u:

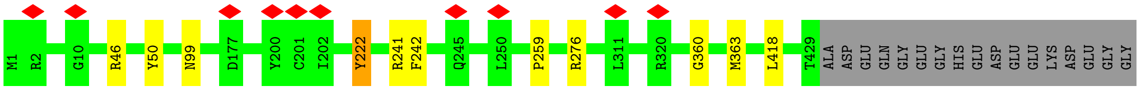




- Molecule 1: Tubulin beta chain

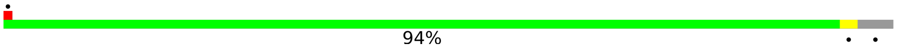
Chain v:

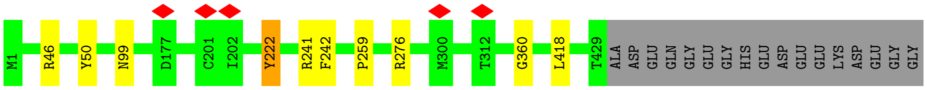




- Molecule 1: Tubulin beta chain

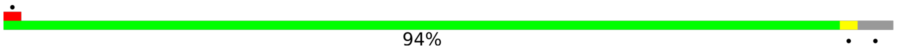
Chain w:

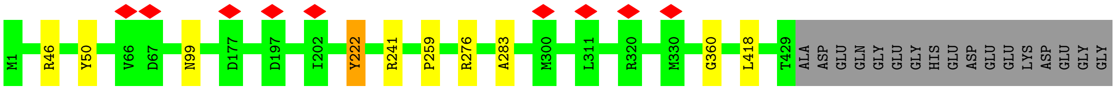




- Molecule 1: Tubulin beta chain

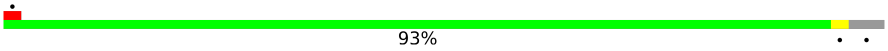
Chain x:

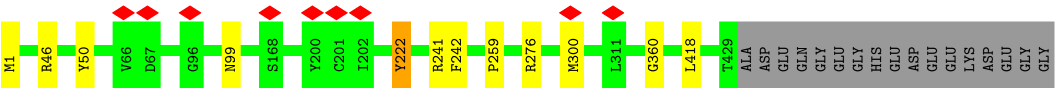




- Molecule 1: Tubulin beta chain

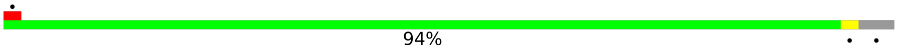
Chain y:

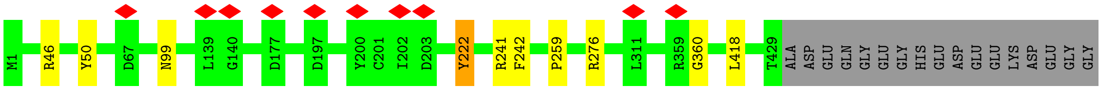




- Molecule 1: Tubulin beta chain

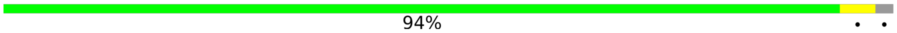
Chain z:

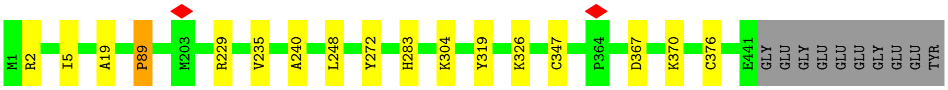




- Molecule 2: Tubulin alpha-1B chain

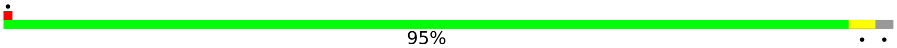
Chain N:

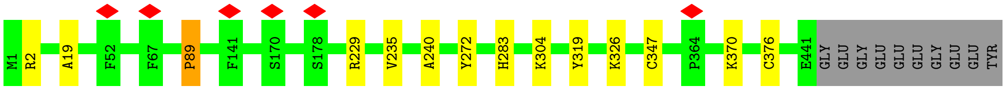




- Molecule 2: Tubulin alpha-1B chain

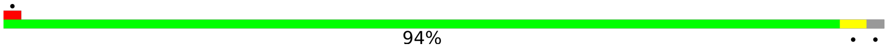
Chain O:

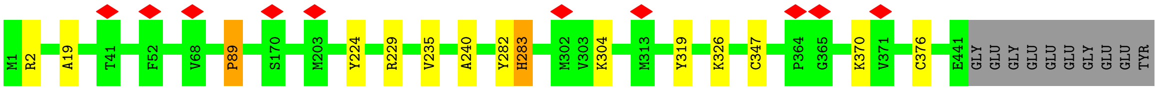




- Molecule 2: Tubulin alpha-1B chain

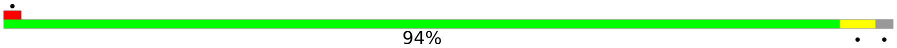
Chain P:

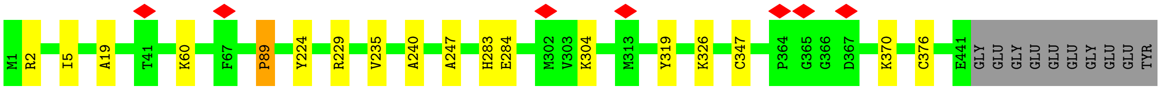




- Molecule 2: Tubulin alpha-1B chain

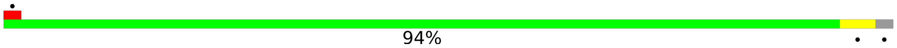
Chain Q:

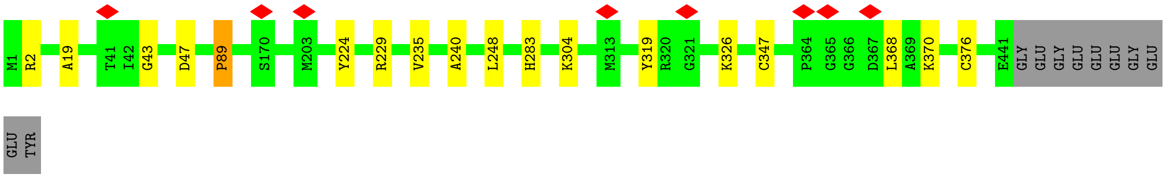




- Molecule 2: Tubulin alpha-1B chain

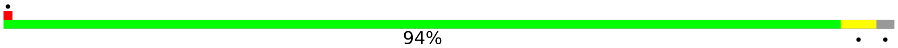
Chain R:

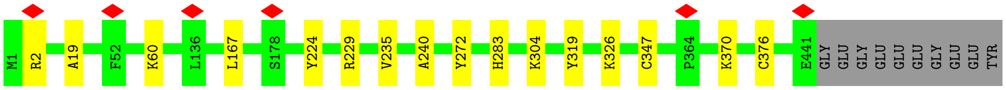




- Molecule 2: Tubulin alpha-1B chain

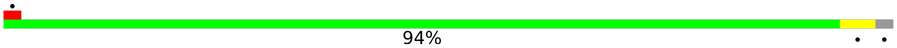
Chain S:

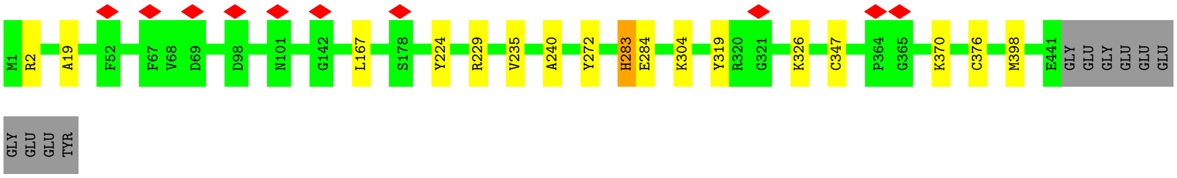




- Molecule 2: Tubulin alpha-1B chain

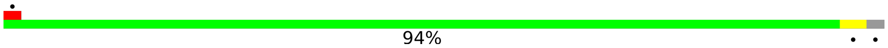
Chain T:

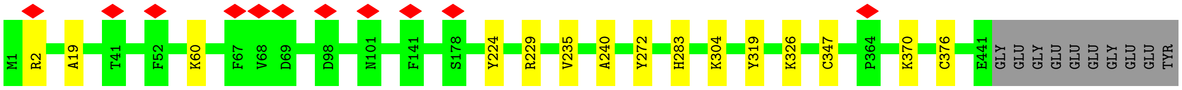




- Molecule 2: Tubulin alpha-1B chain

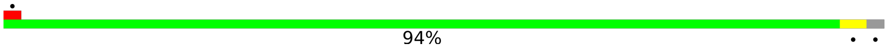
Chain U:

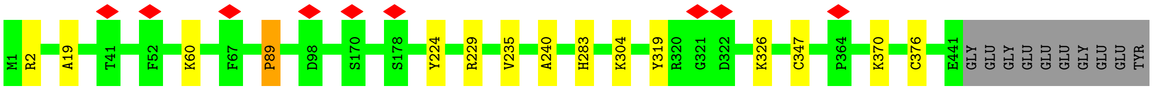




- Molecule 2: Tubulin alpha-1B chain

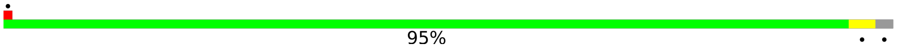
Chain V:

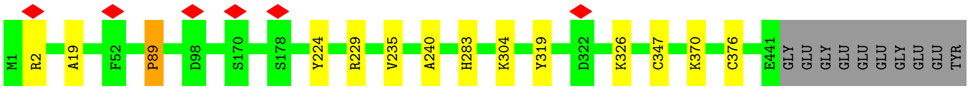




- Molecule 2: Tubulin alpha-1B chain

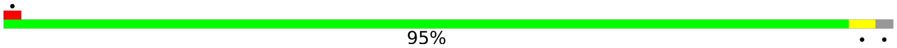
Chain W:

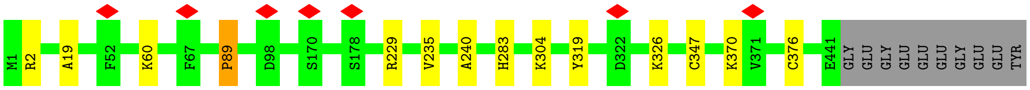




- Molecule 2: Tubulin alpha-1B chain

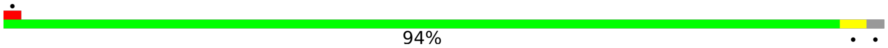
Chain X:

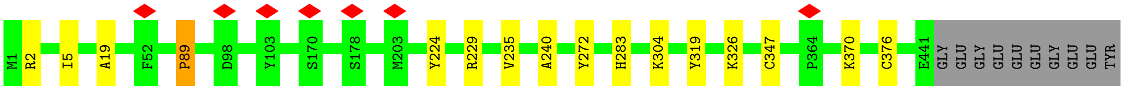




- Molecule 2: Tubulin alpha-1B chain

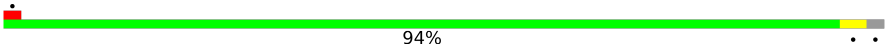
Chain Y:

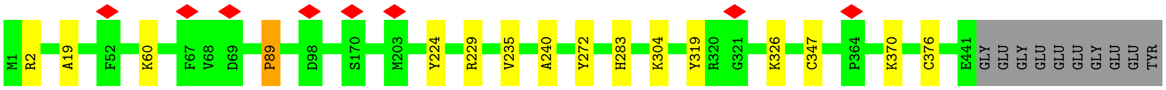




- Molecule 2: Tubulin alpha-1B chain

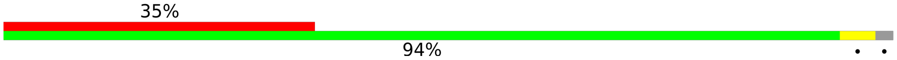
Chain Z:

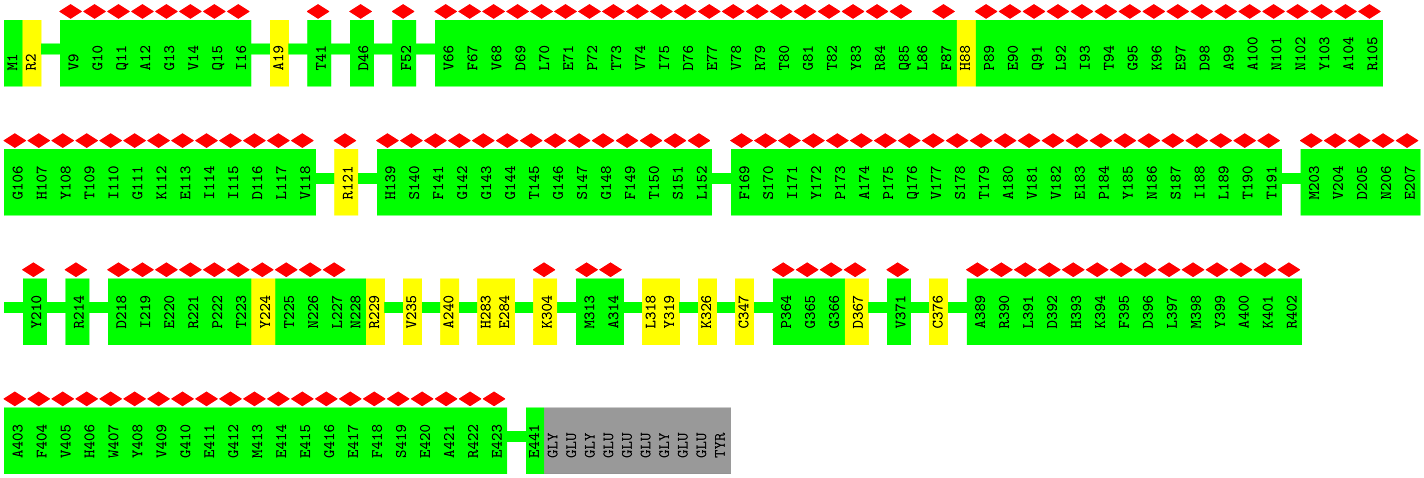




- Molecule 2: Tubulin alpha-1B chain

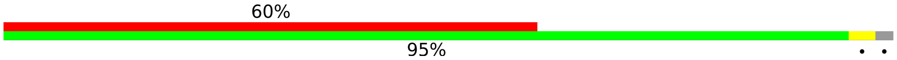
Chain A:

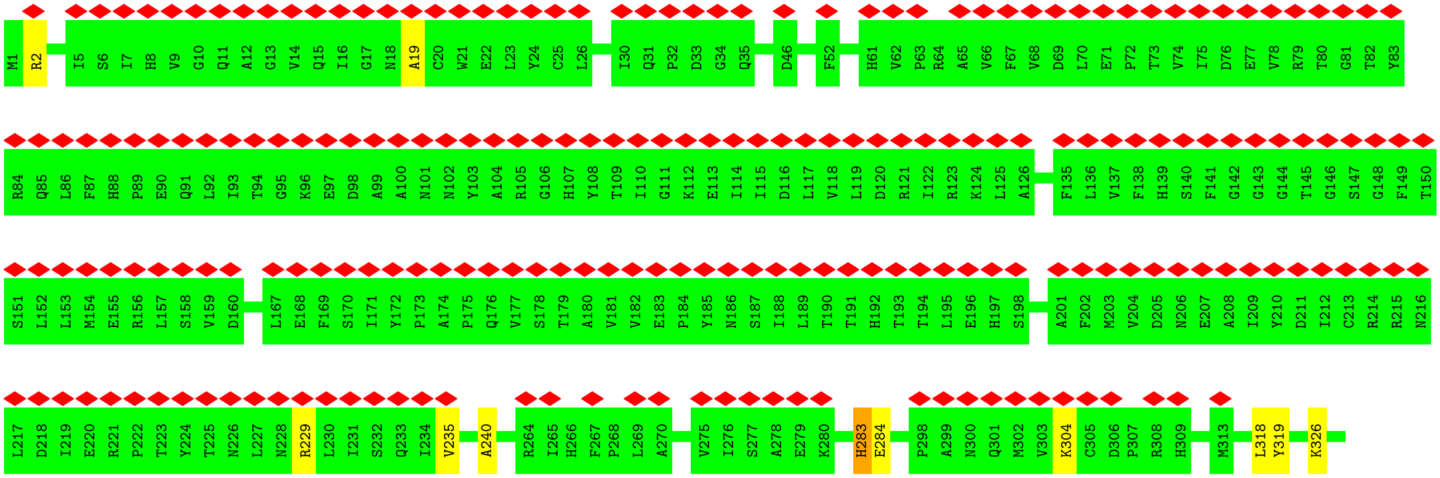




- Molecule 2: Tubulin alpha-1B chain

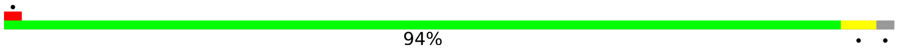
Chain B:

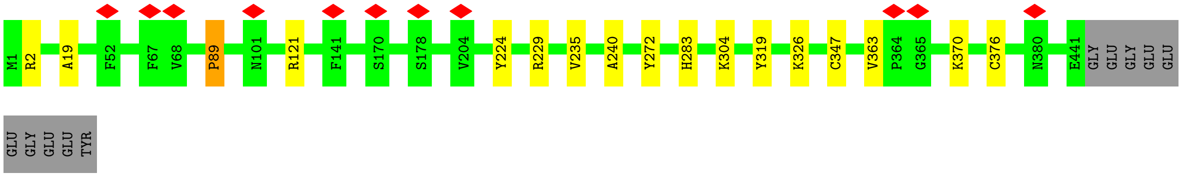




- Molecule 2: Tubulin alpha-1B chain

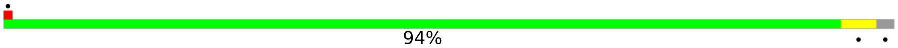
Chain C:

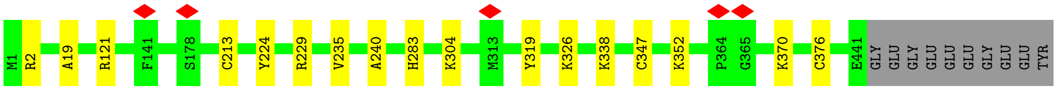




- Molecule 2: Tubulin alpha-1B chain

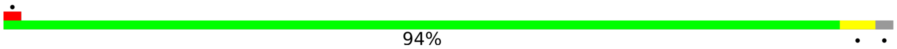
Chain D:

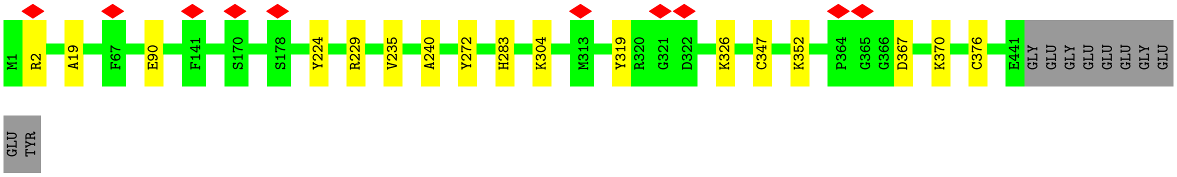




- Molecule 2: Tubulin alpha-1B chain

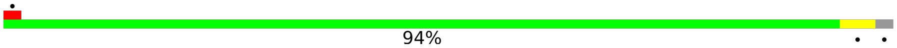
Chain E:

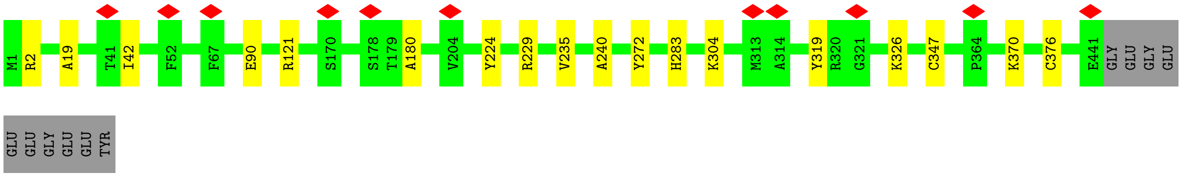




- Molecule 2: Tubulin alpha-1B chain

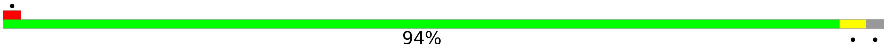
Chain F:

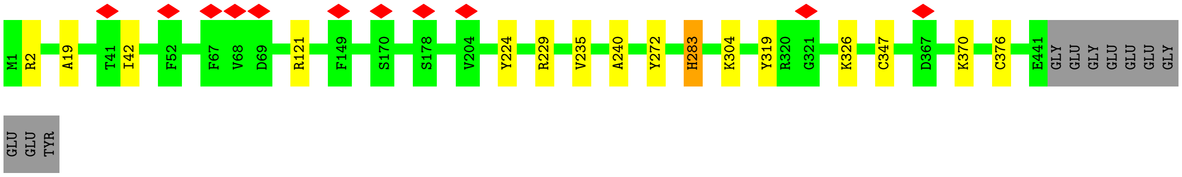




- Molecule 2: Tubulin alpha-1B chain

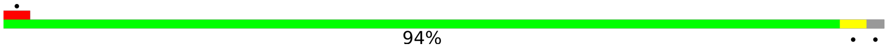
Chain G:

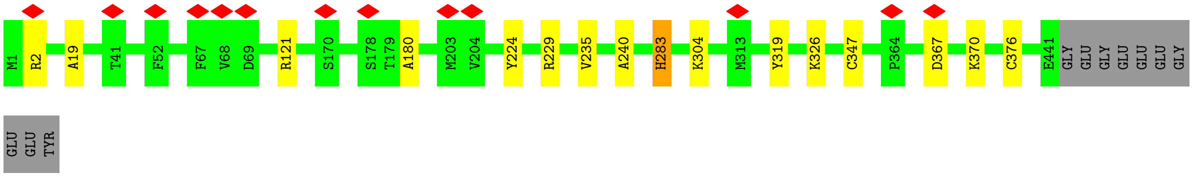




- Molecule 2: Tubulin alpha-1B chain

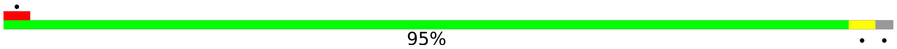
Chain H:

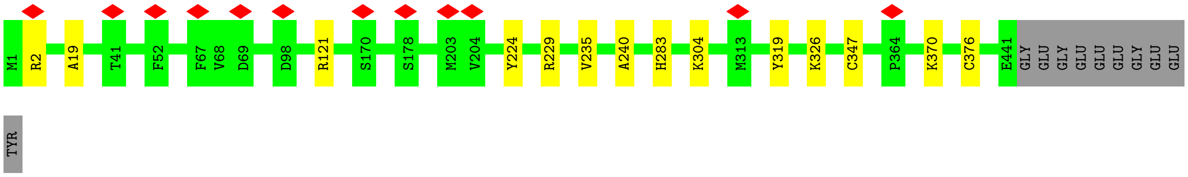




- Molecule 2: Tubulin alpha-1B chain

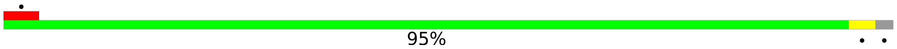
Chain I:

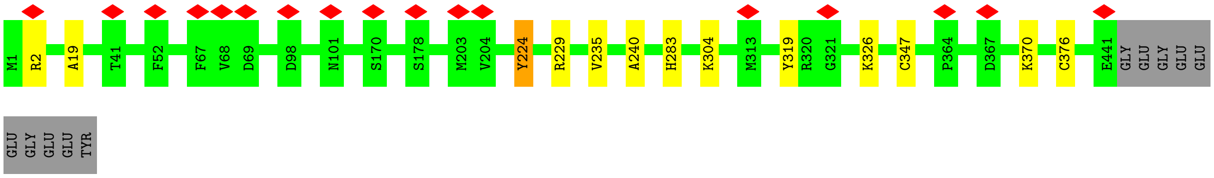




- Molecule 2: Tubulin alpha-1B chain

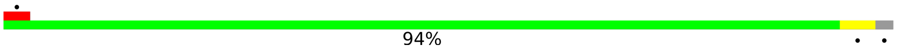
Chain J:

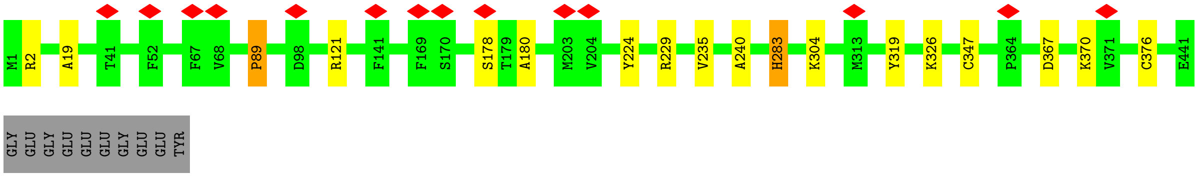




- Molecule 2: Tubulin alpha-1B chain

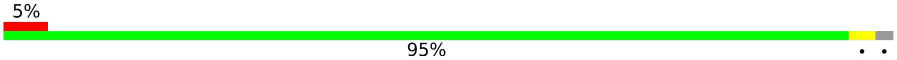
Chain K:

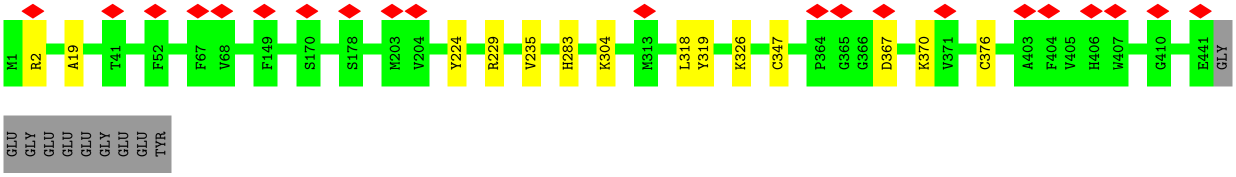




- Molecule 2: Tubulin alpha-1B chain

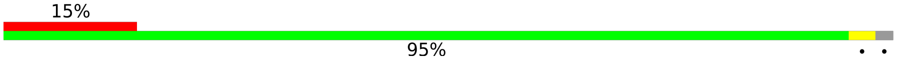
Chain L:

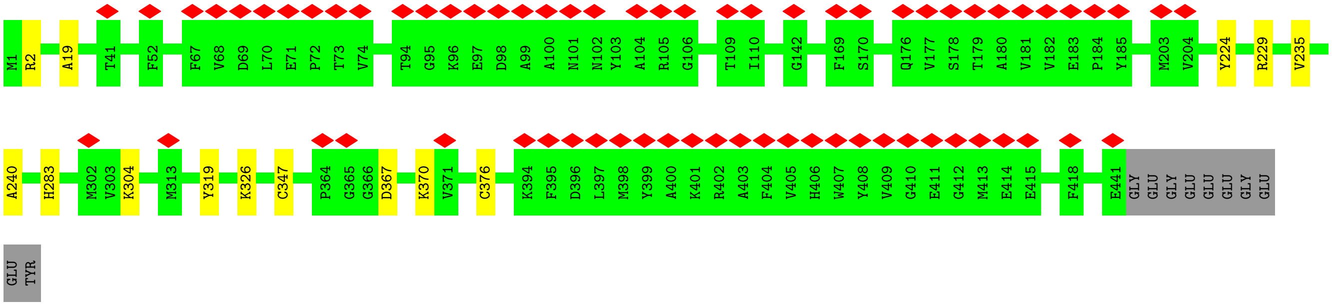




- Molecule 2: Tubulin alpha-1B chain

Chain M:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-27.68°, rise=9.54 Å, axial sym=C1	Depositor
Number of segments used	11670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	627.2, 627.2, 627.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.96, 1.96, 1.96	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, TA1, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.53	0/3451	1.16	9/4674 (0.2%)
1	b	0.54	0/3451	1.16	8/4674 (0.2%)
1	c	0.55	1/3451 (0.0%)	1.16	11/4674 (0.2%)
1	d	0.58	2/3451 (0.1%)	1.18	14/4674 (0.3%)
1	e	0.72	3/3451 (0.1%)	1.22	14/4674 (0.3%)
1	f	0.58	1/3451 (0.0%)	1.14	8/4674 (0.2%)
1	g	0.57	1/3451 (0.0%)	1.15	9/4674 (0.2%)
1	h	0.56	0/3451	1.14	6/4674 (0.1%)
1	i	0.54	0/3451	1.14	7/4674 (0.1%)
1	j	0.55	0/3451	1.14	6/4674 (0.1%)
1	k	0.56	1/3451 (0.0%)	1.15	7/4674 (0.1%)
1	l	0.55	0/3451	1.16	11/4674 (0.2%)
1	m	0.54	0/3451	1.16	9/4674 (0.2%)
1	n	0.55	0/3451	1.18	9/4674 (0.2%)
1	o	0.56	0/3451	1.18	11/4674 (0.2%)
1	p	0.53	0/3451	1.14	10/4674 (0.2%)
1	q	0.54	0/3451	1.15	10/4674 (0.2%)
1	r	0.54	1/3451 (0.0%)	1.15	10/4674 (0.2%)
1	s	0.53	0/3451	1.14	10/4674 (0.2%)
1	t	0.54	0/3451	1.15	9/4674 (0.2%)
1	u	0.53	0/3451	1.15	8/4674 (0.2%)
1	v	0.54	0/3451	1.16	10/4674 (0.2%)
1	w	0.54	0/3451	1.17	9/4674 (0.2%)
1	x	0.54	0/3451	1.18	9/4674 (0.2%)
1	y	0.54	0/3451	1.18	8/4674 (0.2%)
1	z	0.55	0/3451	1.18	9/4674 (0.2%)
2	A	0.57	2/3524 (0.1%)	1.15	12/4784 (0.3%)
2	B	0.58	2/3524 (0.1%)	1.14	10/4784 (0.2%)
2	C	0.55	0/3524	1.18	15/4784 (0.3%)
2	D	0.57	1/3524 (0.0%)	1.19	15/4784 (0.3%)
2	E	0.58	2/3524 (0.1%)	1.17	14/4784 (0.3%)
2	F	0.57	1/3524 (0.0%)	1.18	13/4784 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	G	0.56	0/3524	1.18	14/4784 (0.3%)
2	H	0.57	0/3524	1.19	17/4784 (0.4%)
2	I	0.56	0/3524	1.17	12/4784 (0.3%)
2	J	0.56	0/3524	1.16	10/4784 (0.2%)
2	K	0.56	1/3524 (0.0%)	1.18	18/4784 (0.4%)
2	L	0.54	0/3524	1.16	12/4784 (0.3%)
2	M	0.55	0/3524	1.15	13/4784 (0.3%)
2	N	0.56	0/3524	1.17	14/4784 (0.3%)
2	O	0.56	0/3524	1.17	11/4784 (0.2%)
2	P	0.58	0/3524	1.20	14/4784 (0.3%)
2	Q	0.57	1/3524 (0.0%)	1.21	17/4784 (0.4%)
2	R	0.84	1/3524 (0.0%)	1.20	15/4784 (0.3%)
2	S	0.55	0/3524	1.17	13/4784 (0.3%)
2	T	0.58	2/3524 (0.1%)	1.18	16/4784 (0.3%)
2	U	0.55	0/3524	1.17	11/4784 (0.2%)
2	V	0.55	0/3524	1.17	12/4784 (0.3%)
2	W	0.56	0/3524	1.17	12/4784 (0.3%)
2	X	0.57	0/3524	1.16	11/4784 (0.2%)
2	Y	0.56	0/3524	1.17	14/4784 (0.3%)
2	Z	0.57	0/3524	1.17	13/4784 (0.3%)
All	All	0.57	23/181350 (0.0%)	1.17	589/245908 (0.2%)

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	e	0	1
1	h	0	1
1	i	0	1
2	A	0	1
2	B	0	1
2	C	0	1
2	D	0	1
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	M	0	1
2	N	0	1
2	O	0	1
2	P	0	1
2	Q	0	1
2	R	0	1
2	S	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	W	0	1
2	X	0	1
2	Y	0	1
2	Z	0	1
All	All	0	29

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	43	GLY	C-N	36.46	1.98	1.33
1	e	294	PHE	C-N	21.52	1.83	1.34
1	d	27	GLU	CD-OE2	8.83	1.35	1.25
1	f	22	GLU	CD-OE2	8.82	1.35	1.25
1	e	27	GLU	CD-OE2	8.01	1.34	1.25
1	k	22	GLU	CD-OE2	7.62	1.34	1.25
2	B	284	GLU	CD-OE1	7.61	1.34	1.25
2	B	284	GLU	CD-OE2	7.49	1.33	1.25
2	E	90	GLU	CD-OE2	7.31	1.33	1.25
1	g	22	GLU	CD-OE2	7.11	1.33	1.25
1	e	27	GLU	CD-OE1	6.70	1.33	1.25
2	T	398	MET	CG-SD	6.41	1.97	1.81
2	A	284	GLU	CD-OE1	6.16	1.32	1.25
2	Q	284	GLU	CD-OE2	-6.08	1.19	1.25
1	c	27	GLU	CD-OE2	5.90	1.32	1.25
1	d	27	GLU	CD-OE1	5.75	1.31	1.25
1	r	27	GLU	CD-OE2	5.74	1.31	1.25
2	A	88	HIS	CE1-NE2	5.56	1.45	1.32
2	D	352	LYS	CG-CD	-5.54	1.33	1.52
2	T	284	GLU	CD-OE2	-5.40	1.19	1.25
2	F	90	GLU	CD-OE1	5.34	1.31	1.25
2	K	178	SER	CB-OG	5.28	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	352	LYS	CG-CD	-5.11	1.35	1.52

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	222	TYR	CB-CG-CD1	15.18	130.11	121.00
1	n	222	TYR	CB-CG-CD1	15.07	130.04	121.00
1	w	222	TYR	CB-CG-CD1	14.93	129.96	121.00
1	z	222	TYR	CB-CG-CD1	14.82	129.89	121.00
1	y	222	TYR	CB-CG-CD1	14.44	129.66	121.00
1	v	222	TYR	CB-CG-CD1	14.21	129.53	121.00
2	Q	247	ALA	N-CA-CB	-14.18	90.25	110.10
1	o	222	TYR	CB-CG-CD1	14.18	129.51	121.00
1	b	222	TYR	CB-CG-CD1	13.88	129.33	121.00
1	l	222	TYR	CB-CG-CD1	13.45	129.07	121.00
1	a	222	TYR	CB-CG-CD1	13.43	129.06	121.00
1	t	222	TYR	CB-CG-CD1	13.35	129.01	121.00
1	u	222	TYR	CB-CG-CD1	13.25	128.95	121.00
1	d	222	TYR	CB-CG-CD1	13.06	128.84	121.00
1	p	99	ASN	CB-CA-C	12.98	136.37	110.40
1	s	222	TYR	CB-CG-CD1	12.44	128.46	121.00
1	r	99	ASN	CB-CA-C	12.03	134.45	110.40
2	Q	247	ALA	CB-CA-C	-11.81	92.38	110.10
1	n	99	ASN	CB-CA-C	11.59	133.59	110.40
1	y	99	ASN	CB-CA-C	11.55	133.50	110.40
1	z	222	TYR	CA-CB-CG	11.53	135.31	113.40
1	u	99	ASN	CB-CA-C	11.51	133.42	110.40
1	q	99	ASN	CB-CA-C	11.51	133.41	110.40
1	s	99	ASN	CB-CA-C	11.50	133.41	110.40
1	x	99	ASN	CB-CA-C	11.48	133.37	110.40
1	m	222	TYR	CB-CG-CD1	11.48	127.89	121.00
1	t	99	ASN	CB-CA-C	11.46	133.33	110.40
1	o	99	ASN	CB-CA-C	11.46	133.31	110.40
1	z	99	ASN	CB-CA-C	11.45	133.29	110.40
1	v	99	ASN	CB-CA-C	11.43	133.26	110.40
1	d	99	ASN	CB-CA-C	11.41	133.21	110.40
1	e	294	PHE	CA-C-N	-11.36	92.20	117.20
1	b	99	ASN	CB-CA-C	11.36	133.11	110.40
1	c	99	ASN	CB-CA-C	11.32	133.04	110.40
1	w	99	ASN	CB-CA-C	11.30	133.00	110.40
1	l	99	ASN	CB-CA-C	11.29	132.97	110.40
1	e	99	ASN	CB-CA-C	11.26	132.91	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	99	ASN	CB-CA-C	11.23	132.86	110.40
1	a	99	ASN	CB-CA-C	11.18	132.76	110.40
1	h	99	ASN	CB-CA-C	11.12	132.64	110.40
1	i	99	ASN	CB-CA-C	11.11	132.61	110.40
2	P	283	HIS	CA-CB-CG	11.02	132.33	113.60
1	e	222	TYR	CB-CG-CD1	10.85	127.51	121.00
1	f	99	ASN	CB-CA-C	10.85	132.09	110.40
2	H	224	TYR	CB-CG-CD2	10.76	127.45	121.00
1	e	294	PHE	O-C-N	10.71	139.84	122.70
1	k	99	ASN	CB-CA-C	10.68	131.75	110.40
1	e	294	PHE	C-N-CA	-10.64	95.10	121.70
1	g	99	ASN	CB-CA-C	10.54	131.49	110.40
2	P	370	LYS	CB-CG-CD	10.47	138.81	111.60
1	q	222	TYR	CB-CG-CD1	10.45	127.27	121.00
1	j	99	ASN	CB-CA-C	10.42	131.24	110.40
2	Q	224	TYR	CB-CG-CD2	10.31	127.19	121.00
1	d	282	ARG	NE-CZ-NH2	-10.21	115.19	120.30
2	Q	224	TYR	CB-CG-CD1	-10.16	114.90	121.00
2	T	167	LEU	CB-CG-CD1	10.12	128.21	111.00
1	y	222	TYR	CA-CB-CG	10.06	132.52	113.40
1	o	222	TYR	CA-CB-CG	9.88	132.16	113.40
1	n	222	TYR	CA-CB-CG	9.81	132.03	113.40
2	P	224	TYR	CB-CG-CD1	9.78	126.87	121.00
2	P	224	TYR	CA-CB-CG	9.75	131.92	113.40
1	i	222	TYR	CB-CG-CD1	9.71	126.82	121.00
1	w	222	TYR	CA-CB-CG	9.69	131.81	113.40
1	p	222	TYR	CB-CG-CD1	9.58	126.75	121.00
1	x	222	TYR	CA-CB-CG	9.57	131.58	113.40
2	S	167	LEU	CB-CG-CD1	9.50	127.16	111.00
1	v	222	TYR	CA-CB-CG	9.37	131.19	113.40
2	U	376	CYS	CB-CA-C	-9.33	91.75	110.40
1	t	222	TYR	CA-CB-CG	9.32	131.12	113.40
1	s	222	TYR	CA-CB-CG	9.32	131.11	113.40
1	u	222	TYR	CA-CB-CG	9.32	131.12	113.40
2	T	376	CYS	CB-CA-C	-9.29	91.82	110.40
2	V	376	CYS	CB-CA-C	-9.28	91.83	110.40
2	S	376	CYS	CB-CA-C	-9.27	91.86	110.40
2	W	376	CYS	CB-CA-C	-9.27	91.86	110.40
2	R	376	CYS	CB-CA-C	-9.25	91.89	110.40
2	R	224	TYR	CB-CG-CD2	9.23	126.54	121.00
2	P	376	CYS	CB-CA-C	-9.23	91.94	110.40
2	X	376	CYS	CB-CA-C	-9.21	91.98	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	376	CYS	CB-CA-C	-9.21	91.99	110.40
2	Q	376	CYS	CB-CA-C	-9.20	91.99	110.40
2	O	376	CYS	CB-CA-C	-9.20	91.99	110.40
2	C	376	CYS	CB-CA-C	-9.19	92.03	110.40
2	G	376	CYS	CB-CA-C	-9.18	92.03	110.40
2	F	376	CYS	CB-CA-C	-9.18	92.04	110.40
1	x	222	TYR	CB-CG-CD2	-9.17	115.50	121.00
2	I	376	CYS	CB-CA-C	-9.16	92.07	110.40
2	M	376	CYS	CB-CA-C	-9.16	92.08	110.40
2	E	376	CYS	CB-CA-C	-9.16	92.08	110.40
2	H	376	CYS	CB-CA-C	-9.15	92.10	110.40
2	J	376	CYS	CB-CA-C	-9.10	92.21	110.40
2	B	376	CYS	CB-CA-C	-9.08	92.24	110.40
2	Z	376	CYS	CB-CA-C	-9.07	92.27	110.40
2	L	376	CYS	CB-CA-C	-9.06	92.28	110.40
2	A	376	CYS	CB-CA-C	-9.05	92.30	110.40
1	c	222	TYR	CB-CG-CD1	9.02	126.41	121.00
2	Y	376	CYS	CB-CA-C	-9.01	92.38	110.40
2	K	376	CYS	CB-CA-C	-9.00	92.41	110.40
2	D	376	CYS	CB-CA-C	-8.96	92.49	110.40
1	f	222	TYR	CB-CG-CD1	8.93	126.36	121.00
1	k	222	TYR	CB-CG-CD1	8.86	126.32	121.00
2	R	224	TYR	CB-CG-CD1	-8.85	115.69	121.00
1	w	222	TYR	CB-CG-CD2	-8.84	115.70	121.00
1	b	222	TYR	CB-CG-CD2	-8.76	115.74	121.00
1	z	222	TYR	CB-CG-CD2	-8.75	115.75	121.00
1	a	222	TYR	CA-CB-CG	8.75	130.02	113.40
1	n	222	TYR	CB-CG-CD2	-8.74	115.75	121.00
2	D	121	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	q	222	TYR	CA-CB-CG	8.62	129.78	113.40
1	r	222	TYR	CB-CG-CD1	8.56	126.14	121.00
1	b	222	TYR	CA-CB-CG	8.53	129.60	113.40
1	r	222	TYR	CA-CB-CG	8.46	129.48	113.40
1	y	222	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	p	222	TYR	CA-CB-CG	8.32	129.22	113.40
1	v	222	TYR	CB-CG-CD2	-8.31	116.02	121.00
1	j	222	TYR	CB-CG-CD1	8.30	125.98	121.00
2	H	121	ARG	NE-CZ-NH2	8.09	124.34	120.30
2	D	229	ARG	CG-CD-NE	-8.04	94.91	111.80
1	m	222	TYR	CA-CB-CG	7.99	128.59	113.40
2	U	224	TYR	CB-CG-CD1	-7.94	116.24	121.00
2	T	224	TYR	CB-CG-CD1	-7.93	116.24	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	222	TYR	CB-CG-CD2	-7.80	116.32	121.00
2	I	224	TYR	CB-CG-CD2	7.80	125.68	121.00
1	g	222	TYR	CB-CG-CD1	7.77	125.66	121.00
1	a	222	TYR	CB-CG-CD2	-7.75	116.35	121.00
2	M	224	TYR	CB-CG-CD1	7.74	125.64	121.00
2	O	229	ARG	CG-CD-NE	-7.70	95.62	111.80
2	G	224	TYR	CB-CG-CD2	7.58	125.55	121.00
1	t	222	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	e	286	VAL	CA-CB-CG2	7.53	122.20	110.90
1	d	222	TYR	CB-CG-CD2	-7.52	116.49	121.00
2	D	213	CYS	CA-CB-SG	-7.44	100.60	114.00
2	E	90	GLU	OE1-CD-OE2	7.42	132.20	123.30
2	Z	19	ALA	CB-CA-C	7.35	121.12	110.10
2	Q	229	ARG	CG-CD-NE	-7.33	96.41	111.80
1	e	222	TYR	CA-CB-CG	7.31	127.30	113.40
1	d	222	TYR	CA-CB-CG	7.27	127.20	113.40
1	p	99	ASN	CB-CG-ND2	7.25	134.11	116.70
2	R	229	ARG	CG-CD-NE	-7.25	96.58	111.80
2	V	224	TYR	CB-CG-CD1	-7.21	116.68	121.00
1	c	222	TYR	CA-CB-CG	7.20	127.08	113.40
2	O	229	ARG	NE-CZ-NH2	-7.19	116.71	120.30
2	N	229	ARG	CG-CD-NE	-7.18	96.71	111.80
2	U	229	ARG	CG-CD-NE	-7.15	96.79	111.80
2	I	121	ARG	NE-CZ-NH2	7.13	123.86	120.30
2	X	89	PRO	N-CD-CG	-7.13	92.51	103.20
2	P	229	ARG	CG-CD-NE	-7.12	96.84	111.80
2	X	229	ARG	CG-CD-NE	-7.12	96.84	111.80
2	Y	229	ARG	CG-CD-NE	-7.12	96.85	111.80
2	T	229	ARG	CG-CD-NE	-7.10	96.89	111.80
1	f	222	TYR	CA-CB-CG	7.09	126.87	113.40
2	Z	229	ARG	CG-CD-NE	-7.08	96.92	111.80
2	M	229	ARG	CG-CD-NE	-7.08	96.93	111.80
1	u	222	TYR	CB-CG-CD2	-7.08	116.75	121.00
2	L	229	ARG	CG-CD-NE	-7.06	96.97	111.80
2	V	229	ARG	CG-CD-NE	-7.06	96.97	111.80
2	C	229	ARG	CG-CD-NE	-7.05	97.00	111.80
2	H	224	TYR	CA-CB-CG	7.04	126.77	113.40
2	A	229	ARG	CG-CD-NE	-7.03	97.04	111.80
2	C	121	ARG	NE-CZ-NH2	7.02	123.81	120.30
2	W	229	ARG	CG-CD-NE	-7.02	97.06	111.80
1	q	119	VAL	CA-CB-CG1	-7.01	100.39	110.90
2	E	229	ARG	CG-CD-NE	-6.96	97.17	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	229	ARG	CG-CD-NE	-6.95	97.21	111.80
2	S	229	ARG	CG-CD-NE	-6.93	97.24	111.80
2	K	121	ARG	NE-CZ-NH2	6.92	123.76	120.30
2	B	229	ARG	CG-CD-NE	-6.91	97.30	111.80
2	H	229	ARG	CG-CD-NE	-6.90	97.30	111.80
2	I	229	ARG	CG-CD-NE	-6.88	97.35	111.80
2	F	229	ARG	CG-CD-NE	-6.88	97.36	111.80
2	J	229	ARG	CG-CD-NE	-6.79	97.54	111.80
2	C	224	TYR	CA-CB-CG	6.79	126.29	113.40
2	G	229	ARG	CG-CD-NE	-6.79	97.55	111.80
2	Y	224	TYR	CB-CG-CD1	-6.78	116.93	121.00
2	A	121	ARG	NE-CZ-NH2	6.78	123.69	120.30
2	Y	19	ALA	CB-CA-C	6.77	120.25	110.10
2	S	224	TYR	CB-CG-CD1	-6.76	116.95	121.00
2	R	43	GLY	CA-C-O	-6.70	108.54	120.60
2	K	178	SER	O-C-N	6.67	133.38	122.70
1	s	222	TYR	CB-CG-CD2	-6.65	117.01	121.00
2	P	224	TYR	CB-CG-CD2	-6.64	117.02	121.00
2	T	19	ALA	CB-CA-C	6.63	120.04	110.10
2	P	282	TYR	O-C-N	-6.62	112.11	122.70
2	W	19	ALA	CB-CA-C	6.60	120.00	110.10
2	F	224	TYR	CA-CB-CG	6.60	125.93	113.40
2	M	370	LYS	CB-CG-CD	6.57	128.69	111.60
2	S	19	ALA	CB-CA-C	6.57	119.95	110.10
2	Y	89	PRO	N-CD-CG	-6.56	93.36	103.20
2	G	224	TYR	CA-CB-CG	6.54	125.82	113.40
1	l	222	TYR	CA-CB-CG	6.52	125.79	113.40
2	N	19	ALA	CB-CA-C	6.51	119.87	110.10
2	V	19	ALA	CB-CA-C	6.51	119.86	110.10
2	U	19	ALA	CB-CA-C	6.51	119.86	110.10
2	N	248	LEU	CB-CG-CD2	-6.47	100.00	111.00
2	I	224	TYR	CA-CB-CG	6.46	125.68	113.40
2	A	19	ALA	CB-CA-C	6.45	119.78	110.10
2	X	19	ALA	CB-CA-C	6.45	119.77	110.10
1	o	350	LYS	CB-CG-CD	6.41	128.28	111.60
2	F	121	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	P	19	ALA	CB-CA-C	6.40	119.70	110.10
2	R	89	PRO	N-CD-CG	-6.37	93.64	103.20
2	S	60	LYS	CD-CE-NZ	-6.37	97.05	111.70
2	D	370	LYS	CB-CG-CD	6.37	128.16	111.60
2	K	178	SER	CB-CA-C	6.36	122.19	110.10
2	O	19	ALA	CB-CA-C	6.36	119.64	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	89	PRO	N-CD-CG	-6.36	93.67	103.20
2	L	224	TYR	CA-CB-CG	6.36	125.48	113.40
2	R	19	ALA	CB-CA-C	6.35	119.62	110.10
1	g	276	ARG	CB-CG-CD	6.34	128.09	111.60
2	Y	235	VAL	N-CA-CB	-6.33	97.56	111.50
2	Z	224	TYR	CB-CG-CD1	-6.32	117.21	121.00
2	Y	319	TYR	CB-CA-C	-6.32	97.77	110.40
2	X	235	VAL	N-CA-CB	-6.32	97.61	111.50
2	Z	235	VAL	N-CA-CB	-6.31	97.61	111.50
2	Z	319	TYR	CB-CA-C	-6.31	97.78	110.40
2	D	235	VAL	N-CA-CB	-6.30	97.64	111.50
2	M	19	ALA	CB-CA-C	6.30	119.55	110.10
2	V	235	VAL	N-CA-CB	-6.30	97.65	111.50
2	N	235	VAL	N-CA-CB	-6.29	97.65	111.50
2	K	235	VAL	N-CA-CB	-6.29	97.66	111.50
2	E	319	TYR	CB-CA-C	-6.29	97.82	110.40
2	Q	60	LYS	CD-CE-NZ	-6.29	97.25	111.70
2	W	235	VAL	N-CA-CB	-6.28	97.69	111.50
2	P	319	TYR	CB-CA-C	-6.28	97.85	110.40
2	C	319	TYR	CB-CA-C	-6.28	97.85	110.40
2	R	319	TYR	CB-CA-C	-6.27	97.85	110.40
2	B	319	TYR	CB-CA-C	-6.27	97.86	110.40
2	U	235	VAL	N-CA-CB	-6.27	97.71	111.50
2	A	319	TYR	CB-CA-C	-6.27	97.86	110.40
2	B	19	ALA	CB-CA-C	6.26	119.49	110.10
2	B	235	VAL	N-CA-CB	-6.26	97.72	111.50
2	E	235	VAL	N-CA-CB	-6.25	97.74	111.50
2	A	235	VAL	N-CA-CB	-6.25	97.74	111.50
2	R	235	VAL	N-CA-CB	-6.25	97.75	111.50
2	G	319	TYR	CB-CA-C	-6.25	97.89	110.40
2	J	235	VAL	N-CA-CB	-6.25	97.75	111.50
2	E	224	TYR	CA-CB-CG	6.25	125.27	113.40
2	O	235	VAL	N-CA-CB	-6.25	97.76	111.50
2	K	319	TYR	CB-CA-C	-6.24	97.92	110.40
2	J	319	TYR	CB-CA-C	-6.24	97.93	110.40
2	X	319	TYR	CB-CA-C	-6.23	97.94	110.40
2	G	235	VAL	N-CA-CB	-6.23	97.80	111.50
2	S	235	VAL	N-CA-CB	-6.23	97.80	111.50
2	O	319	TYR	CB-CA-C	-6.22	97.95	110.40
2	Q	19	ALA	CB-CA-C	6.22	119.44	110.10
1	r	241	ARG	CB-CA-C	-6.22	97.96	110.40
2	I	319	TYR	CB-CA-C	-6.22	97.96	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	319	TYR	CB-CA-C	-6.21	97.97	110.40
2	O	229	ARG	CB-CA-C	-6.21	97.98	110.40
2	H	319	TYR	CB-CA-C	-6.21	97.98	110.40
2	C	235	VAL	N-CA-CB	-6.21	97.84	111.50
2	Q	235	VAL	N-CA-CB	-6.21	97.84	111.50
2	L	319	TYR	CB-CA-C	-6.21	97.99	110.40
2	D	319	TYR	CB-CA-C	-6.20	97.99	110.40
2	T	235	VAL	N-CA-CB	-6.20	97.86	111.50
2	T	319	TYR	CB-CA-C	-6.20	98.00	110.40
2	K	19	ALA	CB-CA-C	6.20	119.40	110.10
2	K	224	TYR	CA-CB-CG	6.20	125.18	113.40
2	P	235	VAL	N-CA-CB	-6.19	97.88	111.50
2	W	319	TYR	CB-CA-C	-6.19	98.02	110.40
2	N	319	TYR	CB-CA-C	-6.19	98.03	110.40
2	S	319	TYR	CB-CA-C	-6.19	98.02	110.40
2	I	235	VAL	N-CA-CB	-6.19	97.89	111.50
2	G	121	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	k	276	ARG	CB-CG-CD	6.18	127.67	111.60
2	L	235	VAL	N-CA-CB	-6.18	97.91	111.50
2	V	319	TYR	CB-CA-C	-6.17	98.05	110.40
2	H	235	VAL	N-CA-CB	-6.17	97.92	111.50
2	C	19	ALA	CB-CA-C	6.17	119.36	110.10
1	e	46	ARG	CG-CD-NE	6.16	124.74	111.80
2	F	235	VAL	N-CA-CB	-6.16	97.96	111.50
2	M	319	TYR	CB-CA-C	-6.15	98.10	110.40
2	M	235	VAL	N-CA-CB	-6.15	97.98	111.50
2	U	319	TYR	CB-CA-C	-6.13	98.13	110.40
1	g	87	PRO	N-CA-CB	6.13	110.65	103.30
2	J	224	TYR	CA-CB-CG	6.13	125.04	113.40
2	J	19	ALA	CB-CA-C	6.12	119.28	110.10
1	e	282	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	D	19	ALA	CB-CA-C	6.11	119.27	110.10
1	h	276	ARG	CB-CG-CD	6.11	127.49	111.60
2	F	319	TYR	CB-CA-C	-6.11	98.18	110.40
1	a	276	ARG	CB-CG-CD	6.11	127.48	111.60
1	d	50	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	d	46	ARG	CG-CD-NE	6.08	124.57	111.80
2	F	19	ALA	CB-CA-C	6.08	119.22	110.10
2	Z	89	PRO	N-CD-CG	-6.07	94.09	103.20
1	q	241	ARG	CB-CA-C	-6.07	98.26	110.40
1	d	241	ARG	CB-CA-C	-6.06	98.28	110.40
2	H	180	ALA	CB-CA-C	-6.06	101.02	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	19	ALA	CB-CA-C	6.05	119.17	110.10
2	L	224	TYR	CB-CG-CD2	6.05	124.63	121.00
2	L	19	ALA	CB-CA-C	6.04	119.16	110.10
2	C	89	PRO	N-CD-CG	-6.03	94.16	103.20
1	u	241	ARG	CB-CA-C	-6.03	98.34	110.40
1	k	46	ARG	CG-CD-NE	6.02	124.45	111.80
2	Y	229	ARG	CB-CA-C	-6.02	98.36	110.40
1	w	241	ARG	CB-CA-C	-6.02	98.36	110.40
2	I	235	VAL	CA-CB-CG1	6.02	119.92	110.90
1	o	241	ARG	CB-CA-C	-6.02	98.37	110.40
2	G	19	ALA	CB-CA-C	6.01	119.12	110.10
2	I	19	ALA	CB-CA-C	6.01	119.12	110.10
1	e	276	ARG	CB-CG-CD	6.00	127.21	111.60
1	f	46	ARG	CG-CD-NE	6.00	124.39	111.80
1	c	241	ARG	CB-CA-C	-5.99	98.42	110.40
2	D	224	TYR	CA-CB-CG	5.99	124.77	113.40
1	a	241	ARG	CB-CA-C	-5.98	98.44	110.40
1	t	242	PHE	CB-CG-CD2	-5.97	116.62	120.80
2	T	229	ARG	CB-CA-C	-5.97	98.46	110.40
2	V	229	ARG	CB-CA-C	-5.96	98.47	110.40
1	e	241	ARG	CB-CA-C	-5.96	98.48	110.40
1	l	241	ARG	CB-CA-C	-5.96	98.49	110.40
1	n	241	ARG	CB-CA-C	-5.95	98.50	110.40
2	Z	229	ARG	CB-CA-C	-5.95	98.50	110.40
2	R	229	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	y	242	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	x	241	ARG	CB-CA-C	-5.94	98.52	110.40
1	c	363	MET	CB-CG-SD	5.93	130.20	112.40
2	X	229	ARG	CB-CA-C	-5.93	98.54	110.40
2	M	224	TYR	CA-CB-CG	5.93	124.67	113.40
2	H	19	ALA	CB-CA-C	5.93	118.99	110.10
1	k	241	ARG	CB-CA-C	-5.92	98.56	110.40
2	W	229	ARG	CB-CA-C	-5.92	98.56	110.40
2	F	272	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	m	276	ARG	CB-CG-CD	5.91	126.97	111.60
2	R	229	ARG	CB-CA-C	-5.91	98.58	110.40
1	b	241	ARG	CB-CA-C	-5.91	98.59	110.40
2	Q	89	PRO	N-CD-CG	-5.91	94.34	103.20
2	U	229	ARG	CB-CA-C	-5.90	98.59	110.40
1	m	241	ARG	CB-CA-C	-5.90	98.59	110.40
2	D	229	ARG	CB-CA-C	-5.90	98.60	110.40
2	Y	272	TYR	CB-CG-CD2	-5.90	117.46	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	241	ARG	CB-CA-C	-5.90	98.61	110.40
2	V	229	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	s	242	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	i	241	ARG	CB-CA-C	-5.89	98.62	110.40
1	s	46	ARG	CG-CD-NE	5.89	124.16	111.80
1	v	241	ARG	CB-CA-C	-5.88	98.63	110.40
1	z	242	PHE	CB-CG-CD1	-5.88	116.68	120.80
1	z	241	ARG	CB-CA-C	-5.88	98.64	110.40
2	R	248	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	q	358	PRO	N-CA-CB	5.87	110.34	103.30
2	N	229	ARG	CB-CA-C	-5.87	98.67	110.40
1	q	46	ARG	CG-CD-NE	5.86	124.10	111.80
2	Q	229	ARG	CB-CA-C	-5.85	98.69	110.40
2	W	224	TYR	CB-CG-CD1	-5.84	117.50	121.00
2	X	229	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	j	241	ARG	CB-CA-C	-5.84	98.73	110.40
1	m	46	ARG	CG-CD-NE	5.83	124.05	111.80
2	W	89	PRO	N-CD-CG	-5.83	94.45	103.20
1	i	46	ARG	CG-CD-NE	5.82	124.03	111.80
2	S	229	ARG	CB-CA-C	-5.82	98.76	110.40
1	q	50	TYR	CB-CG-CD2	-5.81	117.51	121.00
2	G	235	VAL	CA-CB-CG1	5.81	119.61	110.90
2	N	89	PRO	N-CD-CG	-5.81	94.49	103.20
2	D	352	LYS	CB-CG-CD	5.80	126.69	111.60
1	l	222	TYR	CB-CG-CD2	-5.79	117.52	121.00
2	E	352	LYS	CB-CG-CD	5.79	126.66	111.60
2	P	89	PRO	N-CD-CG	-5.79	94.52	103.20
2	H	235	VAL	CA-CB-CG1	5.78	119.58	110.90
1	j	276	ARG	CB-CG-CD	5.76	126.57	111.60
1	v	46	ARG	CG-CD-NE	5.75	123.88	111.80
1	d	363	MET	CB-CG-SD	5.75	129.65	112.40
2	P	229	ARG	CB-CA-C	-5.75	98.90	110.40
2	A	229	ARG	CB-CA-C	-5.75	98.91	110.40
1	g	241	ARG	CB-CA-C	-5.74	98.91	110.40
1	p	46	ARG	CG-CD-NE	5.74	123.86	111.80
2	B	229	ARG	CB-CA-C	-5.74	98.92	110.40
1	p	242	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	h	241	ARG	CB-CA-C	-5.73	98.93	110.40
1	c	276	ARG	CB-CG-CD	5.73	126.50	111.60
1	l	276	ARG	CB-CG-CD	5.73	126.50	111.60
1	e	50	TYR	CB-CG-CD2	-5.73	117.56	121.00
2	W	229	ARG	NE-CZ-NH2	-5.73	117.44	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	229	ARG	CB-CA-C	-5.73	98.94	110.40
2	J	229	ARG	CB-CA-C	-5.73	98.95	110.40
2	Y	229	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	b	46	ARG	CG-CD-NE	5.72	123.81	111.80
1	f	241	ARG	CB-CA-C	-5.71	98.98	110.40
2	E	229	ARG	CB-CA-C	-5.70	99.00	110.40
1	u	46	ARG	CG-CD-NE	5.69	123.75	111.80
2	V	89	PRO	N-CD-CG	-5.68	94.67	103.20
1	t	46	ARG	CG-CD-NE	5.68	123.74	111.80
2	K	229	ARG	CB-CA-C	-5.68	99.05	110.40
1	r	50	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	j	46	ARG	CG-CD-NE	5.67	123.70	111.80
2	Q	229	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	I	229	ARG	CB-CA-C	-5.65	99.09	110.40
2	L	229	ARG	CB-CA-C	-5.65	99.09	110.40
1	r	46	ARG	CG-CD-NE	5.65	123.67	111.80
2	N	272	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	e	368	ILE	CB-CG1-CD1	5.63	129.65	113.90
2	M	229	ARG	CB-CA-C	-5.62	99.15	110.40
1	c	46	ARG	CG-CD-NE	5.61	123.58	111.80
2	H	229	ARG	CB-CA-C	-5.60	99.20	110.40
1	x	46	ARG	CG-CD-NE	5.59	123.55	111.80
1	l	46	ARG	CG-CD-NE	5.59	123.54	111.80
2	R	47	ASP	CB-CG-OD1	5.59	123.33	118.30
2	S	272	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	C	363	VAL	CA-CB-CG2	5.58	119.27	110.90
1	z	46	ARG	CG-CD-NE	5.57	123.50	111.80
2	U	224	TYR	CB-CG-CD2	5.56	124.33	121.00
2	W	235	VAL	CA-CB-CG1	5.56	119.24	110.90
2	F	180	ALA	CB-CA-C	-5.55	101.77	110.10
1	f	276	ARG	CB-CG-CD	5.54	126.01	111.60
1	z	50	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	F	229	ARG	CB-CA-C	-5.52	99.36	110.40
2	O	272	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	D	229	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	M	370	LYS	CD-CE-NZ	5.52	124.39	111.70
2	H	283	HIS	CA-CB-CG	5.52	122.98	113.60
1	y	46	ARG	CG-CD-NE	5.52	123.38	111.80
2	Z	272	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	p	241	ARG	CB-CG-CD	-5.51	97.27	111.60
2	T	398	MET	CG-SD-CE	-5.51	91.39	100.20
2	G	229	ARG	CB-CA-C	-5.50	99.39	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	46	ARG	CG-CD-NE	5.50	123.34	111.80
2	U	272	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	t	50	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	d	241	ARG	CB-CG-CD	-5.47	97.37	111.60
2	V	370	LYS	CB-CG-CD	5.47	125.83	111.60
2	K	89	PRO	N-CD-CG	-5.46	95.01	103.20
1	i	276	ARG	CB-CG-CD	5.46	125.79	111.60
2	N	229	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	H	224	TYR	CB-CG-CD1	-5.46	117.73	121.00
2	F	370	LYS	CB-CG-CD	5.45	125.78	111.60
1	w	241	ARG	CB-CG-CD	-5.45	97.42	111.60
1	q	241	ARG	CB-CG-CD	-5.45	97.43	111.60
2	C	272	TYR	CB-CG-CD2	-5.44	117.73	121.00
1	b	241	ARG	CB-CG-CD	-5.44	97.46	111.60
2	T	229	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	o	50	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	g	222	TYR	CA-CB-CG	5.43	123.72	113.40
2	L	235	VAL	CA-CB-CG1	5.43	119.04	110.90
1	c	50	TYR	CB-CG-CD2	-5.43	117.74	121.00
2	I	370	LYS	CB-CG-CD	5.42	125.70	111.60
1	a	50	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	h	46	ARG	CG-CD-NE	5.42	123.18	111.80
1	e	241	ARG	CB-CG-CD	-5.41	97.53	111.60
2	K	283	HIS	CA-CB-CG	5.41	122.80	113.60
1	x	283	ALA	CB-CA-C	5.41	118.21	110.10
2	F	235	VAL	CA-CB-CG1	5.41	119.01	110.90
1	c	241	ARG	CB-CG-CD	-5.40	97.56	111.60
2	S	370	LYS	CB-CG-CD	5.40	125.64	111.60
1	a	46	ARG	CG-CD-NE	5.40	123.14	111.80
2	C	229	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	s	241	ARG	CB-CG-CD	-5.39	97.59	111.60
1	r	358	PRO	N-CA-CB	5.39	109.77	103.30
2	G	272	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	t	241	ARG	CB-CG-CD	-5.38	97.62	111.60
1	u	241	ARG	CB-CG-CD	-5.38	97.63	111.60
1	y	50	TYR	CB-CG-CD2	-5.38	117.78	121.00
1	a	241	ARG	CB-CG-CD	-5.37	97.64	111.60
1	r	241	ARG	CB-CG-CD	-5.37	97.65	111.60
2	L	318	LEU	CB-CG-CD1	5.36	120.11	111.00
2	X	370	LYS	CB-CG-CD	5.36	125.52	111.60
2	A	318	LEU	CB-CG-CD1	5.35	120.10	111.00
2	Q	370	LYS	CB-CG-CD	5.33	125.45	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	276	ARG	CB-CG-CD	5.32	125.43	111.60
2	T	272	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	o	46	ARG	CG-CD-NE	5.32	122.97	111.80
2	K	178	SER	CA-C-O	-5.32	108.94	120.10
1	d	276	ARG	CB-CG-CD	5.31	125.41	111.60
1	p	241	ARG	CB-CA-C	-5.31	99.78	110.40
1	s	241	ARG	CB-CA-C	-5.31	99.78	110.40
1	t	241	ARG	CB-CA-C	-5.31	99.78	110.40
1	s	50	TYR	CB-CG-CD2	-5.31	117.82	121.00
2	Y	370	LYS	CB-CG-CD	5.30	125.39	111.60
2	Z	60	LYS	CD-CE-NZ	-5.30	99.50	111.70
1	x	241	ARG	CB-CG-CD	-5.30	97.83	111.60
2	T	370	LYS	CB-CG-CD	5.29	125.37	111.60
1	d	282	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	l	241	ARG	CB-CG-CD	-5.29	97.86	111.60
1	o	241	ARG	CB-CG-CD	-5.29	97.86	111.60
2	E	272	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	v	241	ARG	CB-CG-CD	-5.28	97.87	111.60
1	j	241	ARG	CB-CG-CD	-5.27	97.90	111.60
2	J	235	VAL	CA-CB-CG1	5.27	118.80	110.90
2	Z	229	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	n	50	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	H	370	LYS	CB-CG-CD	5.26	125.28	111.60
2	W	240	ALA	CB-CA-C	5.26	117.99	110.10
2	E	370	LYS	CB-CG-CD	5.25	125.24	111.60
2	L	370	LYS	CB-CG-CD	5.25	125.24	111.60
1	n	241	ARG	CB-CG-CD	-5.25	97.96	111.60
2	M	235	VAL	CA-CB-CG1	5.23	118.74	110.90
1	l	87	PRO	N-CA-CB	5.22	109.57	103.30
1	k	241	ARG	CB-CG-CD	-5.22	98.02	111.60
1	f	241	ARG	CB-CG-CD	-5.22	98.03	111.60
1	d	50	TYR	CB-CG-CD1	5.22	124.13	121.00
2	Z	240	ALA	CB-CA-C	5.21	117.92	110.10
2	D	338	LYS	CG-CD-CE	5.21	127.54	111.90
1	p	50	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	g	46	ARG	CG-CD-NE	5.21	122.74	111.80
2	J	370	LYS	CB-CG-CD	5.21	125.15	111.60
2	A	224	TYR	CB-CG-CD1	5.21	124.12	121.00
1	r	241	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	n	46	ARG	CG-CD-NE	5.20	122.71	111.80
1	p	276	ARG	CB-CG-CD	5.19	125.10	111.60
2	V	240	ALA	CB-CA-C	5.19	117.89	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	50	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	q	363	MET	CB-CG-SD	5.18	127.94	112.40
2	H	224	TYR	CG-CD2-CE2	5.18	125.44	121.30
2	R	240	ALA	CB-CA-C	5.17	117.86	110.10
1	g	50	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	X	89	PRO	CA-CB-CG	-5.17	94.18	104.00
2	X	240	ALA	CB-CA-C	5.17	117.86	110.10
1	v	363	MET	CB-CG-SD	5.17	127.90	112.40
1	h	50	TYR	CB-CG-CD2	-5.16	117.90	121.00
2	U	240	ALA	CB-CA-C	5.16	117.84	110.10
2	B	283	HIS	CA-CB-CG	5.16	122.38	113.60
2	U	370	LYS	CB-CG-CD	5.16	125.02	111.60
1	k	50	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	m	241	ARG	CB-CG-CD	-5.16	98.20	111.60
2	Z	370	LYS	CB-CG-CD	5.16	125.00	111.60
2	C	370	LYS	CB-CG-CD	5.16	125.01	111.60
2	Q	5	ILE	CA-CB-CG2	-5.14	100.61	110.90
2	K	370	LYS	CB-CG-CD	5.14	124.98	111.60
2	O	240	ALA	CB-CA-C	5.14	117.81	110.10
2	C	224	TYR	CB-CG-CD2	5.14	124.08	121.00
1	u	50	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	l	242	PHE	CB-CG-CD1	-5.14	117.20	120.80
2	N	240	ALA	CB-CA-C	5.13	117.79	110.10
2	K	240	ALA	CB-CA-C	5.12	117.79	110.10
2	Y	240	ALA	CB-CA-C	5.12	117.78	110.10
2	G	283	HIS	CA-CB-CG	5.12	122.31	113.60
1	o	50	TYR	CB-CG-CD1	5.12	124.07	121.00
2	O	370	LYS	CB-CG-CD	5.12	124.91	111.60
2	K	180	ALA	CB-CA-C	-5.12	102.42	110.10
1	w	242	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	x	50	TYR	CB-CG-CD2	-5.11	117.93	121.00
2	H	240	ALA	CB-CA-C	5.11	117.77	110.10
2	N	370	LYS	CB-CG-CD	5.11	124.88	111.60
2	T	240	ALA	CB-CA-C	5.11	117.76	110.10
2	B	318	LEU	CB-CG-CD1	5.10	119.68	111.00
1	i	50	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	B	367	ASP	CB-CA-C	5.10	120.61	110.40
1	z	241	ARG	CB-CG-CD	-5.10	98.33	111.60
2	A	367	ASP	CB-CA-C	5.10	120.60	110.40
1	c	242	PHE	CB-CG-CD1	-5.10	117.23	120.80
2	W	370	LYS	CB-CG-CD	5.10	124.86	111.60
2	G	370	LYS	CB-CG-CD	5.10	124.85	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	283	HIS	CA-CB-CG	5.09	122.25	113.60
2	S	235	VAL	CA-CB-CG1	5.09	118.53	110.90
2	Y	235	VAL	CA-CB-CG1	5.09	118.53	110.90
2	F	240	ALA	CB-CA-C	5.09	117.73	110.10
1	v	50	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	B	240	ALA	CB-CA-C	5.08	117.72	110.10
1	m	50	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	Q	240	ALA	CB-CA-C	5.08	117.71	110.10
2	C	240	ALA	CB-CA-C	5.08	117.71	110.10
2	D	235	VAL	CA-CB-CG1	5.08	118.51	110.90
1	n	276	ARG	CB-CG-CD	5.08	124.80	111.60
2	E	367	ASP	CB-CA-C	5.07	120.54	110.40
1	v	242	PHE	CB-CG-CD1	-5.07	117.25	120.80
2	J	240	ALA	CB-CA-C	5.06	117.69	110.10
1	i	241	ARG	CB-CG-CD	-5.06	98.45	111.60
2	K	367	ASP	CB-CA-C	5.06	120.52	110.40
1	f	50	TYR	CB-CG-CD2	-5.06	117.97	121.00
2	Q	235	VAL	CA-CB-CG1	5.05	118.48	110.90
2	R	370	LYS	CB-CG-CD	5.05	124.73	111.60
2	I	240	ALA	CB-CA-C	5.05	117.67	110.10
2	G	240	ALA	CB-CA-C	5.04	117.67	110.10
1	h	241	ARG	CB-CG-CD	-5.04	98.50	111.60
1	r	392	LYS	CB-CG-CD	5.04	124.70	111.60
2	V	235	VAL	CA-CB-CG1	5.04	118.45	110.90
1	m	185	ALA	CB-CA-C	5.03	117.65	110.10
2	M	240	ALA	CB-CA-C	5.03	117.65	110.10
1	l	50	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	S	240	ALA	CB-CA-C	5.03	117.64	110.10
2	Y	5	ILE	CA-CB-CG2	-5.03	100.85	110.90
2	T	235	VAL	CA-CB-CG1	5.02	118.43	110.90
2	A	240	ALA	CB-CA-C	5.02	117.63	110.10
2	P	240	ALA	CB-CA-C	5.02	117.63	110.10
1	d	283	ALA	CB-CA-C	5.02	117.63	110.10
2	A	235	VAL	CA-CB-CG1	5.02	118.42	110.90
2	L	367	ASP	CB-CA-C	5.02	120.43	110.40
2	D	240	ALA	CB-CA-C	5.01	117.62	110.10
2	E	235	VAL	CA-CB-CG1	5.01	118.42	110.90
1	s	276	ARG	CB-CG-CD	5.01	124.64	111.60
1	c	392	LYS	CB-CG-CD	5.01	124.63	111.60
2	T	224	TYR	CB-CG-CD2	5.01	124.01	121.00
2	M	367	ASP	CB-CA-C	5.01	120.42	110.40
2	K	224	TYR	CB-CG-CD2	5.01	124.01	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	241	ARG	CB-CG-CD	-5.01	98.58	111.60
2	N	367	ASP	CB-CA-C	5.01	120.41	110.40
2	H	367	ASP	CB-CA-C	5.01	120.41	110.40
1	o	276	ARG	CB-CG-CD	5.00	124.61	111.60
2	N	5	ILE	CA-CB-CG2	-5.00	100.90	110.90
2	E	240	ALA	CB-CA-C	5.00	117.60	110.10

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	347	CYS	Peptide
2	B	347	CYS	Peptide
2	C	347	CYS	Peptide
2	D	347	CYS	Peptide
2	E	347	CYS	Peptide
2	F	347	CYS	Peptide
2	G	347	CYS	Peptide
2	H	347	CYS	Peptide
2	I	347	CYS	Peptide
2	J	347	CYS	Peptide
2	K	347	CYS	Peptide
2	L	347	CYS	Peptide
2	M	347	CYS	Peptide
2	N	347	CYS	Peptide
2	O	347	CYS	Peptide
2	P	347	CYS	Peptide
2	Q	347	CYS	Peptide
2	R	347	CYS	Peptide
2	S	347	CYS	Peptide
2	T	347	CYS	Peptide
2	U	347	CYS	Peptide
2	V	347	CYS	Peptide
2	W	347	CYS	Peptide
2	X	347	CYS	Peptide
2	Y	347	CYS	Peptide
2	Z	347	CYS	Peptide
1	e	285	THR	Mainchain
1	h	222	TYR	Sidechain
1	i	310	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

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	427/446 (96%)	389 (91%)	36 (8%)	2 (0%)	29	69
1	b	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	c	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	d	427/446 (96%)	389 (91%)	36 (8%)	2 (0%)	29	69
1	e	427/446 (96%)	388 (91%)	37 (9%)	2 (0%)	29	69
1	f	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
1	g	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
1	h	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	i	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	j	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	k	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	l	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	m	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	n	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	o	427/446 (96%)	392 (92%)	33 (8%)	2 (0%)	29	69
1	p	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	q	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	r	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
1	s	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
1	t	427/446 (96%)	392 (92%)	33 (8%)	2 (0%)	29	69
1	u	427/446 (96%)	392 (92%)	33 (8%)	2 (0%)	29	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
1	w	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
1	x	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	y	427/446 (96%)	390 (91%)	35 (8%)	2 (0%)	29	69
1	z	427/446 (96%)	391 (92%)	34 (8%)	2 (0%)	29	69
2	A	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	B	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	C	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	D	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	E	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	F	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	G	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	H	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	I	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	J	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	K	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	L	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	M	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	N	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	O	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	P	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	Q	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	R	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	S	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	T	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	U	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	V	439/451 (97%)	402 (92%)	36 (8%)	1 (0%)	47	81
2	W	439/451 (97%)	404 (92%)	34 (8%)	1 (0%)	47	81
2	X	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	Y	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81
2	Z	439/451 (97%)	403 (92%)	35 (8%)	1 (0%)	47	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	22516/23322 (96%)	20640 (92%)	1798 (8%)	78 (0%)	44	76

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	304	LYS
2	F	304	LYS
2	G	304	LYS
2	H	304	LYS
2	J	304	LYS
2	L	304	LYS
2	N	304	LYS
2	O	304	LYS
2	P	304	LYS
2	Q	304	LYS
2	R	304	LYS
2	S	304	LYS
2	T	304	LYS
2	U	304	LYS
2	V	304	LYS
2	W	304	LYS
2	X	304	LYS
2	Y	304	LYS
2	Z	304	LYS
2	A	304	LYS
2	C	304	LYS
2	D	304	LYS
2	E	304	LYS
2	I	304	LYS
2	K	304	LYS
2	M	304	LYS
1	e	360	GLY
1	a	360	GLY
1	b	360	GLY
1	c	259	PRO
1	c	360	GLY
1	d	360	GLY
1	f	259	PRO
1	f	360	GLY
1	g	360	GLY
1	h	259	PRO
1	h	360	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	259	PRO
1	i	360	GLY
1	j	259	PRO
1	j	360	GLY
1	k	259	PRO
1	k	360	GLY
1	l	259	PRO
1	l	360	GLY
1	m	259	PRO
1	m	360	GLY
1	n	259	PRO
1	o	259	PRO
1	q	259	PRO
1	r	259	PRO
1	u	360	GLY
1	y	259	PRO
1	y	360	GLY
1	z	259	PRO
1	a	259	PRO
1	b	259	PRO
1	d	259	PRO
1	e	259	PRO
1	g	259	PRO
1	n	360	GLY
1	o	360	GLY
1	p	259	PRO
1	p	360	GLY
1	r	360	GLY
1	s	259	PRO
1	s	360	GLY
1	t	259	PRO
1	t	360	GLY
1	u	259	PRO
1	v	259	PRO
1	v	360	GLY
1	w	259	PRO
1	w	360	GLY
1	x	259	PRO
1	x	360	GLY
1	z	360	GLY
1	q	360	GLY

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	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	b	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	c	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	d	371/383 (97%)	366 (99%)	5 (1%)	69	82
1	e	371/383 (97%)	366 (99%)	5 (1%)	69	82
1	f	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	g	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	h	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	i	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	j	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	k	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	l	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	m	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	n	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	o	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	p	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	q	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	r	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	s	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	t	371/383 (97%)	367 (99%)	4 (1%)	73	84
1	u	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	v	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	w	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	x	371/383 (97%)	368 (99%)	3 (1%)	81	89
1	y	371/383 (97%)	366 (99%)	5 (1%)	69	82
1	z	371/383 (97%)	368 (99%)	3 (1%)	81	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	B	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	D	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	E	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	F	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	G	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	H	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	I	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	J	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	K	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	L	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	M	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	N	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	O	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	P	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	Q	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	R	372/379 (98%)	367 (99%)	5 (1%)	69	82
2	S	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	T	372/379 (98%)	369 (99%)	3 (1%)	81	89
2	U	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	V	372/379 (98%)	367 (99%)	5 (1%)	69	82
2	W	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	X	372/379 (98%)	367 (99%)	5 (1%)	69	82
2	Y	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	Z	372/379 (98%)	368 (99%)	4 (1%)	73	84
All	All	19318/19812 (98%)	19128 (99%)	190 (1%)	77	86

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	222	TYR
1	a	276	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	418	LEU
1	b	1	MET
1	b	222	TYR
1	b	276	ARG
1	b	418	LEU
1	c	1	MET
1	c	222	TYR
1	c	276	ARG
1	c	418	LEU
1	d	1	MET
1	d	222	TYR
1	d	276	ARG
1	d	300	MET
1	d	418	LEU
1	e	1	MET
1	e	222	TYR
1	e	276	ARG
1	e	300	MET
1	e	418	LEU
1	f	1	MET
1	f	222	TYR
1	f	276	ARG
1	f	418	LEU
1	g	1	MET
1	g	276	ARG
1	g	418	LEU
1	h	1	MET
1	h	222	TYR
1	h	276	ARG
1	h	418	LEU
1	i	1	MET
1	i	222	TYR
1	i	276	ARG
1	i	418	LEU
1	j	222	TYR
1	j	276	ARG
1	j	418	LEU
1	k	1	MET
1	k	222	TYR
1	k	276	ARG
1	k	418	LEU
1	l	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	l	276	ARG
1	l	418	LEU
1	m	1	MET
1	m	222	TYR
1	m	276	ARG
1	m	418	LEU
2	N	2	ARG
2	N	89	PRO
2	N	283	HIS
2	N	326	LYS
2	O	2	ARG
2	O	89	PRO
2	O	283	HIS
2	O	326	LYS
2	P	2	ARG
2	P	89	PRO
2	P	283	HIS
2	P	326	LYS
2	Q	2	ARG
2	Q	89	PRO
2	Q	283	HIS
2	Q	326	LYS
2	R	2	ARG
2	R	89	PRO
2	R	283	HIS
2	R	326	LYS
2	R	368	LEU
2	S	2	ARG
2	S	283	HIS
2	S	326	LYS
2	T	2	ARG
2	T	283	HIS
2	T	326	LYS
2	U	2	ARG
2	U	60	LYS
2	U	283	HIS
2	U	326	LYS
2	V	2	ARG
2	V	60	LYS
2	V	89	PRO
2	V	283	HIS
2	V	326	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	W	2	ARG
2	W	89	PRO
2	W	283	HIS
2	W	326	LYS
2	X	2	ARG
2	X	60	LYS
2	X	89	PRO
2	X	283	HIS
2	X	326	LYS
2	Y	2	ARG
2	Y	89	PRO
2	Y	283	HIS
2	Y	326	LYS
2	Z	2	ARG
2	Z	89	PRO
2	Z	283	HIS
2	Z	326	LYS
2	A	2	ARG
2	A	283	HIS
2	A	326	LYS
2	B	2	ARG
2	B	283	HIS
2	B	326	LYS
2	C	2	ARG
2	C	89	PRO
2	C	283	HIS
2	C	326	LYS
2	D	2	ARG
2	D	283	HIS
2	D	326	LYS
2	E	2	ARG
2	E	283	HIS
2	E	326	LYS
2	F	2	ARG
2	F	42	ILE
2	F	283	HIS
2	F	326	LYS
2	G	2	ARG
2	G	42	ILE
2	G	283	HIS
2	G	326	LYS
2	H	2	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	283	HIS
2	H	326	LYS
2	I	2	ARG
2	I	283	HIS
2	I	326	LYS
2	J	2	ARG
2	J	224	TYR
2	J	283	HIS
2	J	326	LYS
2	K	2	ARG
2	K	89	PRO
2	K	283	HIS
2	K	326	LYS
2	L	2	ARG
2	L	283	HIS
2	L	326	LYS
2	M	2	ARG
2	M	283	HIS
2	M	326	LYS
1	n	222	TYR
1	n	276	ARG
1	n	418	LEU
1	o	222	TYR
1	o	276	ARG
1	o	300	MET
1	o	418	LEU
1	p	222	TYR
1	p	276	ARG
1	p	418	LEU
1	q	222	TYR
1	q	276	ARG
1	q	418	LEU
1	r	222	TYR
1	r	276	ARG
1	r	418	LEU
1	s	222	TYR
1	s	276	ARG
1	s	418	LEU
1	t	122	LYS
1	t	222	TYR
1	t	276	ARG
1	t	418	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	u	222	TYR
1	u	276	ARG
1	u	418	LEU
1	v	222	TYR
1	v	276	ARG
1	v	418	LEU
1	w	222	TYR
1	w	276	ARG
1	w	418	LEU
1	x	222	TYR
1	x	276	ARG
1	x	418	LEU
1	y	1	MET
1	y	222	TYR
1	y	276	ARG
1	y	300	MET
1	y	418	LEU
1	z	222	TYR
1	z	276	ARG
1	z	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	347	ASN
1	b	347	ASN
1	c	347	ASN
1	d	347	ASN
1	e	347	ASN
1	f	347	ASN
1	g	347	ASN
1	h	347	ASN
1	i	347	ASN
1	j	347	ASN
1	k	347	ASN
1	l	347	ASN
1	m	347	ASN
2	N	258	ASN
2	N	285	GLN
2	O	258	ASN
2	P	258	ASN
2	Q	258	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	258	ASN
2	S	258	ASN
2	T	258	ASN
2	U	258	ASN
2	V	258	ASN
2	W	258	ASN
2	W	283	HIS
2	W	285	GLN
2	X	101	ASN
2	X	258	ASN
2	X	285	GLN
2	Y	258	ASN
2	Y	285	GLN
2	Z	258	ASN
2	Z	285	GLN
2	A	258	ASN
2	B	258	ASN
2	C	258	ASN
2	D	258	ASN
2	E	258	ASN
2	F	258	ASN
2	F	342	GLN
2	G	258	ASN
2	G	342	GLN
2	H	258	ASN
2	H	342	GLN
2	I	258	ASN
2	J	228	ASN
2	J	258	ASN
2	K	258	ASN
2	L	258	ASN
2	M	258	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 13 are monoatomic - leaving 39 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	$\#\|Z\| > 2$
6	GTP	P	502	5	26,34,34	1.39	3 (11%)	32,54,54	2.71	10 (31%)
3	TA1	m	601	-	68,68,68	1.27	7 (10%)	105,105,105	1.48	16 (15%)
4	GDP	f	602	-	24,30,30	1.23	3 (12%)	30,47,47	2.04	10 (33%)
3	TA1	g	601	-	68,68,68	1.67	14 (20%)	105,105,105	3.19	39 (37%)
4	GDP	e	602	-	24,30,30	1.20	3 (12%)	30,47,47	1.83	7 (23%)
4	GDP	i	602	-	24,30,30	1.30	4 (16%)	30,47,47	2.06	10 (33%)
4	GDP	c	602	-	24,30,30	1.68	6 (25%)	30,47,47	2.00	9 (30%)
3	TA1	a	601	-	68,68,68	1.00	3 (4%)	105,105,105	1.20	11 (10%)
6	GTP	O	502	5	26,34,34	1.36	3 (11%)	32,54,54	1.68	6 (18%)
4	GDP	h	602	-	24,30,30	1.32	3 (12%)	30,47,47	2.17	11 (36%)
4	GDP	j	602	-	24,30,30	1.15	1 (4%)	30,47,47	1.90	9 (30%)
6	GTP	Q	502	5	26,34,34	1.65	6 (23%)	32,54,54	1.81	9 (28%)
4	GDP	d	602	-	24,30,30	1.23	2 (8%)	30,47,47	2.06	11 (36%)
4	GDP	k	602	-	24,30,30	1.14	1 (4%)	30,47,47	1.87	8 (26%)
3	TA1	j	601	-	68,68,68	1.03	4 (5%)	105,105,105	1.35	13 (12%)
3	TA1	c	601	-	68,68,68	1.06	5 (7%)	105,105,105	1.45	15 (14%)
3	TA1	i	601	-	68,68,68	1.02	4 (5%)	105,105,105	1.26	11 (10%)
3	TA1	d	601	-	68,68,68	1.12	6 (8%)	105,105,105	1.25	12 (11%)
6	GTP	R	502	5	26,34,34	1.80	4 (15%)	32,54,54	1.91	10 (31%)
3	TA1	k	601	-	68,68,68	1.62	12 (17%)	105,105,105	1.96	22 (20%)
3	TA1	h	601	-	68,68,68	1.20	7 (10%)	105,105,105	1.66	15 (14%)
6	GTP	Y	502	5	26,34,34	1.20	1 (3%)	32,54,54	1.58	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\vert Z\vert > 2$	Counts	RMSZ	$\#\vert Z\vert > 2$
4	GDP	l	602	-	24,30,30	1.01	1 (4%)	30,47,47	1.81	8 (26%)
6	GTP	S	502	5	26,34,34	1.70	4 (15%)	32,54,54	2.23	11 (34%)
6	GTP	V	502	5	26,34,34	1.70	4 (15%)	32,54,54	1.73	8 (25%)
4	GDP	m	602	-	24,30,30	1.20	3 (12%)	30,47,47	1.88	7 (23%)
6	GTP	N	502	5	26,34,34	1.49	3 (11%)	32,54,54	1.25	3 (9%)
6	GTP	U	502	5	26,34,34	2.20	7 (26%)	32,54,54	2.61	13 (40%)
4	GDP	a	602	-	24,30,30	1.27	2 (8%)	30,47,47	1.76	4 (13%)
6	GTP	W	502	5	26,34,34	2.39	7 (26%)	32,54,54	2.20	8 (25%)
3	TA1	f	601	-	68,68,68	1.49	11 (16%)	105,105,105	1.59	20 (19%)
3	TA1	e	601	-	68,68,68	1.18	6 (8%)	105,105,105	1.47	18 (17%)
6	GTP	X	502	5	26,34,34	1.10	2 (7%)	32,54,54	1.39	5 (15%)
4	GDP	b	602	-	24,30,30	1.42	4 (16%)	30,47,47	1.83	7 (23%)
3	TA1	l	601	-	68,68,68	1.06	5 (7%)	105,105,105	1.21	13 (12%)
6	GTP	Z	502	5	26,34,34	1.70	4 (15%)	32,54,54	2.04	4 (12%)
4	GDP	g	602	1	24,30,30	1.36	4 (16%)	30,47,47	1.97	11 (36%)
3	TA1	b	601	-	68,68,68	1.16	6 (8%)	105,105,105	1.37	13 (12%)
6	GTP	T	502	5	26,34,34	1.90	7 (26%)	32,54,54	3.39	15 (46%)

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
6	GTP	P	502	5	-	5/18/38/38	0/3/3/3
3	TA1	m	601	-	-	10/41/127/127	0/7/7/7
4	GDP	f	602	-	-	4/12/32/32	0/3/3/3
3	TA1	g	601	-	-	14/41/127/127	0/7/7/7
4	GDP	e	602	-	-	5/12/32/32	0/3/3/3
4	GDP	i	602	-	-	4/12/32/32	0/3/3/3
4	GDP	c	602	-	-	4/12/32/32	0/3/3/3
3	TA1	a	601	-	-	8/41/127/127	0/7/7/7
6	GTP	O	502	5	-	2/18/38/38	0/3/3/3
4	GDP	h	602	-	-	5/12/32/32	0/3/3/3
4	GDP	j	602	-	-	5/12/32/32	0/3/3/3
6	GTP	Q	502	5	-	4/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	d	602	-	-	4/12/32/32	0/3/3/3
4	GDP	k	602	-	-	5/12/32/32	0/3/3/3
3	TA1	j	601	-	-	10/41/127/127	0/7/7/7
3	TA1	c	601	-	-	9/41/127/127	0/7/7/7
3	TA1	i	601	-	-	12/41/127/127	0/7/7/7
3	TA1	d	601	-	-	8/41/127/127	0/7/7/7
6	GTP	R	502	5	-	2/18/38/38	0/3/3/3
3	TA1	k	601	-	-	9/41/127/127	0/7/7/7
3	TA1	h	601	-	-	13/41/127/127	0/7/7/7
6	GTP	Y	502	5	-	4/18/38/38	0/3/3/3
4	GDP	l	602	-	-	5/12/32/32	0/3/3/3
6	GTP	S	502	5	-	4/18/38/38	0/3/3/3
6	GTP	V	502	5	-	3/18/38/38	0/3/3/3
4	GDP	m	602	-	-	5/12/32/32	0/3/3/3
6	GTP	N	502	5	-	3/18/38/38	0/3/3/3
6	GTP	U	502	5	-	2/18/38/38	0/3/3/3
4	GDP	a	602	-	-	4/12/32/32	0/3/3/3
6	GTP	W	502	5	-	3/18/38/38	0/3/3/3
3	TA1	f	601	-	-	6/41/127/127	0/7/7/7
3	TA1	e	601	-	-	8/41/127/127	0/7/7/7
6	GTP	X	502	5	-	3/18/38/38	0/3/3/3
4	GDP	b	602	-	-	5/12/32/32	0/3/3/3
3	TA1	l	601	-	-	10/41/127/127	0/7/7/7
6	GTP	Z	502	5	-	6/18/38/38	0/3/3/3
4	GDP	g	602	1	-	5/12/32/32	0/3/3/3
3	TA1	b	601	-	-	10/41/127/127	0/7/7/7
6	GTP	T	502	5	-	2/18/38/38	0/3/3/3

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	502	GTP	C6-N1	8.27	1.50	1.37
6	U	502	GTP	C6-N1	6.72	1.47	1.37
6	R	502	GTP	C6-N1	5.60	1.46	1.37
3	f	601	TA1	C45-C24	5.60	1.64	1.54
4	c	602	GDP	O4'-C1'	5.52	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	502	GTP	C5-C6	-5.35	1.36	1.47
6	N	502	GTP	C6-N1	5.35	1.45	1.37
6	U	502	GTP	C2'-C1'	5.30	1.61	1.53
6	S	502	GTP	C5-C6	-5.09	1.37	1.47
3	k	601	TA1	C45-C24	4.98	1.62	1.54
6	Z	502	GTP	C2'-C1'	4.96	1.61	1.53
6	W	502	GTP	C4-N3	4.81	1.49	1.37
3	k	601	TA1	C18-C10	4.77	1.68	1.57
6	T	502	GTP	O4'-C1'	4.64	1.47	1.41
6	T	502	GTP	C2'-C1'	4.62	1.60	1.53
3	g	601	TA1	C31-C30	4.57	1.59	1.50
6	V	502	GTP	C8-N7	-4.43	1.27	1.35
6	Q	502	GTP	C6-N1	4.40	1.44	1.37
3	f	601	TA1	C18-C10	4.17	1.66	1.57
6	Z	502	GTP	O4'-C1'	4.09	1.46	1.41
3	g	601	TA1	C30-N01	4.07	1.43	1.34
3	m	601	TA1	C45-C24	4.04	1.61	1.54
6	O	502	GTP	C6-N1	4.03	1.43	1.37
3	b	601	TA1	C45-C24	3.99	1.61	1.54
4	k	602	GDP	O4'-C1'	3.95	1.46	1.41
3	g	601	TA1	C04-C03	-3.92	1.40	1.50
3	h	601	TA1	O07-C17	-3.90	1.37	1.43
3	m	601	TA1	C43-C26	3.86	1.60	1.52
3	k	601	TA1	C21-C24	3.86	1.60	1.51
6	W	502	GTP	C2'-C1'	3.86	1.59	1.53
3	g	601	TA1	C42-C37	3.85	1.45	1.39
6	S	502	GTP	C8-N7	-3.82	1.28	1.35
3	k	601	TA1	C31-C30	3.81	1.58	1.50
6	R	502	GTP	C2'-C1'	3.75	1.59	1.53
3	m	601	TA1	O11-C26	3.74	1.52	1.45
6	U	502	GTP	O6-C6	3.73	1.30	1.23
6	P	502	GTP	O6-C6	3.72	1.30	1.23
3	e	601	TA1	C45-C24	3.66	1.60	1.54
3	a	601	TA1	C45-C24	3.62	1.60	1.54
4	f	602	GDP	O4'-C1'	3.59	1.46	1.41
3	c	601	TA1	C45-C24	3.57	1.60	1.54
3	g	601	TA1	C38-C37	-3.47	1.33	1.39
3	g	601	TA1	C37-C29	3.46	1.56	1.52
6	Y	502	GTP	C2'-C1'	3.45	1.59	1.53
3	g	601	TA1	C43-C26	3.40	1.59	1.52
3	l	601	TA1	C45-C24	3.39	1.60	1.54
6	S	502	GTP	C6-N1	3.38	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	502	GTP	O6-C6	3.38	1.30	1.23
3	c	601	TA1	C43-C26	3.36	1.59	1.52
6	O	502	GTP	C5-C6	-3.35	1.40	1.47
4	a	602	GDP	C6-N1	-3.34	1.32	1.37
3	g	601	TA1	C32-C31	3.30	1.45	1.39
3	m	601	TA1	C25-C24	3.30	1.39	1.34
6	P	502	GTP	O5'-C5'	3.29	1.57	1.44
3	k	601	TA1	C30-N01	3.24	1.41	1.34
3	l	601	TA1	C43-C26	3.23	1.59	1.52
3	e	601	TA1	C18-C10	3.23	1.64	1.57
3	h	601	TA1	C43-C26	3.22	1.59	1.52
4	b	602	GDP	C2'-C1'	-3.20	1.48	1.53
3	j	601	TA1	O11-C26	3.18	1.51	1.45
4	h	602	GDP	O4'-C1'	3.16	1.45	1.41
3	j	601	TA1	C45-C24	3.15	1.59	1.54
4	l	602	GDP	O4'-C1'	3.15	1.45	1.41
4	d	602	GDP	O4'-C1'	3.14	1.45	1.41
3	k	601	TA1	C32-C31	3.12	1.44	1.39
4	e	602	GDP	O4'-C1'	3.08	1.45	1.41
3	k	601	TA1	C43-C26	3.08	1.58	1.52
3	f	601	TA1	C43-C26	3.07	1.58	1.52
4	d	602	GDP	C2-N3	3.05	1.40	1.33
4	g	602	GDP	O4'-C1'	3.04	1.45	1.41
3	b	601	TA1	O11-C26	3.00	1.51	1.45
4	j	602	GDP	O4'-C1'	2.99	1.45	1.41
3	f	601	TA1	C30-N01	2.99	1.40	1.34
3	i	601	TA1	C45-C24	2.98	1.59	1.54
3	d	601	TA1	C18-C10	2.94	1.63	1.57
3	b	601	TA1	C43-C26	2.89	1.58	1.52
3	k	601	TA1	C10-C02	2.89	1.64	1.57
6	R	502	GTP	C4-N3	2.88	1.44	1.37
4	g	602	GDP	C5-C6	2.87	1.53	1.47
3	f	601	TA1	C31-C30	2.87	1.56	1.50
6	Q	502	GTP	C2'-C1'	2.87	1.58	1.53
4	m	602	GDP	O4'-C1'	2.86	1.45	1.41
6	W	502	GTP	C8-N7	-2.84	1.30	1.35
3	j	601	TA1	C43-C26	2.84	1.58	1.52
6	X	502	GTP	C6-N1	2.84	1.42	1.37
6	U	502	GTP	O2'-C2'	2.84	1.49	1.43
6	P	502	GTP	C6-N1	2.81	1.42	1.37
3	i	601	TA1	C43-C26	2.80	1.58	1.52
3	d	601	TA1	C43-C26	2.80	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	601	TA1	C10-C02	2.79	1.64	1.57
4	i	602	GDP	O4'-C4'	2.76	1.51	1.45
3	a	601	TA1	C43-C26	2.73	1.58	1.52
6	T	502	GTP	C4-N3	2.72	1.44	1.37
3	e	601	TA1	C43-C26	2.72	1.58	1.52
6	Q	502	GTP	C5-C6	2.70	1.52	1.47
6	W	502	GTP	O4'-C1'	2.70	1.44	1.41
6	Z	502	GTP	C4-N3	2.69	1.43	1.37
3	k	601	TA1	C26-C25	2.69	1.56	1.51
3	c	601	TA1	O11-C26	2.66	1.50	1.45
6	N	502	GTP	C8-N7	-2.64	1.30	1.35
3	g	601	TA1	C45-C24	2.61	1.58	1.54
3	l	601	TA1	O11-C26	2.60	1.50	1.45
4	g	602	GDP	C2-N3	2.59	1.39	1.33
3	h	601	TA1	C31-C30	2.57	1.55	1.50
6	T	502	GTP	O2'-C2'	2.55	1.49	1.43
3	d	601	TA1	C45-C24	2.55	1.58	1.54
6	U	502	GTP	C2-N1	2.54	1.43	1.37
3	k	601	TA1	C11-C15	2.52	1.59	1.55
4	e	602	GDP	C2-N3	2.50	1.39	1.33
3	j	601	TA1	C25-C24	2.50	1.38	1.34
3	k	601	TA1	O02-C02	2.49	1.49	1.45
3	d	601	TA1	O11-C26	2.49	1.50	1.45
3	m	601	TA1	C43-C01	2.47	1.59	1.54
3	f	601	TA1	C11-C15	2.47	1.59	1.55
6	Z	502	GTP	O2'-C2'	2.46	1.48	1.43
3	f	601	TA1	C18-C17	2.46	1.63	1.55
3	m	601	TA1	C31-C30	2.45	1.55	1.50
3	i	601	TA1	C31-C30	2.45	1.55	1.50
6	T	502	GTP	C2'-C3'	2.44	1.60	1.53
6	S	502	GTP	O4'-C1'	2.42	1.44	1.41
3	k	601	TA1	C37-C29	2.41	1.55	1.52
6	T	502	GTP	C5-C6	2.39	1.52	1.47
3	a	601	TA1	O11-C26	2.38	1.50	1.45
6	U	502	GTP	C8-N7	-2.36	1.31	1.35
4	m	602	GDP	O2'-C2'	2.36	1.48	1.43
6	Q	502	GTP	C4-N3	2.36	1.43	1.37
6	V	502	GTP	O4'-C1'	2.34	1.44	1.41
3	f	601	TA1	O11-C26	2.33	1.50	1.45
3	d	601	TA1	O09-C21	2.32	1.50	1.45
6	R	502	GTP	O6-C6	2.32	1.28	1.23
4	e	602	GDP	C2'-C1'	-2.32	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	502	GTP	C2-N1	-2.32	1.32	1.37
3	g	601	TA1	O14-C30	2.31	1.28	1.23
3	b	601	TA1	C37-C29	2.31	1.55	1.52
6	N	502	GTP	C4-N3	2.31	1.43	1.37
4	i	602	GDP	C2-N3	2.31	1.38	1.33
4	h	602	GDP	C5-C4	2.30	1.49	1.43
4	c	602	GDP	C8-N7	-2.30	1.31	1.35
4	i	602	GDP	O2'-C2'	2.30	1.48	1.43
3	e	601	TA1	O09-C21	2.29	1.50	1.45
6	V	502	GTP	C5-C4	-2.29	1.37	1.43
4	h	602	GDP	C2-N3	2.29	1.38	1.33
4	m	602	GDP	C2-N3	2.29	1.38	1.33
3	c	601	TA1	C25-C24	2.29	1.38	1.34
3	g	601	TA1	C06-C05	-2.28	1.34	1.38
4	b	602	GDP	C5-C4	2.28	1.48	1.43
6	W	502	GTP	C2-N1	2.28	1.43	1.37
4	b	602	GDP	O6-C6	2.25	1.27	1.23
3	e	601	TA1	C37-C29	2.24	1.55	1.52
3	m	601	TA1	C30-N01	2.23	1.39	1.34
4	f	602	GDP	C2'-C1'	-2.22	1.50	1.53
3	i	601	TA1	O11-C26	2.21	1.50	1.45
3	c	601	TA1	O09-C21	2.21	1.50	1.45
4	g	602	GDP	C5-C4	2.20	1.48	1.43
4	a	602	GDP	C5-C6	2.18	1.51	1.47
6	Q	502	GTP	O4'-C1'	2.18	1.44	1.41
4	c	602	GDP	C3'-C4'	2.18	1.58	1.53
3	g	601	TA1	C11-C10	2.17	1.59	1.54
3	d	601	TA1	C11-C15	2.16	1.59	1.55
3	h	601	TA1	C30-N01	2.15	1.38	1.34
3	h	601	TA1	C45-C24	2.14	1.57	1.54
4	c	602	GDP	O2'-C2'	2.14	1.48	1.43
6	O	502	GTP	C8-N7	-2.13	1.31	1.35
3	f	601	TA1	C25-C24	2.11	1.37	1.34
4	f	602	GDP	C5-C4	2.11	1.48	1.43
3	h	601	TA1	O11-C26	2.10	1.49	1.45
3	g	601	TA1	C01-C02	2.09	1.64	1.57
4	c	602	GDP	C2'-C1'	-2.07	1.50	1.53
3	e	601	TA1	C10-C02	2.07	1.62	1.57
6	U	502	GTP	O4'-C1'	2.06	1.44	1.41
6	X	502	GTP	C2'-C1'	2.06	1.56	1.53
3	h	601	TA1	C25-C24	2.06	1.37	1.34
3	b	601	TA1	C25-C24	2.05	1.37	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	601	TA1	C25-C24	2.04	1.37	1.34
4	i	602	GDP	C5-C6	2.04	1.51	1.47
3	g	601	TA1	O13-C28	-2.04	1.38	1.42
6	W	502	GTP	C2-N2	2.03	1.39	1.34
3	b	601	TA1	C18-C20	2.03	1.61	1.55
3	f	601	TA1	C11-C10	2.02	1.59	1.54
4	c	602	GDP	C5-C4	2.02	1.48	1.43
3	l	601	TA1	C31-C30	2.01	1.54	1.50
4	b	602	GDP	O4'-C1'	2.00	1.43	1.41

All (437) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	g	601	TA1	C42-C37-C29	15.01	144.64	120.78
3	g	601	TA1	C38-C37-C29	-14.24	98.14	120.78
6	T	502	GTP	O6-C6-N1	-12.05	106.42	120.65
3	g	601	TA1	C05-C04-C03	-8.37	101.51	120.40
3	k	601	TA1	C45-C24-C25	-7.33	109.48	119.61
3	g	601	TA1	C09-C04-C05	7.05	128.63	118.59
6	T	502	GTP	PA-O3A-PB	6.93	156.61	132.83
6	Z	502	GTP	O2'-C2'-C1'	6.79	135.93	110.85
6	W	502	GTP	PA-O3A-PB	6.63	155.59	132.83
6	P	502	GTP	O5'-C5'-C4'	6.48	131.31	108.99
6	S	502	GTP	O6-C6-N1	6.38	128.18	120.65
3	g	601	TA1	C11-O04-C12	6.27	135.29	119.06
3	h	601	TA1	O07-C17-C16	-6.26	96.37	109.12
3	g	601	TA1	O02-C03-O03	6.10	133.47	123.53
6	U	502	GTP	PA-O3A-PB	6.05	153.59	132.83
6	P	502	GTP	C5-C6-N1	-5.98	103.40	113.95
6	U	502	GTP	O2'-C2'-C1'	5.83	132.37	110.85
6	U	502	GTP	C5-C6-N1	-5.77	103.76	113.95
4	a	602	GDP	C8-N7-C5	5.54	113.54	102.99
6	T	502	GTP	O2'-C2'-C1'	5.52	131.23	110.85
3	g	601	TA1	C08-C09-C04	-5.44	113.90	120.34
3	g	601	TA1	C02-O02-C03	5.38	127.96	117.79
4	d	602	GDP	C8-N7-C5	5.35	113.17	102.99
6	Z	502	GTP	PA-O3A-PB	5.29	150.99	132.83
3	k	601	TA1	C18-C10-C02	5.22	127.35	115.69
3	k	601	TA1	C29-N01-C30	5.21	130.62	122.28
3	f	601	TA1	C01-C02-C10	5.21	126.15	118.18
3	f	601	TA1	C17-C18-C20	5.14	114.48	102.59
3	c	601	TA1	C02-O02-C03	5.14	127.52	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	502	GTP	O2'-C2'-C1'	5.14	129.84	110.85
4	m	602	GDP	C8-N7-C5	5.13	112.76	102.99
6	T	502	GTP	O6-C6-C5	5.06	134.26	124.37
3	h	601	TA1	C11-O04-C12	5.03	132.09	119.06
3	g	601	TA1	O13-C28-C29	-4.97	95.65	109.80
6	P	502	GTP	O6-C6-C5	4.88	133.91	124.37
3	k	601	TA1	C01-C02-C10	4.83	125.57	118.18
4	h	602	GDP	O6-C6-N1	4.82	126.34	120.65
3	b	601	TA1	C17-C18-C20	4.80	113.69	102.59
3	g	601	TA1	C37-C29-N01	4.78	121.48	112.11
4	h	602	GDP	C8-N7-C5	4.76	112.06	102.99
3	e	601	TA1	C29-N01-C30	4.72	129.84	122.28
3	m	601	TA1	C11-O04-C12	4.65	131.08	119.06
3	c	601	TA1	C11-O04-C12	4.64	131.07	119.06
6	P	502	GTP	C5'-C4'-C3'	-4.63	97.84	115.18
4	k	602	GDP	C2'-C3'-C4'	4.60	111.58	102.64
3	j	601	TA1	C11-O04-C12	4.54	130.81	119.06
6	W	502	GTP	N1-C2-N3	-4.50	114.91	123.32
4	i	602	GDP	O6-C6-N1	4.50	125.96	120.65
4	b	602	GDP	O6-C6-N1	4.48	125.94	120.65
6	P	502	GTP	O4'-C4'-C3'	-4.46	96.29	105.11
3	k	601	TA1	C19-C18-C20	-4.45	94.44	106.55
6	R	502	GTP	PA-O5'-C5'	-4.44	95.67	121.68
6	P	502	GTP	O4'-C4'-C5'	4.43	123.94	109.37
6	Q	502	GTP	O6-C6-C5	4.43	133.02	124.37
4	e	602	GDP	C8-N7-C5	4.42	111.42	102.99
4	f	602	GDP	C8-N7-C5	4.42	111.40	102.99
4	f	602	GDP	O3B-PB-O3A	4.42	119.44	104.64
3	f	601	TA1	C29-N01-C30	4.40	129.32	122.28
3	g	601	TA1	C45-C01-C02	4.38	116.71	111.91
6	R	502	GTP	O2'-C2'-C1'	4.37	127.00	110.85
6	V	502	GTP	PA-O3A-PB	4.35	147.77	132.83
3	g	601	TA1	C29-N01-C30	4.33	129.22	122.28
3	g	601	TA1	C36-C31-C32	-4.31	112.45	118.59
4	j	602	GDP	C8-N7-C5	4.25	111.08	102.99
3	h	601	TA1	C10-C18-C17	-4.24	98.28	106.54
3	i	601	TA1	C45-C01-C02	4.21	116.52	111.91
3	f	601	TA1	C19-C18-C20	-4.20	95.12	106.55
6	T	502	GTP	N2-C2-N1	-4.20	107.76	116.71
6	S	502	GTP	PA-O3A-PB	4.19	147.21	132.83
3	k	601	TA1	C10-C18-C20	4.14	123.44	116.31
3	h	601	TA1	C29-N01-C30	4.13	128.90	122.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	502	GTP	PA-O3A-PB	4.13	146.99	132.83
3	h	601	TA1	C02-O02-C03	4.13	125.60	117.79
4	l	602	GDP	C8-N7-C5	4.11	110.82	102.99
3	g	601	TA1	C09-C04-C03	4.10	129.66	120.40
4	i	602	GDP	C8-N7-C5	4.10	110.79	102.99
6	Y	502	GTP	O2'-C2'-C1'	4.08	125.94	110.85
4	c	602	GDP	C2'-C3'-C4'	4.04	110.49	102.64
4	g	602	GDP	N2-C2-N3	4.02	127.57	119.74
3	a	601	TA1	C45-C01-C02	4.00	116.29	111.91
3	m	601	TA1	C42-C37-C29	4.00	127.13	120.78
3	a	601	TA1	C11-O04-C12	3.99	129.40	119.06
6	Z	502	GTP	PB-O3B-PG	3.98	146.49	132.83
3	g	601	TA1	C37-C29-C28	3.96	121.55	111.36
3	m	601	TA1	C21-C24-C25	3.94	125.93	120.40
3	k	601	TA1	C44-C25-C24	-3.93	120.54	125.30
3	i	601	TA1	C11-O04-C12	3.92	129.20	119.06
4	k	602	GDP	C8-N7-C5	3.92	110.45	102.99
6	S	502	GTP	C2-N1-C6	3.90	132.28	125.10
3	d	601	TA1	C45-C01-C02	3.90	116.18	111.91
4	c	602	GDP	C8-N7-C5	3.89	110.41	102.99
6	U	502	GTP	C2-N1-C6	3.89	132.25	125.10
4	f	602	GDP	C2'-C3'-C4'	3.87	110.16	102.64
6	T	502	GTP	O3'-C3'-C2'	3.85	124.28	111.82
6	S	502	GTP	C8-N7-C5	-3.85	95.66	102.99
3	h	601	TA1	C45-C01-C02	3.84	116.11	111.91
4	a	602	GDP	C3'-C2'-C1'	3.84	106.76	100.98
4	d	602	GDP	O6-C6-C5	-3.82	116.91	124.37
6	O	502	GTP	C5-C6-N1	-3.81	107.22	113.95
4	b	602	GDP	O6-C6-C5	-3.81	116.92	124.37
3	k	601	TA1	C45-C24-C21	3.79	131.53	118.78
3	b	601	TA1	C11-O04-C12	3.79	128.87	119.06
4	h	602	GDP	C2'-C3'-C4'	3.79	110.00	102.64
6	Q	502	GTP	O2'-C2'-C1'	3.76	124.75	110.85
3	m	601	TA1	C38-C37-C29	-3.76	114.81	120.78
3	l	601	TA1	C45-C01-C02	3.75	116.02	111.91
4	j	602	GDP	O3B-PB-O3A	3.72	117.13	104.64
3	l	601	TA1	C11-O04-C12	3.72	128.69	119.06
3	g	601	TA1	C17-C18-C20	3.72	111.18	102.59
3	b	601	TA1	C29-N01-C30	3.72	128.23	122.28
4	c	602	GDP	O4'-C1'-C2'	3.71	112.35	106.93
3	j	601	TA1	C02-O02-C03	3.71	124.81	117.79
3	e	601	TA1	C45-C01-C02	3.71	115.97	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	602	GDP	O6-C6-N1	3.71	125.03	120.65
4	i	602	GDP	O3B-PB-O3A	3.70	117.05	104.64
4	b	602	GDP	C8-N7-C5	3.69	110.03	102.99
3	k	601	TA1	C32-C31-C30	3.69	132.57	120.62
6	P	502	GTP	O3'-C3'-C2'	3.68	123.73	111.82
3	g	601	TA1	C32-C31-C30	3.66	132.49	120.62
4	l	602	GDP	C2'-C3'-C4'	3.66	109.76	102.64
4	b	602	GDP	O2B-PB-O3A	-3.65	92.41	104.64
3	j	601	TA1	C42-C37-C29	3.63	126.55	120.78
3	h	601	TA1	C17-C18-C20	3.61	110.93	102.59
3	g	601	TA1	C06-C05-C04	-3.60	116.08	120.34
3	j	601	TA1	C45-C01-C02	3.60	115.85	111.91
6	U	502	GTP	O6-C6-N1	3.60	124.90	120.65
4	d	602	GDP	O6-C6-N1	3.58	124.88	120.65
6	O	502	GTP	O6-C6-N1	3.58	124.88	120.65
3	f	601	TA1	O01-C01-C02	3.58	113.34	105.49
6	U	502	GTP	O3'-C3'-C2'	3.57	123.36	111.82
3	d	601	TA1	C17-C18-C20	3.56	110.83	102.59
6	X	502	GTP	PA-O3A-PB	3.56	145.03	132.83
6	U	502	GTP	O6-C6-C5	3.55	131.31	124.37
4	g	602	GDP	N2-C2-N1	-3.54	109.19	116.71
3	k	601	TA1	O09-C21-C24	3.52	114.54	109.83
4	e	602	GDP	O6-C6-N1	3.52	124.80	120.65
3	f	601	TA1	O04-C11-C14	-3.49	100.46	108.09
3	c	601	TA1	C17-C18-C20	3.49	110.65	102.59
4	h	602	GDP	O2'-C2'-C3'	3.48	123.08	111.82
3	e	601	TA1	C02-O02-C03	3.48	124.37	117.79
6	S	502	GTP	C5'-C4'-C3'	-3.48	102.16	115.18
3	h	601	TA1	C21-C24-C25	3.47	125.28	120.40
3	a	601	TA1	C17-C18-C20	3.46	110.59	102.59
3	g	601	TA1	O04-C11-C15	-3.46	104.05	112.28
3	b	601	TA1	C45-C01-C02	3.44	115.68	111.91
3	g	601	TA1	O02-C02-C10	-3.44	101.80	108.17
4	g	602	GDP	C2'-C3'-C4'	3.42	109.29	102.64
3	e	601	TA1	C17-C18-C20	3.42	110.48	102.59
4	a	602	GDP	O4'-C1'-C2'	-3.41	101.94	106.93
3	j	601	TA1	C17-C18-C20	3.41	110.47	102.59
6	U	502	GTP	PA-O5'-C5'	-3.40	101.72	121.68
3	g	601	TA1	O02-C02-C01	3.38	111.91	104.76
3	b	601	TA1	C02-O02-C03	3.37	124.17	117.79
6	R	502	GTP	C8-N7-C5	3.35	109.37	102.99
4	h	602	GDP	O3B-PB-O3A	3.32	115.77	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	601	TA1	C31-C30-N01	-3.31	110.71	117.06
6	R	502	GTP	O3'-C3'-C4'	3.31	120.62	111.05
3	k	601	TA1	C36-C31-C32	-3.30	113.88	118.59
3	m	601	TA1	C47-C45-C24	3.30	126.25	112.83
4	f	602	GDP	O6-C6-C5	-3.30	117.93	124.37
6	V	502	GTP	O5'-C5'-C4'	3.28	120.29	108.99
3	k	601	TA1	C21-O09-C22	3.28	123.83	116.11
3	g	601	TA1	C33-C32-C31	3.27	124.21	120.34
6	Z	502	GTP	O5'-C5'-C4'	3.26	120.22	108.99
3	c	601	TA1	C45-C01-C02	3.25	115.47	111.91
4	j	602	GDP	C2'-C3'-C4'	3.25	108.95	102.64
6	Q	502	GTP	PA-O3A-PB	3.25	143.97	132.83
6	T	502	GTP	C2-N1-C6	-3.24	119.13	125.10
4	m	602	GDP	O2'-C2'-C3'	3.24	122.30	111.82
6	S	502	GTP	C5-C6-N1	-3.23	108.25	113.95
3	i	601	TA1	C02-O02-C03	3.23	123.89	117.79
6	V	502	GTP	O2'-C2'-C1'	3.22	122.73	110.85
4	e	602	GDP	O6-C6-C5	-3.20	118.13	124.37
3	l	601	TA1	C17-C18-C20	3.18	109.94	102.59
4	c	602	GDP	O3B-PB-O3A	3.17	115.27	104.64
3	k	601	TA1	C02-O02-C03	3.17	123.79	117.79
3	g	601	TA1	C10-C18-C17	-3.16	100.38	106.54
4	e	602	GDP	C2'-C3'-C4'	3.16	108.78	102.64
4	d	602	GDP	N2-C2-N3	3.15	125.87	119.74
4	c	602	GDP	O6-C6-N1	3.15	124.37	120.65
6	T	502	GTP	N2-C2-N3	3.15	125.87	119.74
3	b	601	TA1	C19-C18-C20	-3.15	98.00	106.55
4	h	602	GDP	O6-C6-C5	-3.14	118.24	124.37
3	k	601	TA1	C43-C01-C45	-3.14	105.72	111.50
3	f	601	TA1	C36-C31-C32	-3.12	114.14	118.59
4	g	602	GDP	C8-N7-C5	3.12	108.94	102.99
4	j	602	GDP	O2'-C2'-C3'	3.12	121.91	111.82
3	d	601	TA1	C19-C18-C20	-3.11	98.09	106.55
4	c	602	GDP	O2'-C2'-C3'	3.10	121.84	111.82
4	i	602	GDP	PA-O3A-PB	-3.09	122.22	132.83
4	i	602	GDP	O6-C6-C5	-3.09	118.34	124.37
6	V	502	GTP	O3'-C3'-C4'	3.09	119.98	111.05
3	m	601	TA1	C02-O02-C03	3.08	123.63	117.79
6	R	502	GTP	O6-C6-C5	3.08	130.38	124.37
4	d	602	GDP	O3B-PB-O3A	3.07	114.92	104.64
3	k	601	TA1	O11-C27-C28	-3.05	106.16	111.15
3	k	601	TA1	C45-C01-C02	3.05	115.25	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	602	GDP	O3B-PB-O3A	3.05	114.85	104.64
3	k	601	TA1	C01-C45-C24	3.04	108.22	105.22
6	Y	502	GTP	PA-O5'-C5'	-3.03	103.94	121.68
4	m	602	GDP	C2'-C3'-C4'	3.02	108.52	102.64
6	Y	502	GTP	PA-O3A-PB	3.02	143.19	132.83
6	T	502	GTP	C5-C6-N1	3.02	119.28	113.95
4	m	602	GDP	O6-C6-C5	-3.01	118.50	124.37
3	e	601	TA1	C19-C18-C20	-3.01	98.38	106.55
6	O	502	GTP	C3'-C2'-C1'	2.99	105.48	100.98
3	c	601	TA1	C29-N01-C30	2.98	127.06	122.28
3	m	601	TA1	C05-C04-C03	-2.97	113.69	120.40
3	i	601	TA1	C21-C24-C25	2.96	124.56	120.40
6	Q	502	GTP	C8-N7-C5	2.95	108.62	102.99
4	g	602	GDP	O3B-PB-O3A	2.95	114.53	104.64
6	W	502	GTP	N2-C2-N1	2.95	122.98	116.71
3	m	601	TA1	C17-C18-C20	2.94	109.39	102.59
3	m	601	TA1	O04-C11-C10	2.93	113.93	109.24
3	g	601	TA1	O04-C11-C10	2.93	113.92	109.24
4	g	602	GDP	PA-O3A-PB	-2.91	122.84	132.83
4	k	602	GDP	O6-C6-N1	2.90	124.08	120.65
4	d	602	GDP	C2'-C3'-C4'	2.90	108.28	102.64
6	O	502	GTP	C2-N1-C6	2.89	130.43	125.10
4	k	602	GDP	O2'-C2'-C3'	2.89	121.18	111.82
4	g	602	GDP	O6-C6-N1	2.89	124.06	120.65
4	j	602	GDP	PA-O3A-PB	-2.89	122.92	132.83
4	m	602	GDP	O6-C6-N1	2.89	124.06	120.65
4	l	602	GDP	PA-O3A-PB	-2.89	122.92	132.83
6	S	502	GTP	N1-C2-N3	-2.87	117.95	123.32
3	c	601	TA1	C21-C24-C25	2.87	124.42	120.40
4	i	602	GDP	C2'-C3'-C4'	2.86	108.20	102.64
3	i	601	TA1	C17-C18-C20	2.86	109.21	102.59
4	j	602	GDP	O6-C6-N1	2.86	124.03	120.65
4	l	602	GDP	O6-C6-N1	2.86	124.02	120.65
3	i	601	TA1	C29-N01-C30	2.85	126.85	122.28
3	k	601	TA1	C33-C32-C31	2.85	123.72	120.34
4	i	602	GDP	O3'-C3'-C4'	-2.85	102.80	111.05
3	e	601	TA1	O04-C11-C14	-2.84	101.88	108.09
6	R	502	GTP	O5'-C5'-C4'	2.84	118.75	108.99
6	Q	502	GTP	O6-C6-N1	-2.84	117.30	120.65
3	e	601	TA1	C26-O11-C27	2.83	122.07	116.67
3	e	601	TA1	O14-C30-C31	2.82	125.97	120.94
3	c	601	TA1	C26-O11-C27	2.82	122.05	116.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	601	TA1	O11-C27-C28	-2.81	106.55	111.15
6	W	502	GTP	PB-O3B-PG	2.81	142.46	132.83
3	j	601	TA1	O04-C11-C10	2.81	113.72	109.24
4	b	602	GDP	O3B-PB-O3A	2.79	114.00	104.64
3	m	601	TA1	C26-O11-C27	2.79	121.99	116.67
6	T	502	GTP	PA-O5'-C5'	-2.79	105.34	121.68
3	j	601	TA1	C21-C24-C25	2.79	124.31	120.40
6	T	502	GTP	C8-N7-C5	2.78	108.29	102.99
4	k	602	GDP	O3B-PB-O3A	2.78	113.95	104.64
4	l	602	GDP	O3B-PB-O3A	2.77	113.94	104.64
4	h	602	GDP	PA-O3A-PB	-2.77	123.32	132.83
6	U	502	GTP	PB-O3B-PG	2.77	142.32	132.83
4	d	602	GDP	O4'-C1'-C2'	2.76	110.96	106.93
3	c	601	TA1	O02-C02-C01	2.75	110.57	104.76
3	m	601	TA1	C45-C01-C02	2.74	114.91	111.91
4	k	602	GDP	PA-O3A-PB	-2.74	123.42	132.83
4	f	602	GDP	O3A-PB-O1B	-2.74	96.01	111.19
4	i	602	GDP	O2'-C2'-C3'	2.74	120.67	111.82
4	f	602	GDP	PA-O3A-PB	-2.72	123.49	132.83
4	i	602	GDP	C3'-C2'-C1'	2.72	105.08	100.98
3	e	601	TA1	O04-C11-C10	2.71	113.57	109.24
6	V	502	GTP	O6-C6-N1	2.70	123.83	120.65
6	S	502	GTP	C2'-C3'-C4'	2.69	107.88	102.64
4	k	602	GDP	O6-C6-C5	-2.68	119.13	124.37
4	l	602	GDP	O6-C6-C5	-2.68	119.14	124.37
3	a	601	TA1	C02-O02-C03	2.68	122.85	117.79
3	b	601	TA1	C47-C45-C24	2.67	123.69	112.83
4	l	602	GDP	O2'-C2'-C3'	2.66	120.43	111.82
4	m	602	GDP	O3B-PB-O3A	2.66	113.54	104.64
4	i	602	GDP	O3A-PB-O1B	-2.65	96.47	111.19
3	e	601	TA1	C11-O04-C12	2.65	125.92	119.06
6	O	502	GTP	PB-O3B-PG	2.64	141.90	132.83
3	a	601	TA1	C19-C18-C20	-2.64	99.37	106.55
3	c	601	TA1	C10-C18-C20	2.61	120.81	116.31
3	e	601	TA1	C39-C38-C37	2.61	123.88	120.65
3	e	601	TA1	C37-C29-C28	2.60	118.04	111.36
6	X	502	GTP	C3'-C2'-C1'	2.60	104.89	100.98
6	W	502	GTP	C2'-C3'-C4'	2.60	107.69	102.64
4	c	602	GDP	O2A-PA-O1A	2.59	125.06	112.24
3	f	601	TA1	C35-C36-C31	2.59	123.41	120.34
3	g	601	TA1	C43-C01-C02	2.59	116.37	111.70
3	l	601	TA1	C29-N01-C30	2.59	126.43	122.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	k	601	TA1	C11-O04-C12	2.58	125.74	119.06
3	l	601	TA1	O04-C11-C14	-2.57	102.46	108.09
3	d	601	TA1	C11-O04-C12	2.57	125.71	119.06
4	l	602	GDP	O3'-C3'-C4'	-2.57	103.63	111.05
6	U	502	GTP	C2'-C3'-C4'	2.56	107.62	102.64
3	l	601	TA1	C02-O02-C03	2.56	122.63	117.79
6	N	502	GTP	C3'-C2'-C1'	2.56	104.83	100.98
3	g	601	TA1	C35-C36-C31	2.55	123.37	120.34
3	j	601	TA1	C38-C37-C29	-2.55	116.73	120.78
4	m	602	GDP	PA-O3A-PB	-2.55	124.08	132.83
3	d	601	TA1	O04-C11-C14	-2.54	102.54	108.09
3	c	601	TA1	O04-C11-C10	2.53	113.29	109.24
6	T	502	GTP	O2'-C2'-C3'	2.53	120.01	111.82
3	f	601	TA1	C45-C01-C02	2.53	114.68	111.91
3	h	601	TA1	C36-C31-C32	-2.52	114.99	118.59
4	j	602	GDP	O6-C6-C5	-2.52	119.45	124.37
3	f	601	TA1	C37-C29-N01	2.52	117.05	112.11
6	P	502	GTP	PB-O3B-PG	2.52	141.47	132.83
6	Y	502	GTP	C8-N7-C5	2.52	107.78	102.99
6	V	502	GTP	PA-O5'-C5'	-2.51	106.96	121.68
3	a	601	TA1	C10-C18-C20	2.51	120.63	116.31
3	i	601	TA1	O09-C21-C24	2.50	113.17	109.83
4	f	602	GDP	O2'-C2'-C3'	2.50	119.91	111.82
3	g	601	TA1	O06-C15-C16	2.49	117.95	113.21
3	g	601	TA1	C08-C07-C06	2.48	124.54	119.93
3	d	601	TA1	C21-C24-C25	2.48	123.88	120.40
6	V	502	GTP	O2'-C2'-C3'	2.47	119.83	111.82
3	j	601	TA1	C29-N01-C30	2.47	126.23	122.28
4	g	602	GDP	O6-C6-C5	-2.46	119.56	124.37
6	Q	502	GTP	C5-C6-N1	-2.46	109.61	113.95
3	j	601	TA1	C47-C45-C24	2.44	122.76	112.83
3	g	601	TA1	O14-C30-N01	-2.44	117.96	122.45
3	f	601	TA1	C43-C01-C02	-2.44	107.31	111.70
3	h	601	TA1	C26-O11-C27	2.43	121.30	116.67
3	b	601	TA1	O08-C20-C21	-2.42	116.14	119.30
3	f	601	TA1	C11-C10-C02	2.42	116.39	111.66
6	X	502	GTP	O2'-C2'-C1'	2.42	119.78	110.85
6	S	502	GTP	PB-O3B-PG	2.41	141.11	132.83
3	i	601	TA1	C10-C18-C20	2.41	120.46	116.31
3	b	601	TA1	C11-C10-C02	2.41	116.37	111.66
3	j	601	TA1	C26-O11-C27	2.40	121.25	116.67
6	N	502	GTP	PA-O5'-C5'	-2.40	107.63	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	601	TA1	O09-C21-C24	2.39	113.02	109.83
3	f	601	TA1	C18-C10-C02	2.39	121.02	115.69
3	g	601	TA1	O06-C15-C11	2.38	93.25	90.58
6	R	502	GTP	C3'-C2'-C1'	2.37	104.55	100.98
4	d	602	GDP	C5-C6-N1	2.37	118.14	113.95
3	m	601	TA1	C01-C45-C24	-2.37	102.89	105.22
4	a	602	GDP	O3B-PB-O3A	2.36	112.56	104.64
3	l	601	TA1	C21-C24-C25	2.36	123.72	120.40
3	b	601	TA1	C47-C45-C46	-2.36	99.32	106.26
6	P	502	GTP	O4'-C1'-C2'	-2.36	103.48	106.93
4	k	602	GDP	O3'-C3'-C4'	-2.35	104.24	111.05
6	T	502	GTP	O5'-C5'-C4'	2.34	117.06	108.99
3	g	601	TA1	C47-C45-C24	2.34	122.35	112.83
4	g	602	GDP	O3A-PB-O1B	-2.34	98.20	111.19
3	e	601	TA1	C10-C18-C20	2.34	120.33	116.31
6	N	502	GTP	O2'-C2'-C1'	2.33	119.47	110.85
3	m	601	TA1	C47-C45-C46	-2.33	99.40	106.26
4	j	602	GDP	O3A-PB-O1B	-2.33	98.29	111.19
3	b	601	TA1	C26-O11-C27	2.32	121.10	116.67
6	U	502	GTP	O3G-PG-O3B	2.32	112.42	104.64
3	f	601	TA1	O09-C21-C24	2.32	112.92	109.83
4	c	602	GDP	O5'-PA-O1A	-2.31	100.03	109.07
3	f	601	TA1	O04-C11-C10	2.31	112.94	109.24
3	d	601	TA1	C29-N01-C30	2.31	125.98	122.28
4	h	602	GDP	O3'-C3'-C4'	-2.31	104.38	111.05
6	T	502	GTP	PB-O3B-PG	2.30	140.73	132.83
6	Q	502	GTP	O3'-C3'-C2'	2.30	119.25	111.82
3	a	601	TA1	C39-C38-C37	2.29	123.48	120.65
6	Q	502	GTP	O2'-C2'-C3'	2.29	119.22	111.82
4	h	602	GDP	O3A-PB-O1B	-2.28	98.53	111.19
3	i	601	TA1	C47-C45-C46	-2.28	99.56	106.26
4	d	602	GDP	N2-C2-N1	-2.27	111.87	116.71
6	U	502	GTP	O4'-C1'-C2'	2.27	110.24	106.93
3	g	601	TA1	O14-C30-C31	2.27	124.98	120.94
3	m	601	TA1	C09-C04-C03	2.27	125.52	120.40
3	g	601	TA1	C21-C24-C25	2.27	123.58	120.40
3	f	601	TA1	C47-C45-C46	-2.26	99.60	106.26
3	d	601	TA1	C21-O09-C22	2.26	121.44	116.11
3	e	601	TA1	C47-C45-C46	-2.26	99.60	106.26
3	l	601	TA1	C10-C18-C20	2.26	120.20	116.31
3	m	601	TA1	O11-C26-C25	2.26	115.26	109.78
4	g	602	GDP	O3'-C3'-C4'	-2.26	104.52	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	601	TA1	C02-O02-C03	2.24	122.02	117.79
3	k	601	TA1	C36-C31-C30	-2.23	113.39	120.62
4	b	602	GDP	C3'-C2'-C1'	2.23	104.34	100.98
3	f	601	TA1	C02-O02-C03	2.23	122.01	117.79
6	O	502	GTP	O3G-PG-O3B	2.23	112.11	104.64
3	k	601	TA1	C37-C29-C28	2.23	117.09	111.36
3	l	601	TA1	C47-C45-C24	2.23	121.88	112.83
3	a	601	TA1	C01-C02-C10	2.23	121.59	118.18
4	b	602	GDP	O3B-PB-O2B	2.22	116.14	107.64
6	W	502	GTP	O5'-C5'-C4'	2.22	116.62	108.99
3	l	601	TA1	C47-C45-C46	-2.22	99.74	106.26
6	R	502	GTP	O6-C6-N1	-2.22	118.03	120.65
3	c	601	TA1	O01-C01-C02	-2.21	100.64	105.49
6	W	502	GTP	C2-N1-C6	2.20	129.15	125.10
3	d	601	TA1	C47-C45-C46	-2.20	99.78	106.26
3	h	601	TA1	C16-C17-C18	2.20	117.78	112.31
3	e	601	TA1	C42-C37-C38	-2.19	115.56	118.29
6	S	502	GTP	O3'-C3'-C4'	-2.19	104.72	111.05
3	g	601	TA1	O01-C01-C43	-2.18	101.58	107.03
3	h	601	TA1	C47-C45-C46	-2.18	99.85	106.26
3	d	601	TA1	C10-C18-C20	2.18	120.06	116.31
3	a	601	TA1	O04-C11-C10	2.18	112.72	109.24
3	d	601	TA1	O04-C11-C10	2.17	112.71	109.24
4	h	602	GDP	C5'-C4'-C3'	2.17	123.31	115.18
4	j	602	GDP	O3'-C3'-C4'	-2.17	104.79	111.05
4	g	602	GDP	O4'-C1'-C2'	2.16	110.08	106.93
3	j	601	TA1	C47-C45-C46	-2.15	99.92	106.26
4	f	602	GDP	C5'-C4'-C3'	2.15	123.25	115.18
6	X	502	GTP	O5'-C5'-C4'	2.15	116.40	108.99
3	c	601	TA1	O09-C21-C24	2.14	112.68	109.83
4	d	602	GDP	O2A-PA-O1A	2.13	122.76	112.24
3	h	601	TA1	C46-C45-C24	-2.13	104.19	112.83
4	h	602	GDP	N2-C2-N3	2.12	123.86	119.74
3	c	601	TA1	O11-C26-C25	2.11	114.91	109.78
3	m	601	TA1	C10-C18-C20	2.11	119.95	116.31
3	b	601	TA1	O08-C20-C18	2.11	124.06	119.18
4	e	602	GDP	O3A-PB-O1B	-2.11	99.48	111.19
4	e	602	GDP	O2A-PA-O1A	2.11	122.67	112.24
3	l	601	TA1	C19-C18-C20	-2.11	100.81	106.55
3	k	601	TA1	O11-C27-O12	2.11	127.87	123.94
6	V	502	GTP	O3G-PG-O3B	2.11	111.70	104.64
3	g	601	TA1	C11-C10-C02	2.10	115.77	111.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	502	GTP	N2-C2-N1	2.10	121.19	116.71
6	U	502	GTP	N2-C2-N1	2.09	121.15	116.71
6	R	502	GTP	PA-O3A-PB	2.09	139.98	132.83
3	f	601	TA1	O08-C20-C21	-2.08	116.58	119.30
3	h	601	TA1	O09-C21-C24	2.08	112.61	109.83
3	l	601	TA1	O04-C11-C10	2.07	112.56	109.24
3	b	601	TA1	C01-C02-C10	2.07	121.36	118.18
3	j	601	TA1	O11-C26-C25	2.06	114.78	109.78
3	g	601	TA1	C47-C45-C46	-2.06	100.19	106.26
6	Q	502	GTP	PA-O5'-C5'	-2.06	109.62	121.68
6	T	502	GTP	C2'-C3'-C4'	2.06	106.64	102.64
4	c	602	GDP	PA-O3A-PB	-2.05	125.80	132.83
6	Y	502	GTP	C5-C6-N1	-2.05	110.34	113.95
3	f	601	TA1	C45-C24-C25	-2.05	116.78	119.61
3	e	601	TA1	O11-C26-C25	2.04	114.73	109.78
6	X	502	GTP	O3G-PG-O3B	2.04	111.47	104.64
3	a	601	TA1	C26-O11-C27	2.04	120.56	116.67
3	a	601	TA1	C29-N01-C30	2.04	125.54	122.28
3	h	601	TA1	C16-C15-C11	-2.03	116.75	119.61
4	f	602	GDP	O4'-C1'-C2'	2.03	109.89	106.93
3	l	601	TA1	C01-C02-C10	2.03	121.29	118.18
3	c	601	TA1	O02-C03-O03	2.03	126.83	123.53
3	i	601	TA1	C36-C31-C32	-2.02	115.71	118.59
6	S	502	GTP	N2-C2-N1	2.02	121.01	116.71
3	g	601	TA1	O11-C27-O12	2.02	127.70	123.94
3	e	601	TA1	O11-C27-C28	-2.01	107.86	111.15
4	d	602	GDP	PA-O3A-PB	-2.01	125.93	132.83
3	c	601	TA1	O06-C15-C16	2.01	117.03	113.21
3	i	601	TA1	C47-C45-C24	2.00	120.98	112.83
3	f	601	TA1	C33-C32-C31	2.00	122.71	120.34

There are no chirality outliers.

All (230) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	601	TA1	O02-C03-C04-C05
3	g	601	TA1	C27-C28-C29-N01
4	a	602	GDP	PA-O3A-PB-O2B
4	a	602	GDP	C5'-O5'-PA-O3A
4	a	602	GDP	C5'-O5'-PA-O1A
4	b	602	GDP	PA-O3A-PB-O2B
4	b	602	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	c	602	GDP	PA-O3A-PB-O2B
4	c	602	GDP	C5'-O5'-PA-O3A
4	d	602	GDP	PA-O3A-PB-O2B
4	d	602	GDP	C5'-O5'-PA-O3A
4	e	602	GDP	PA-O3A-PB-O2B
4	e	602	GDP	C5'-O5'-PA-O3A
4	f	602	GDP	PA-O3A-PB-O2B
4	f	602	GDP	C5'-O5'-PA-O3A
4	g	602	GDP	PA-O3A-PB-O2B
4	g	602	GDP	C5'-O5'-PA-O3A
4	h	602	GDP	PA-O3A-PB-O2B
4	h	602	GDP	C5'-O5'-PA-O3A
4	i	602	GDP	PA-O3A-PB-O2B
4	i	602	GDP	C5'-O5'-PA-O3A
4	j	602	GDP	PA-O3A-PB-O2B
4	j	602	GDP	C5'-O5'-PA-O3A
4	k	602	GDP	PA-O3A-PB-O2B
4	k	602	GDP	C5'-O5'-PA-O3A
4	l	602	GDP	PA-O3A-PB-O2B
4	l	602	GDP	C5'-O5'-PA-O3A
4	m	602	GDP	PA-O3A-PB-O2B
4	m	602	GDP	C5'-O5'-PA-O3A
6	N	502	GTP	C5'-O5'-PA-O3A
6	N	502	GTP	C5'-O5'-PA-O2A
6	O	502	GTP	C5'-O5'-PA-O3A
6	O	502	GTP	C5'-O5'-PA-O2A
6	P	502	GTP	C5'-O5'-PA-O3A
6	P	502	GTP	C5'-O5'-PA-O1A
6	P	502	GTP	C5'-O5'-PA-O2A
6	Q	502	GTP	C5'-O5'-PA-O3A
6	Q	502	GTP	C5'-O5'-PA-O1A
6	Q	502	GTP	C5'-O5'-PA-O2A
6	R	502	GTP	C5'-O5'-PA-O3A
6	R	502	GTP	C5'-O5'-PA-O2A
6	S	502	GTP	C5'-O5'-PA-O1A
6	S	502	GTP	C5'-O5'-PA-O2A
6	T	502	GTP	C5'-O5'-PA-O3A
6	T	502	GTP	C5'-O5'-PA-O2A
6	U	502	GTP	C5'-O5'-PA-O3A
6	U	502	GTP	C5'-O5'-PA-O2A
6	V	502	GTP	C5'-O5'-PA-O1A
6	V	502	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	W	502	GTP	C5'-O5'-PA-O3A
6	W	502	GTP	C5'-O5'-PA-O2A
6	X	502	GTP	C5'-O5'-PA-O3A
6	X	502	GTP	C5'-O5'-PA-O2A
6	Y	502	GTP	C5'-O5'-PA-O1A
6	Y	502	GTP	C5'-O5'-PA-O2A
6	Z	502	GTP	C5'-O5'-PA-O1A
6	Z	502	GTP	C5'-O5'-PA-O2A
3	c	601	TA1	O02-C03-C04-C09
3	g	601	TA1	O02-C03-C04-C09
3	h	601	TA1	O02-C03-C04-C09
3	j	601	TA1	O02-C03-C04-C09
3	k	601	TA1	O02-C03-C04-C09
3	a	601	TA1	O02-C03-C04-C09
3	b	601	TA1	O02-C03-C04-C05
3	b	601	TA1	O02-C03-C04-C09
3	c	601	TA1	O03-C03-C04-C05
3	e	601	TA1	O02-C03-C04-C05
3	h	601	TA1	O02-C03-C04-C05
3	j	601	TA1	O02-C03-C04-C05
3	k	601	TA1	O02-C03-C04-C05
3	m	601	TA1	O02-C03-C04-C05
3	m	601	TA1	O02-C03-C04-C09
3	a	601	TA1	O02-C03-C04-C05
3	c	601	TA1	O03-C03-C04-C09
3	e	601	TA1	O02-C03-C04-C09
3	g	601	TA1	O02-C03-C04-C05
3	c	601	TA1	O14-C30-C31-C36
3	g	601	TA1	O14-C30-C31-C36
3	c	601	TA1	O14-C30-C31-C32
3	g	601	TA1	N01-C30-C31-C36
3	i	601	TA1	O02-C03-C04-C05
3	c	601	TA1	N01-C30-C31-C32
3	c	601	TA1	N01-C30-C31-C36
3	f	601	TA1	N01-C30-C31-C36
3	g	601	TA1	N01-C30-C31-C32
3	g	601	TA1	O14-C30-C31-C32
3	h	601	TA1	N01-C30-C31-C36
3	b	601	TA1	N01-C30-C31-C36
3	b	601	TA1	O14-C30-C31-C36
3	d	601	TA1	O02-C03-C04-C05
3	d	601	TA1	N01-C30-C31-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	e	601	TA1	N01-C30-C31-C36
3	f	601	TA1	N01-C30-C31-C32
3	f	601	TA1	O14-C30-C31-C32
3	f	601	TA1	O14-C30-C31-C36
3	i	601	TA1	O02-C03-C04-C09
3	m	601	TA1	N01-C30-C31-C36
3	b	601	TA1	N01-C30-C31-C32
3	m	601	TA1	N01-C30-C31-C32
3	e	601	TA1	O14-C30-C31-C36
3	j	601	TA1	O03-C03-C04-C05
3	a	601	TA1	C31-C30-N01-C29
3	k	601	TA1	C31-C30-N01-C29
3	l	601	TA1	C31-C30-N01-C29
3	m	601	TA1	C31-C30-N01-C29
3	a	601	TA1	O03-C03-C04-C09
3	d	601	TA1	N01-C30-C31-C32
3	h	601	TA1	O03-C03-C04-C05
3	h	601	TA1	O03-C03-C04-C09
3	m	601	TA1	O14-C30-C31-C36
3	b	601	TA1	O14-C30-C31-C32
3	h	601	TA1	N01-C30-C31-C32
3	j	601	TA1	N01-C30-C31-C36
3	d	601	TA1	O02-C03-C04-C09
3	i	601	TA1	N01-C30-C31-C36
3	k	601	TA1	O03-C03-C04-C05
3	k	601	TA1	O03-C03-C04-C09
3	a	601	TA1	O03-C03-C04-C05
3	b	601	TA1	O03-C03-C04-C05
3	j	601	TA1	O03-C03-C04-C09
3	m	601	TA1	O03-C03-C04-C05
3	e	601	TA1	O03-C03-C04-C05
3	l	601	TA1	O02-C03-C04-C05
3	h	601	TA1	O14-C30-C31-C36
3	e	601	TA1	N01-C30-C31-C32
3	m	601	TA1	O03-C03-C04-C09
3	m	601	TA1	O14-C30-C31-C32
3	j	601	TA1	N01-C30-C31-C32
3	d	601	TA1	O14-C30-C31-C36
3	i	601	TA1	O14-C30-C31-C36
3	b	601	TA1	O03-C03-C04-C09
3	j	601	TA1	O14-C30-C31-C36
3	i	601	TA1	N01-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	h	601	TA1	C31-C30-N01-C29
3	i	601	TA1	C31-C30-N01-C29
3	j	601	TA1	C31-C30-N01-C29
3	e	601	TA1	O03-C03-C04-C09
3	g	601	TA1	O03-C03-C04-C09
3	b	601	TA1	C31-C30-N01-C29
3	d	601	TA1	O14-C30-C31-C32
3	l	601	TA1	O02-C03-C04-C09
3	l	601	TA1	O14-C30-N01-C29
3	i	601	TA1	O03-C03-C04-C09
3	h	601	TA1	O14-C30-C31-C32
3	a	601	TA1	O14-C30-N01-C29
3	d	601	TA1	O03-C03-C04-C05
3	i	601	TA1	O03-C03-C04-C05
3	i	601	TA1	O14-C30-C31-C32
3	d	601	TA1	O03-C03-C04-C09
3	i	601	TA1	C23-C22-O09-C21
3	j	601	TA1	O14-C30-C31-C32
3	e	601	TA1	O14-C30-C31-C32
3	g	601	TA1	O03-C03-C04-C05
3	m	601	TA1	O14-C30-N01-C29
3	l	601	TA1	N01-C30-C31-C36
3	k	601	TA1	N01-C30-C31-C36
3	b	601	TA1	O14-C30-N01-C29
3	k	601	TA1	O14-C30-N01-C29
3	i	601	TA1	O14-C30-N01-C29
3	f	601	TA1	C31-C30-N01-C29
3	l	601	TA1	O03-C03-C04-C05
3	j	601	TA1	O14-C30-N01-C29
6	Z	502	GTP	PB-O3A-PA-O1A
3	f	601	TA1	O14-C30-N01-C29
3	l	601	TA1	O14-C30-C31-C36
3	h	601	TA1	O14-C30-N01-C29
3	l	601	TA1	O03-C03-C04-C09
3	i	601	TA1	O10-C22-O09-C21
3	l	601	TA1	N01-C30-C31-C32
6	S	502	GTP	C5'-O5'-PA-O3A
6	Z	502	GTP	PB-O3A-PA-O2A
3	a	601	TA1	N01-C30-C31-C36
4	c	602	GDP	C5'-O5'-PA-O1A
4	d	602	GDP	C5'-O5'-PA-O1A
4	e	602	GDP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	f	602	GDP	C5'-O5'-PA-O1A
4	g	602	GDP	C5'-O5'-PA-O1A
4	h	602	GDP	C5'-O5'-PA-O1A
4	i	602	GDP	C5'-O5'-PA-O1A
4	j	602	GDP	C5'-O5'-PA-O1A
4	k	602	GDP	C5'-O5'-PA-O1A
4	l	602	GDP	C5'-O5'-PA-O1A
4	m	602	GDP	C5'-O5'-PA-O1A
3	k	601	TA1	N01-C30-C31-C32
3	g	601	TA1	C14-C11-O04-C12
3	g	601	TA1	C37-C29-N01-C30
3	a	601	TA1	C23-C22-O09-C21
3	k	601	TA1	O14-C30-C31-C36
3	g	601	TA1	C15-C11-O04-C12
3	g	601	TA1	O13-C28-C29-N01
6	X	502	GTP	PG-O3B-PB-O3A
3	h	601	TA1	C14-C11-O04-C12
6	Y	502	GTP	PG-O3B-PB-O3A
4	b	602	GDP	PA-O3A-PB-O1B
4	e	602	GDP	PA-O3A-PB-O1B
4	g	602	GDP	PA-O3A-PB-O1B
4	h	602	GDP	PA-O3A-PB-O1B
4	j	602	GDP	PA-O3A-PB-O1B
4	k	602	GDP	PA-O3A-PB-O1B
4	l	602	GDP	PA-O3A-PB-O1B
4	m	602	GDP	PA-O3A-PB-O1B
3	g	601	TA1	C10-C11-O04-C12
4	a	602	GDP	PA-O3A-PB-O3B
4	b	602	GDP	PA-O3A-PB-O3B
4	c	602	GDP	PA-O3A-PB-O3B
4	d	602	GDP	PA-O3A-PB-O3B
4	e	602	GDP	PA-O3A-PB-O3B
4	g	602	GDP	PA-O3A-PB-O3B
4	h	602	GDP	PA-O3A-PB-O3B
4	j	602	GDP	PA-O3A-PB-O3B
4	k	602	GDP	PA-O3A-PB-O3B
4	l	602	GDP	PA-O3A-PB-O3B
4	m	602	GDP	PA-O3A-PB-O3B
6	N	502	GTP	PG-O3B-PB-O3A
6	Q	502	GTP	PG-O3B-PB-O3A
6	W	502	GTP	PG-O3B-PB-O3A
6	V	502	GTP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

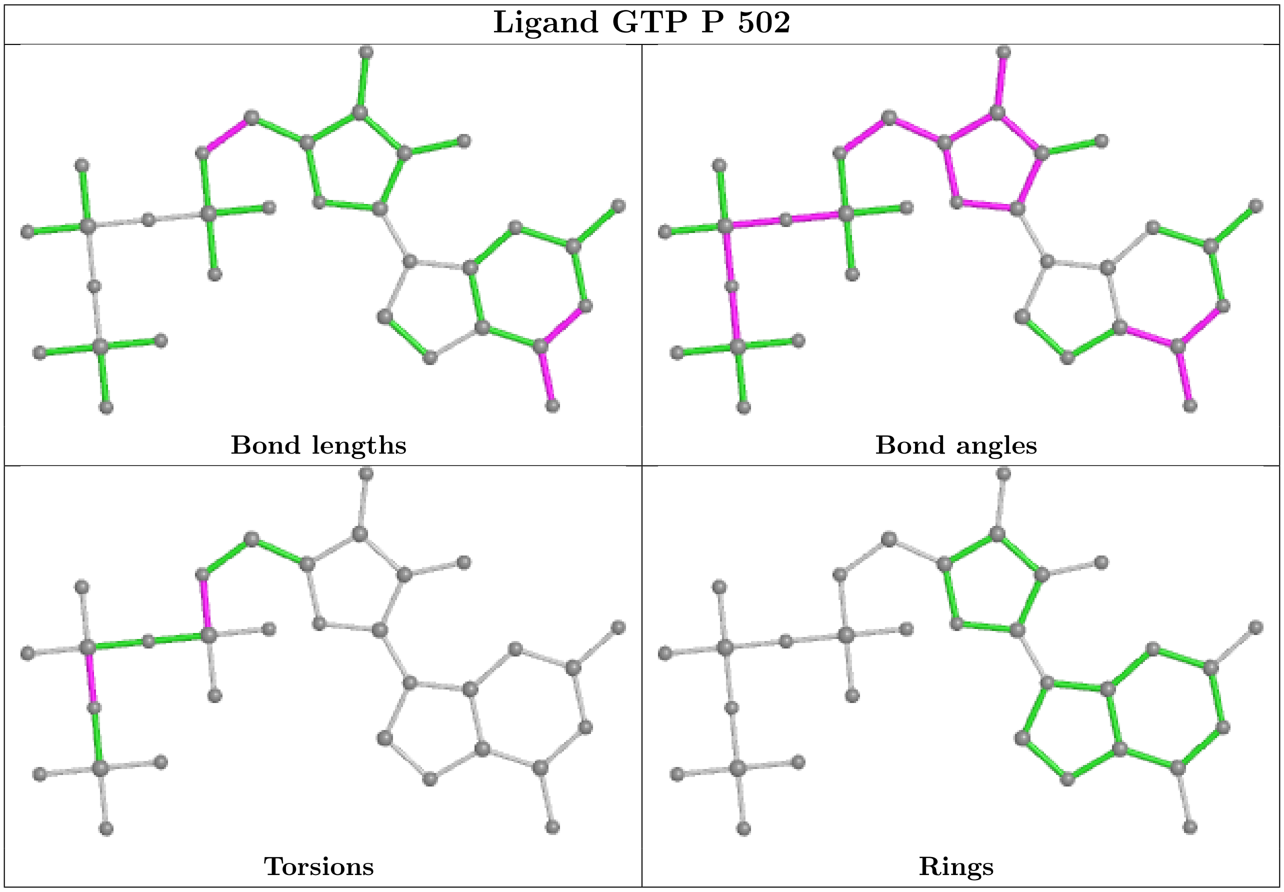
Mol	Chain	Res	Type	Atoms
6	Y	502	GTP	C5'-O5'-PA-O3A
6	Z	502	GTP	C5'-O5'-PA-O3A
4	b	602	GDP	C4'-C5'-O5'-PA
6	P	502	GTP	PG-O3B-PB-O2B
6	S	502	GTP	PG-O3B-PB-O2B
3	c	601	TA1	C15-C11-O04-C12
3	h	601	TA1	C15-C11-O04-C12
3	l	601	TA1	O14-C30-C31-C32
4	f	602	GDP	PA-O3A-PB-O1B
4	i	602	GDP	PA-O3A-PB-O1B
3	h	601	TA1	C20-C21-O09-C22
6	P	502	GTP	PG-O3B-PB-O3A
6	Z	502	GTP	PG-O3B-PB-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 P 502



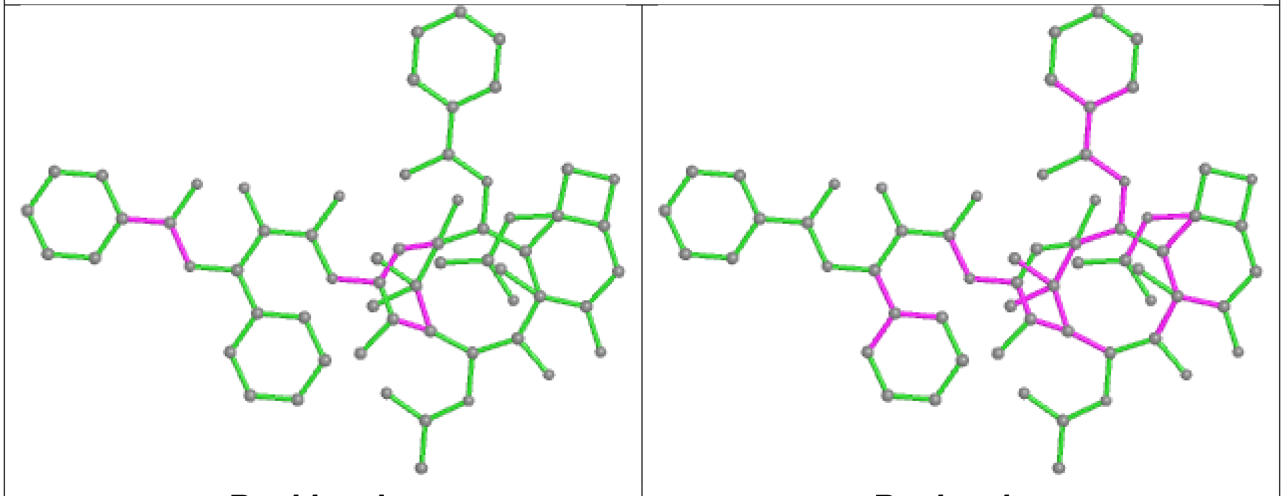
Bond lengths

Bond angles

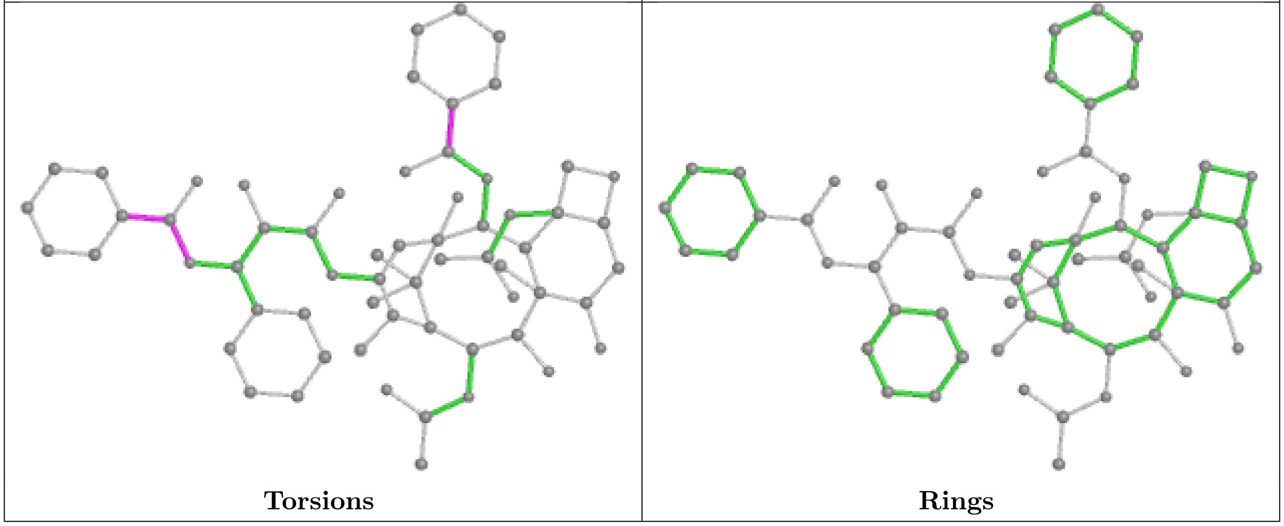
Torsions

Rings

Ligand TA1 m 601

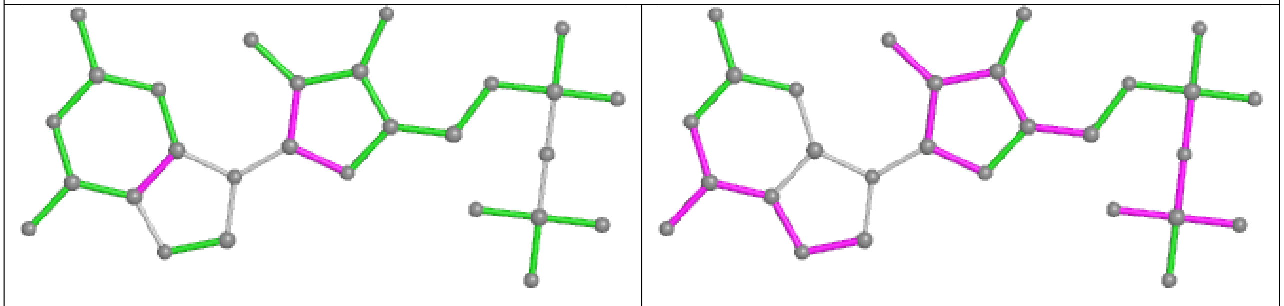


Bond lengths **Bond angles**

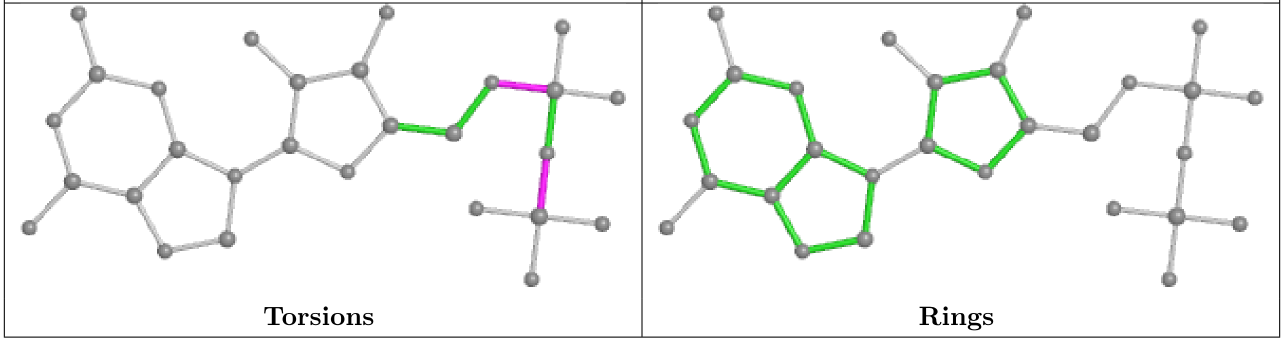


Torsions **Rings**

Ligand GDP f 602

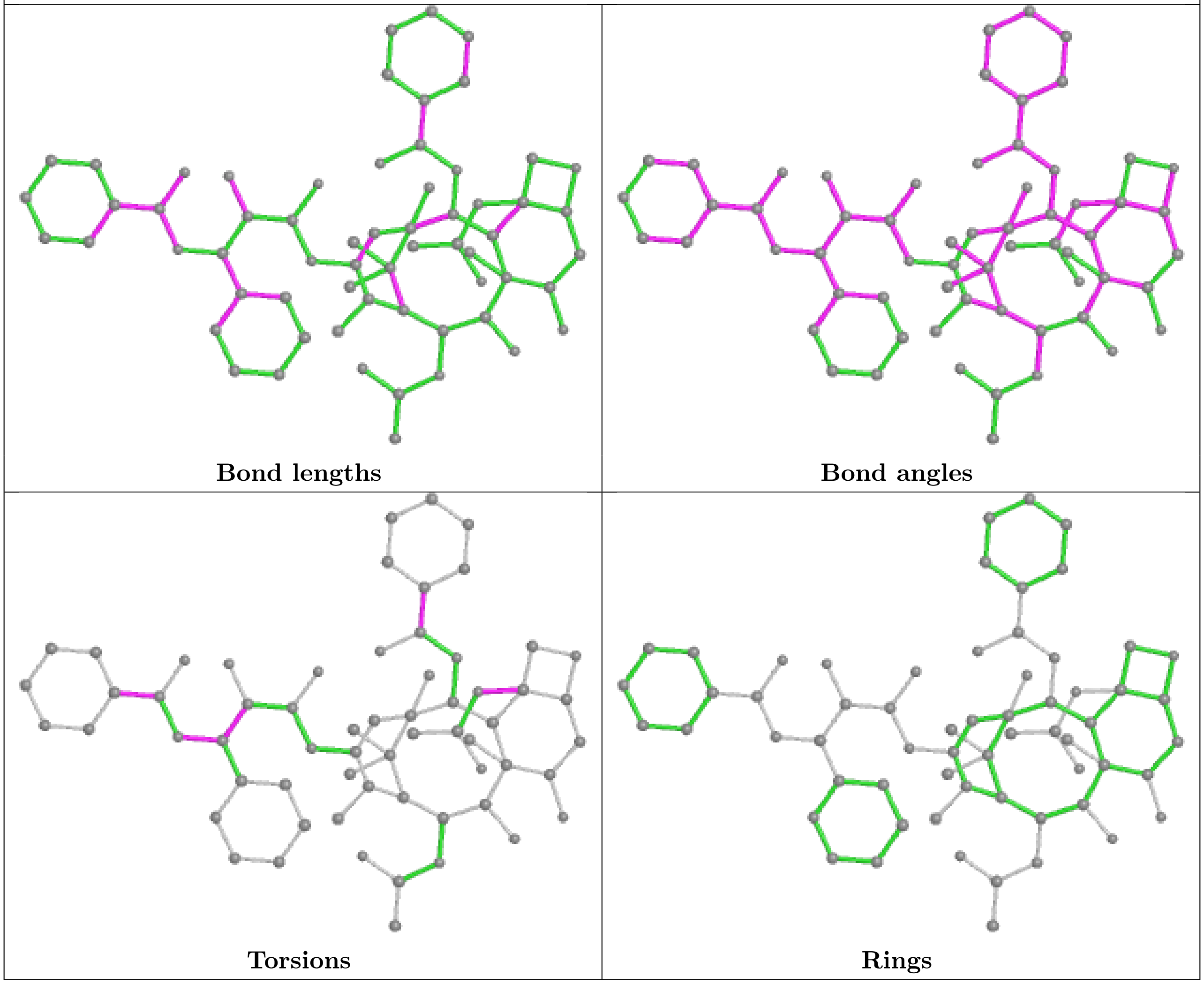


Bond lengths **Bond angles**



Torsions **Rings**

Ligand TA1 g 601



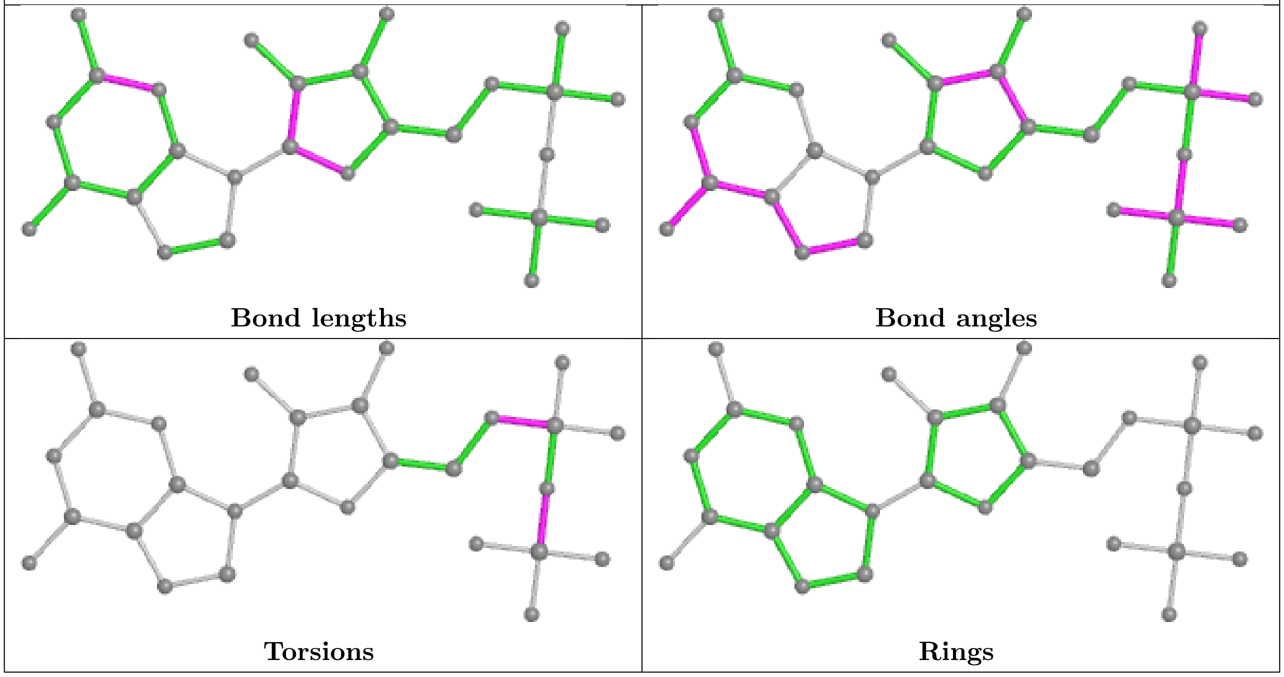
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP e 602



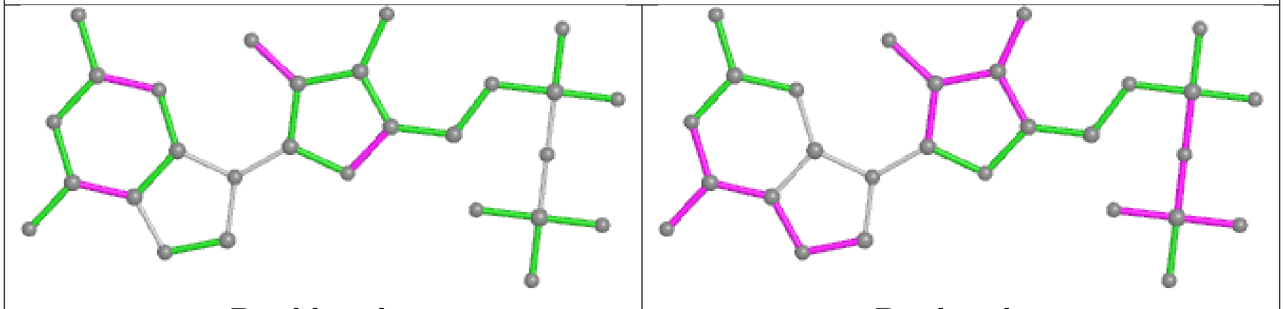
Bond lengths

Bond angles

Torsions

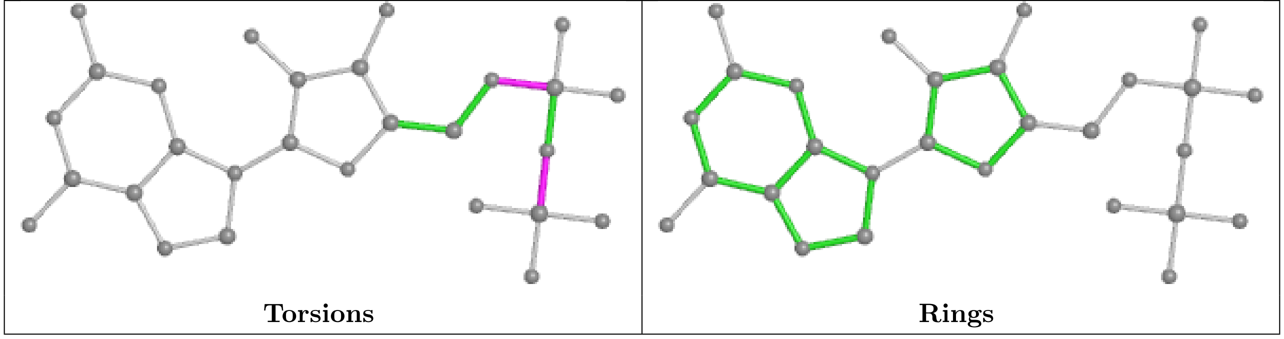
Rings

Ligand GDP i 602



Bond lengths

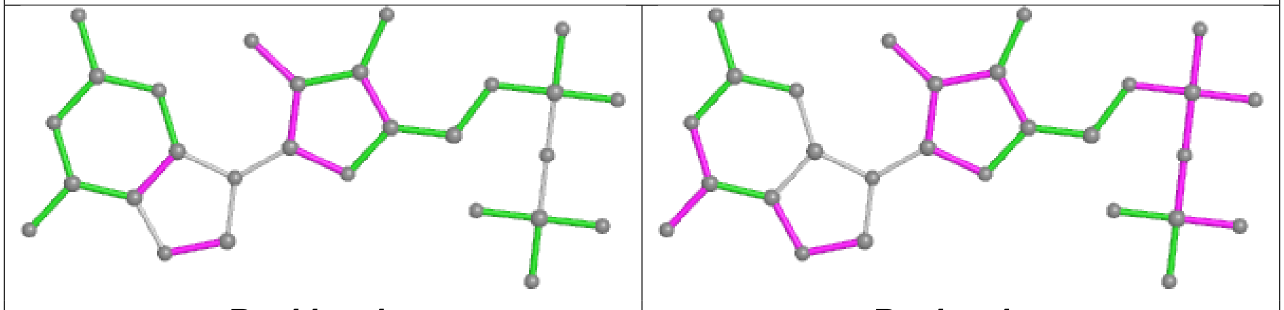
Bond angles



Torsions

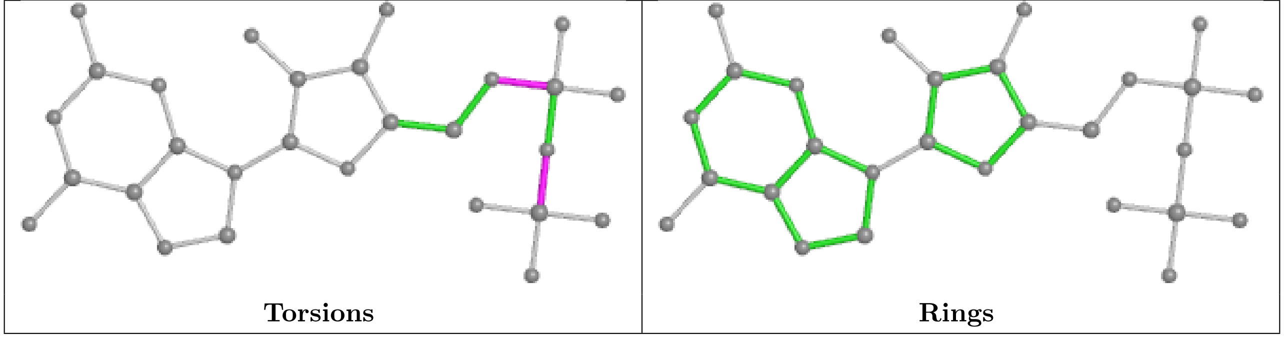
Rings

Ligand GDP c 602



Bond lengths

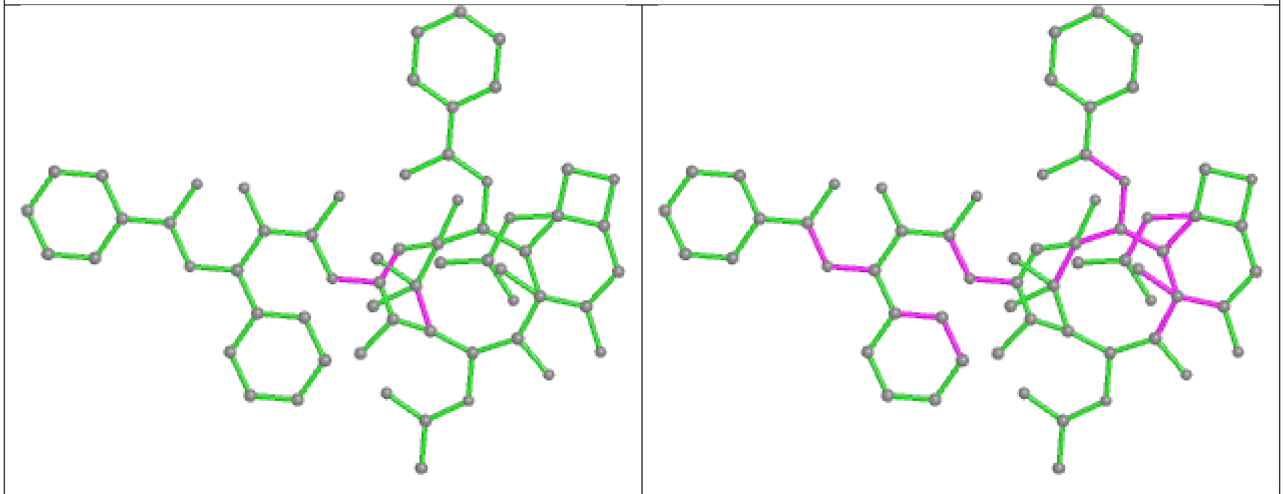
Bond angles



Torsions

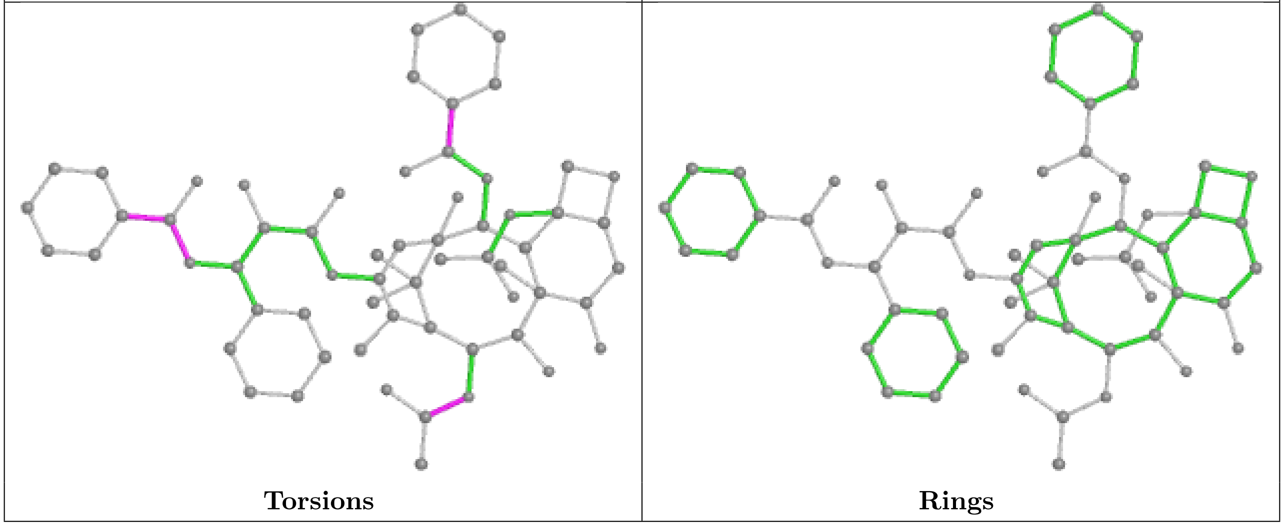
Rings

Ligand TA1 a 601



Bond lengths

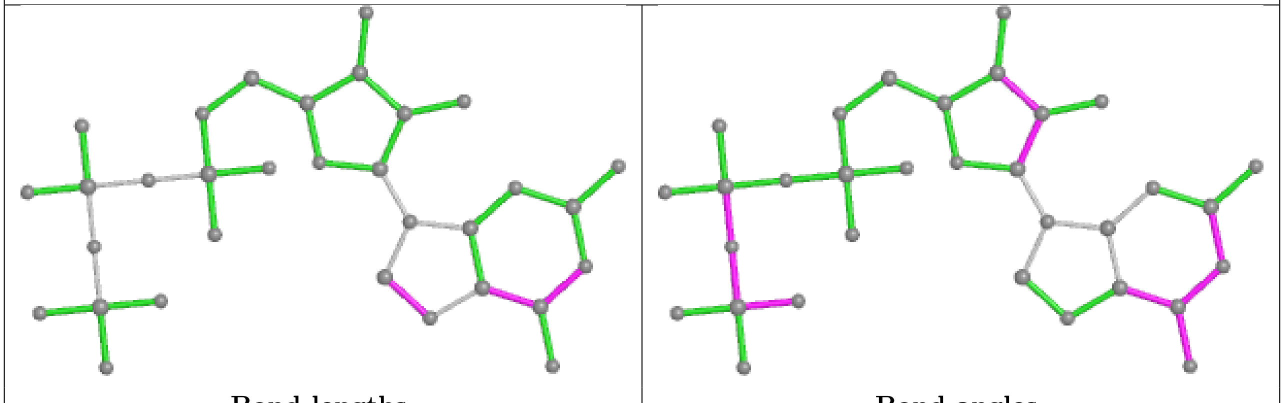
Bond angles



Torsions

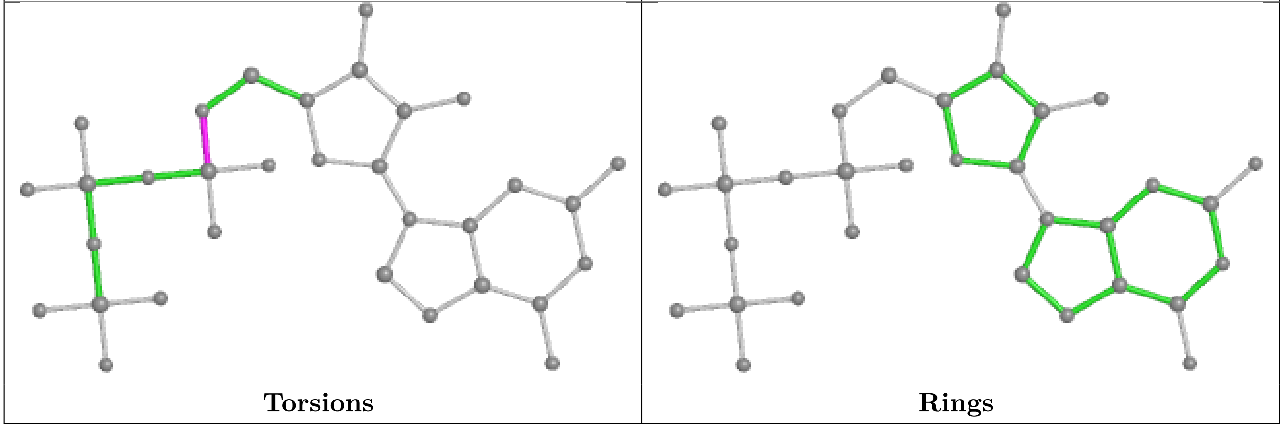
Rings

Ligand GTP O 502



Bond lengths

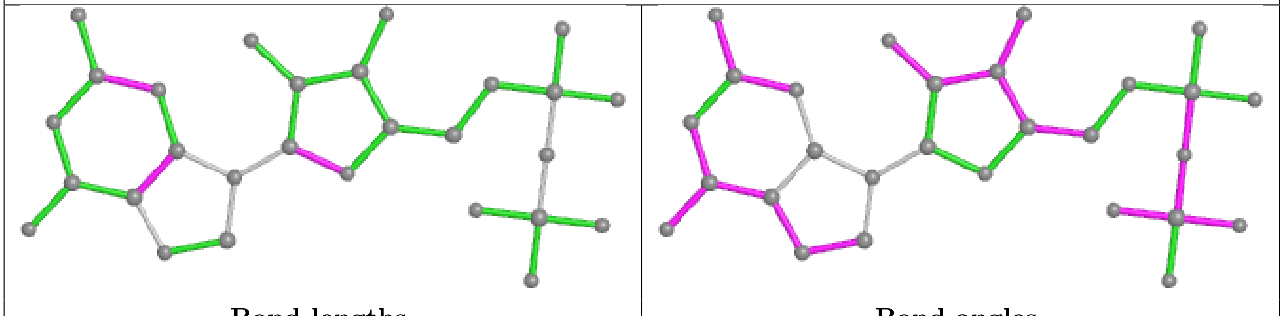
Bond angles



Torsions

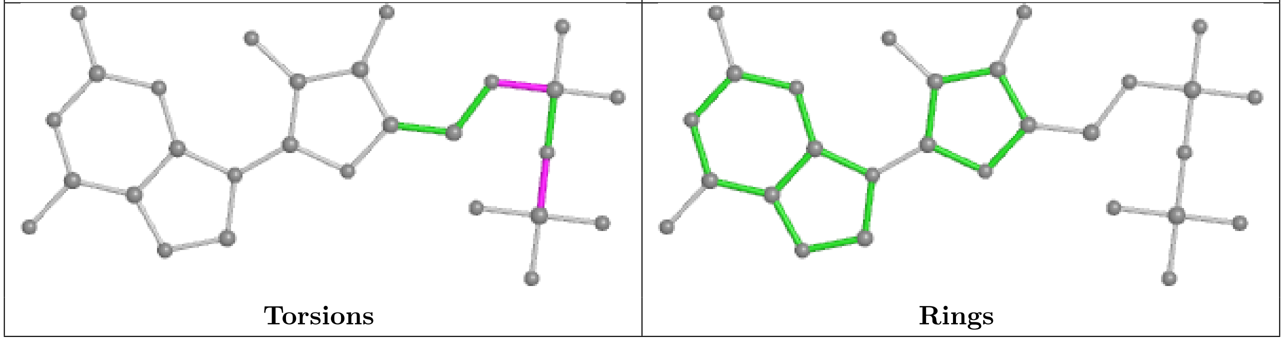
Rings

Ligand GDP h 602



Bond lengths

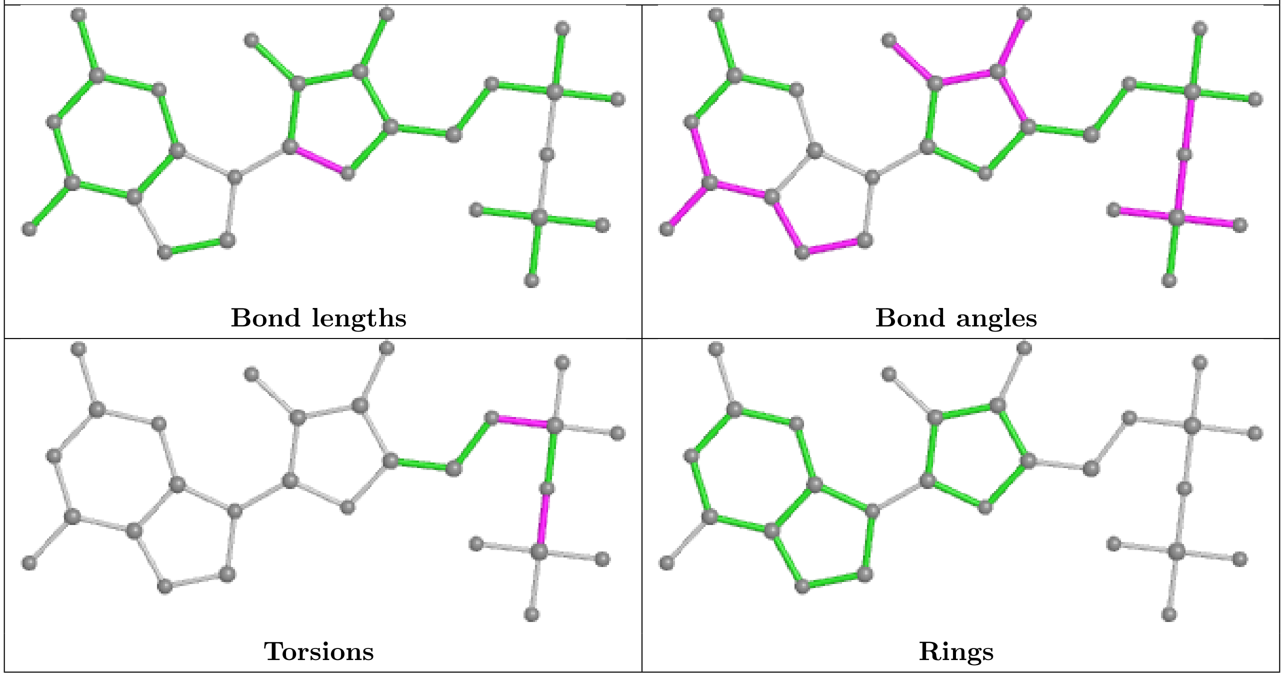
Bond angles



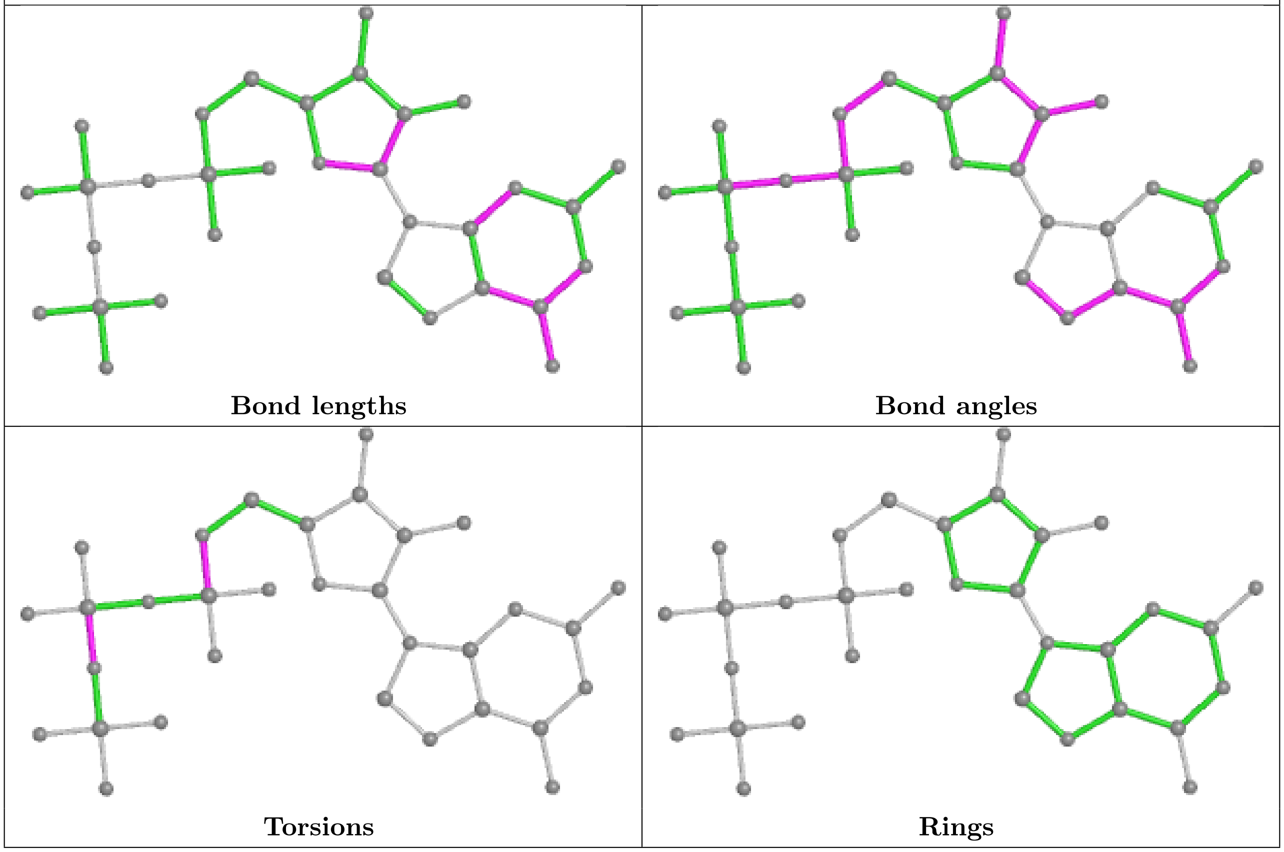
Torsions

Rings

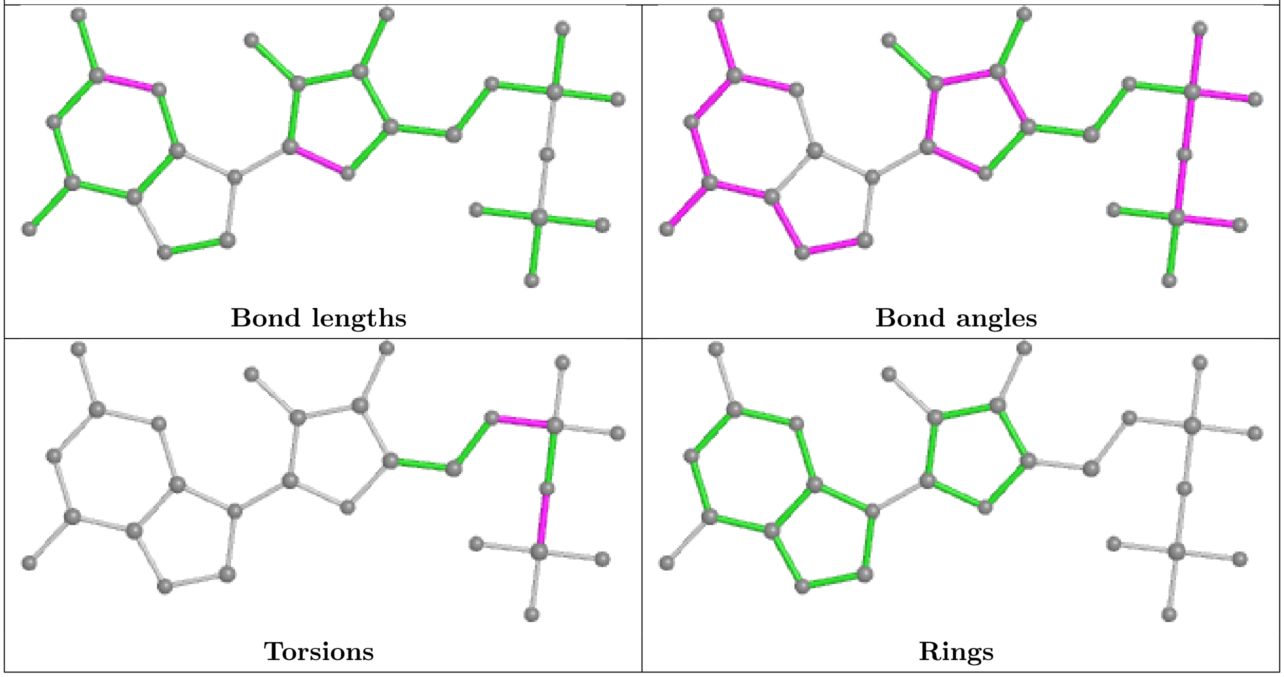
Ligand GDP j 602



Ligand GTP Q 502



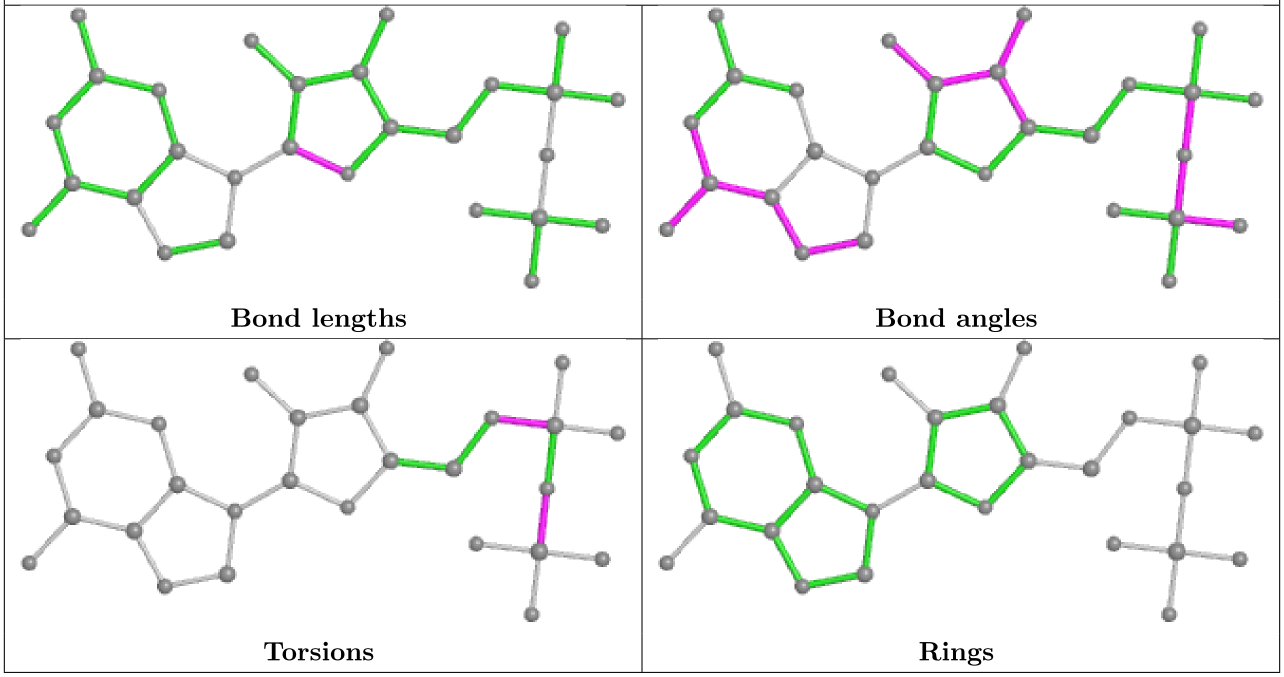
Ligand GDP d 602



Bond lengths Bond angles

Torsions Rings

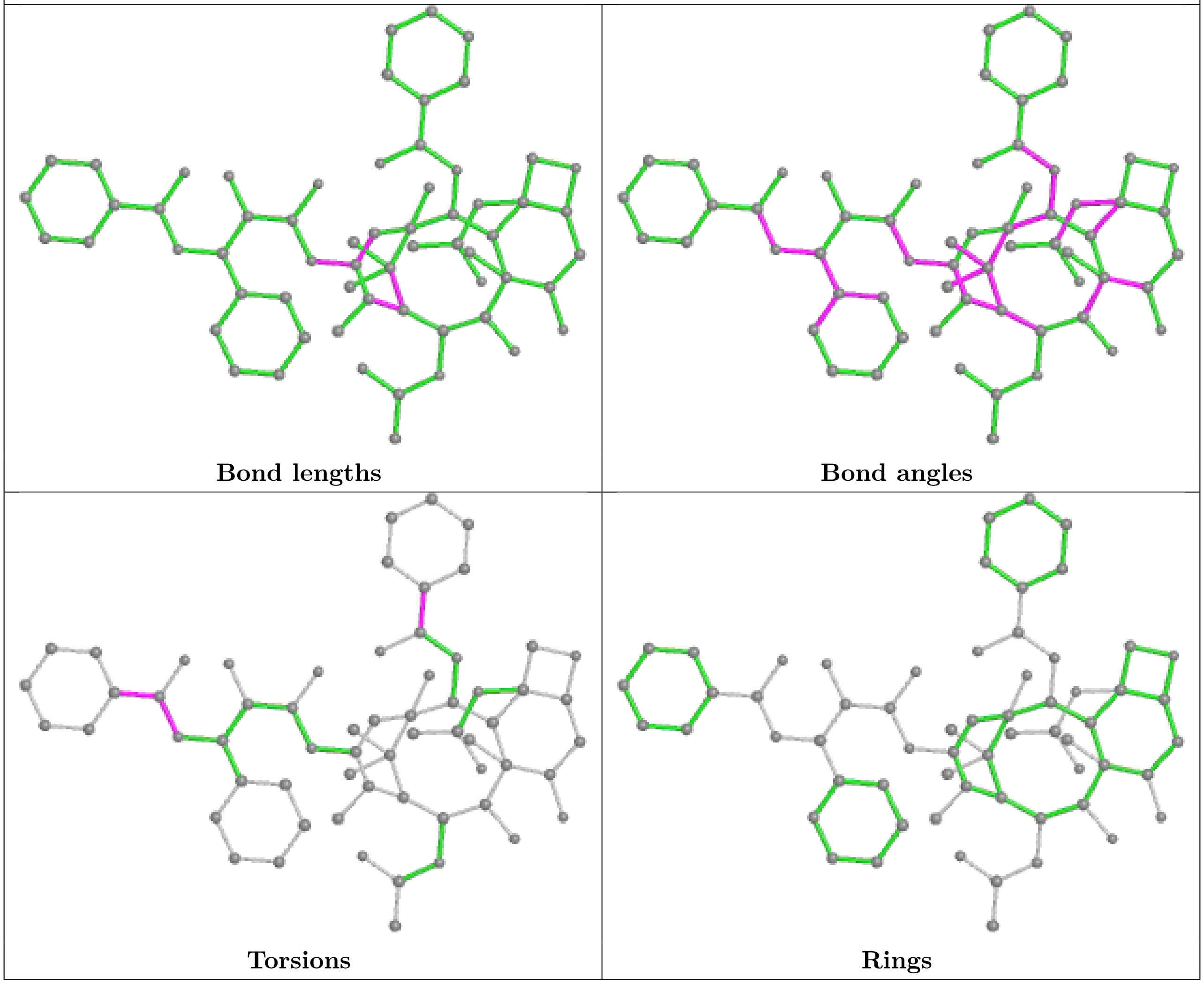
Ligand GDP k 602



Bond lengths Bond angles

Torsions Rings

Ligand TA1 j 601



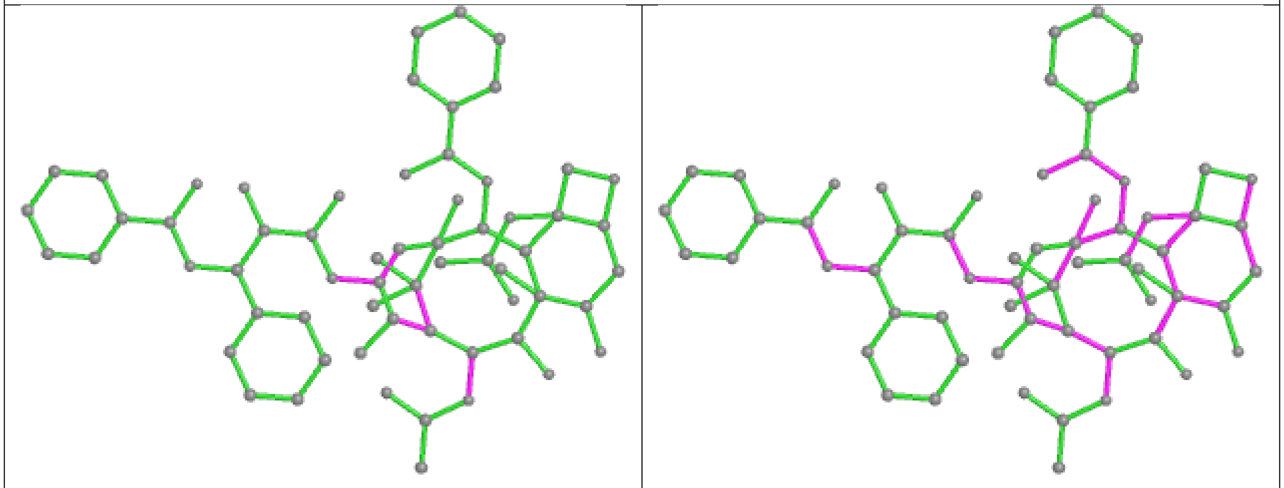
Bond lengths

Bond angles

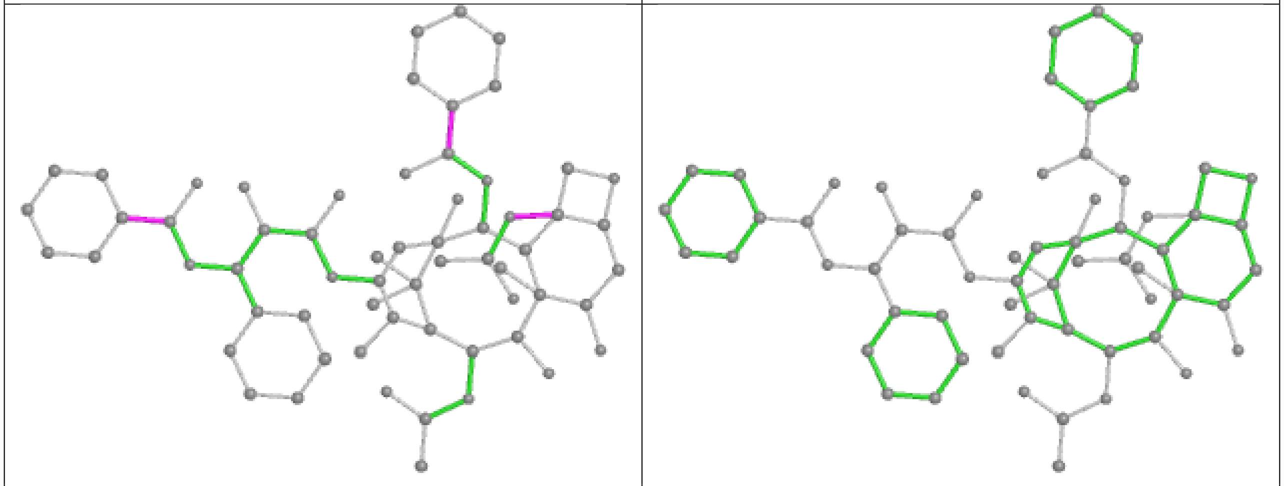
Torsions

Rings

Ligand TA1 c 601

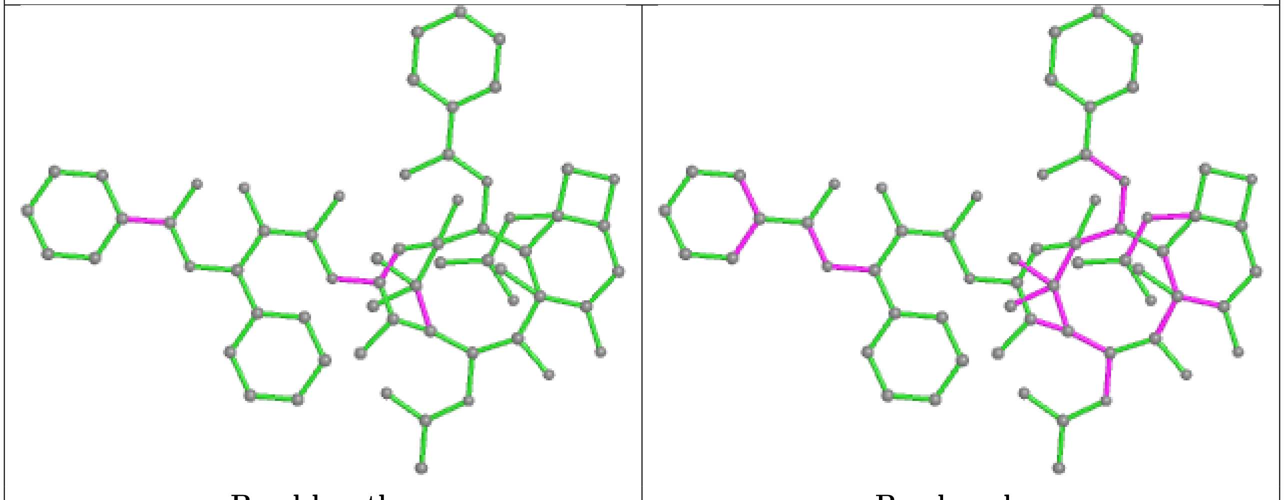


Bond lengths **Bond angles**



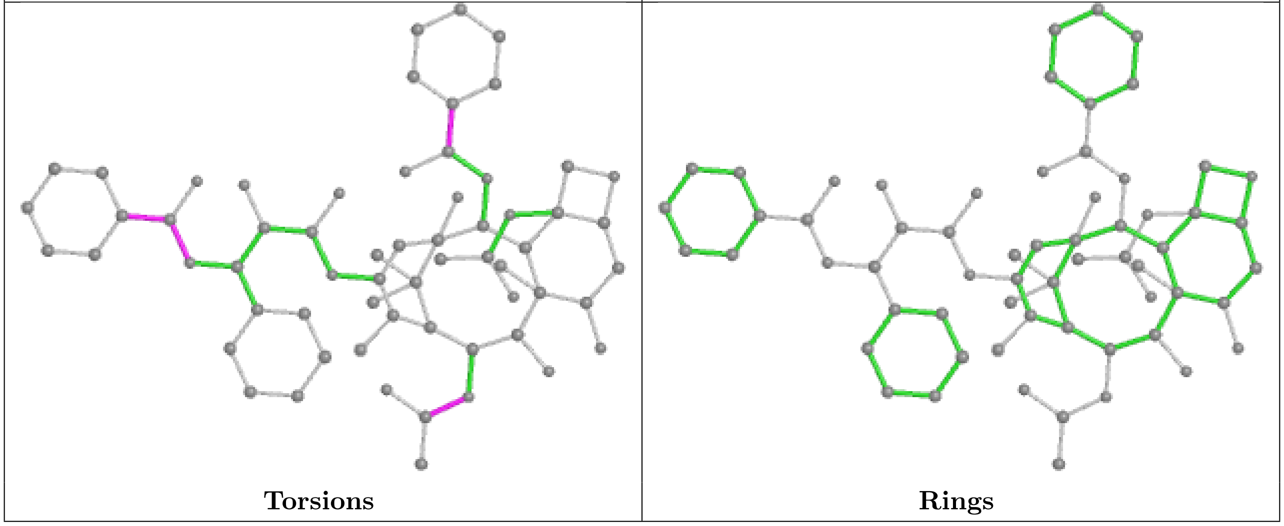
Torsions **Rings**

Ligand TA1 i 601



Bond lengths

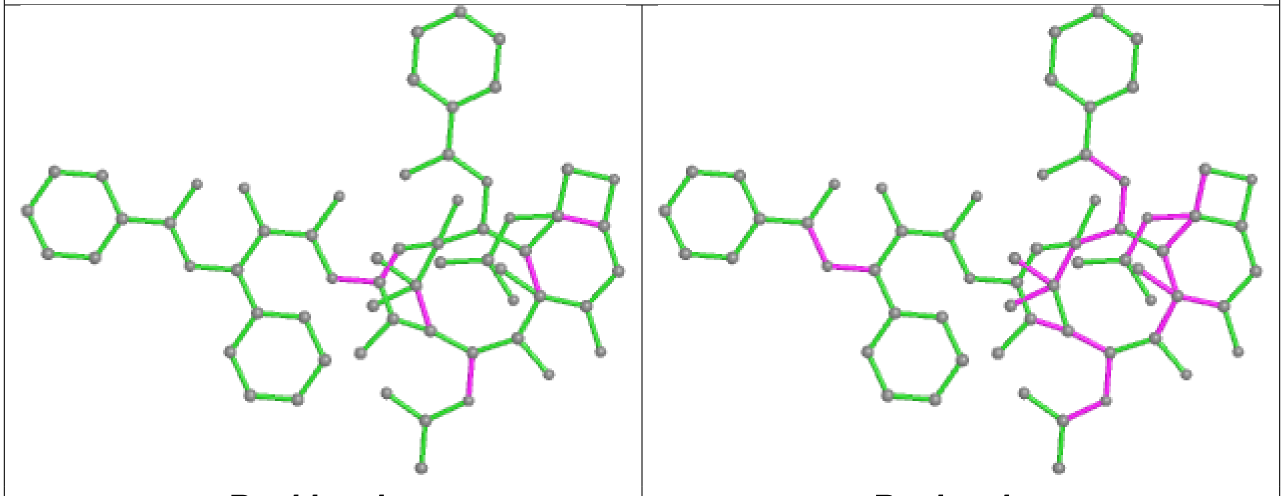
Bond angles



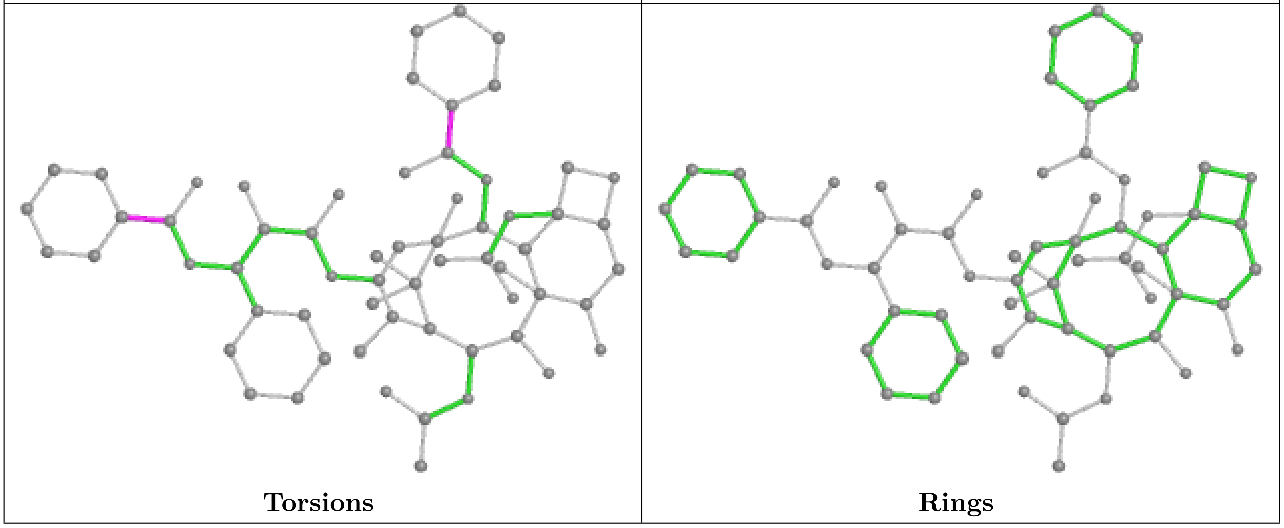
Torsions

Rings

Ligand TA1 d 601

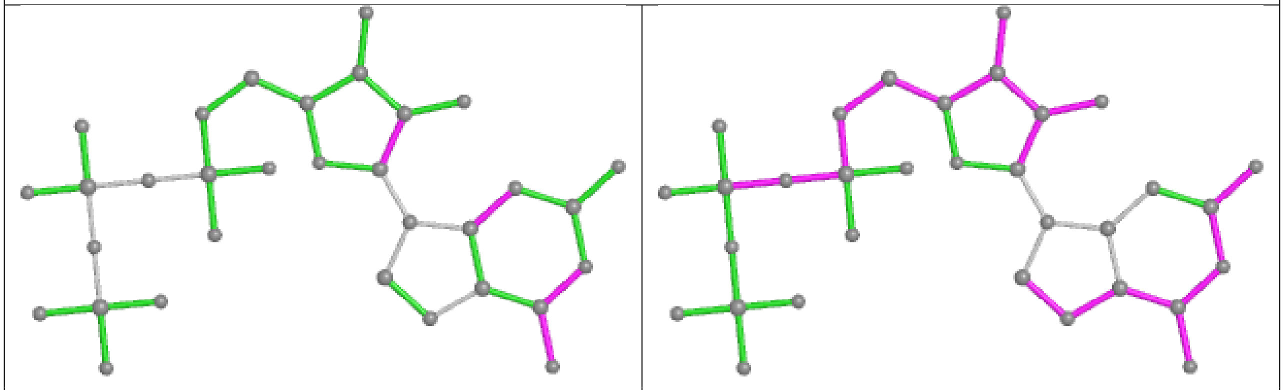


Bond lengths **Bond angles**

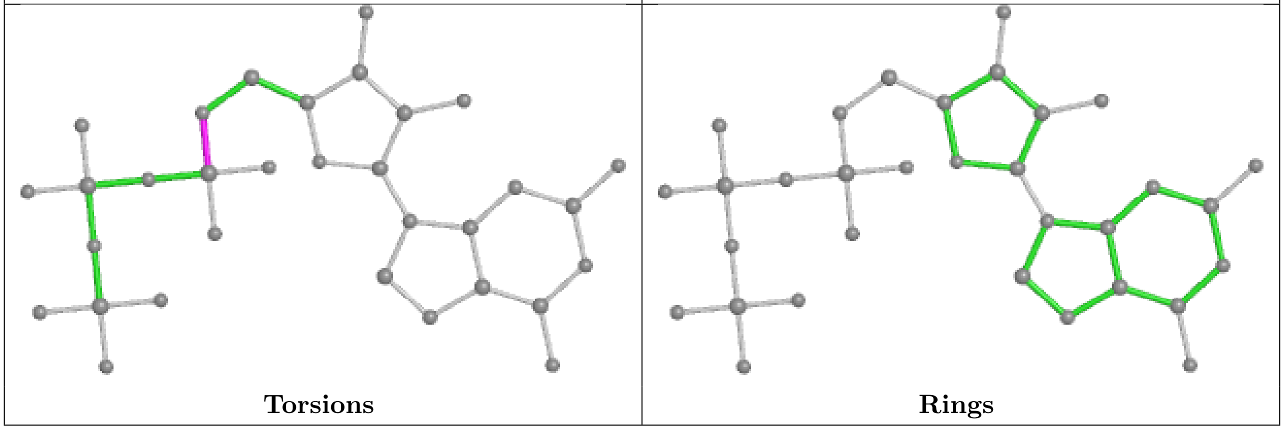


Torsions **Rings**

Ligand GTP R 502

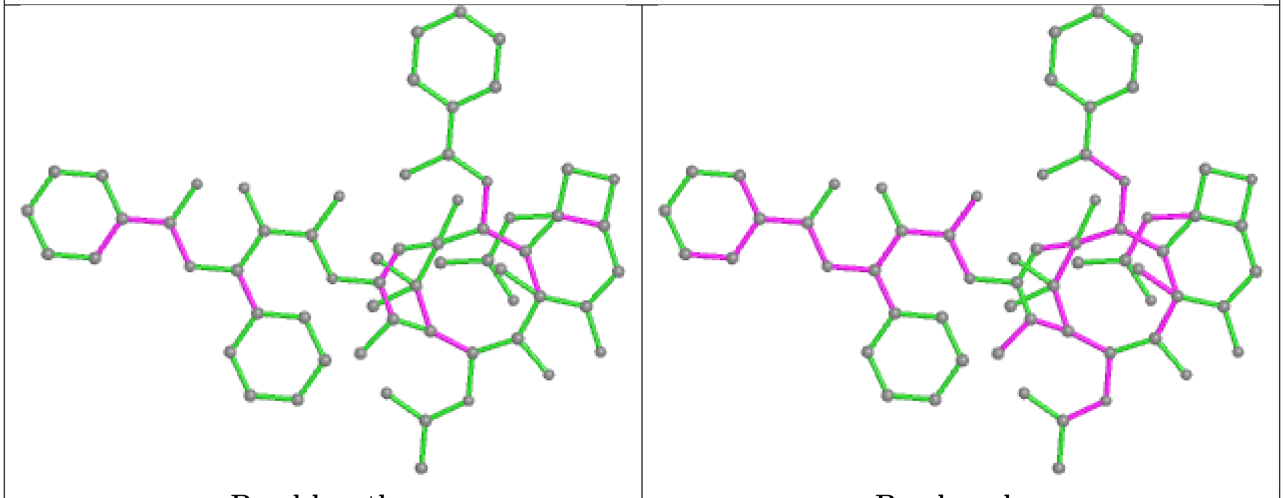


Bond lengths **Bond angles**

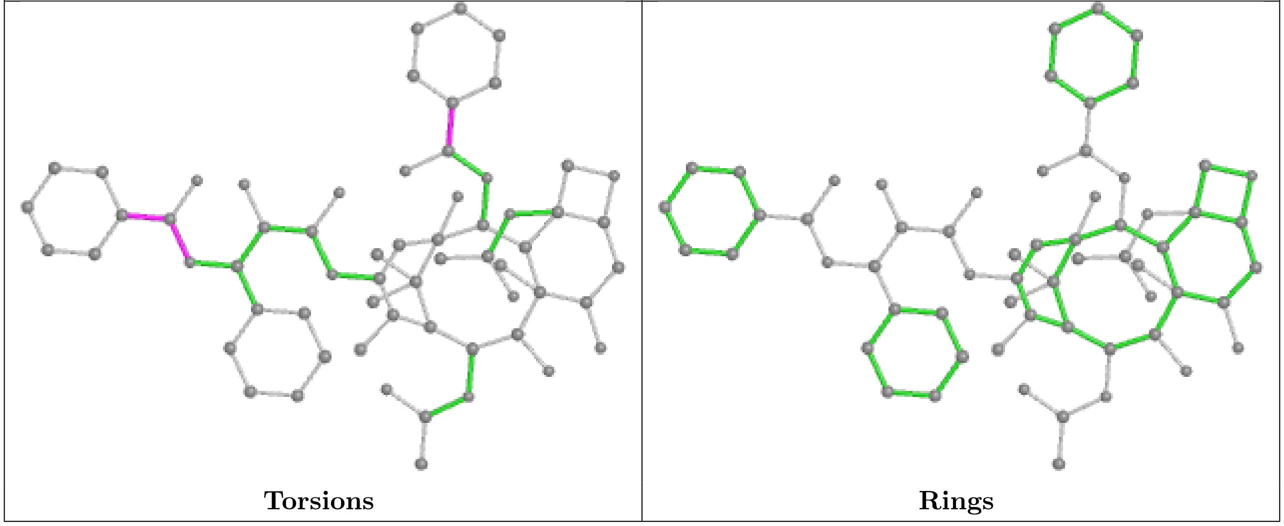


Torsions **Rings**

Ligand TA1 k 601

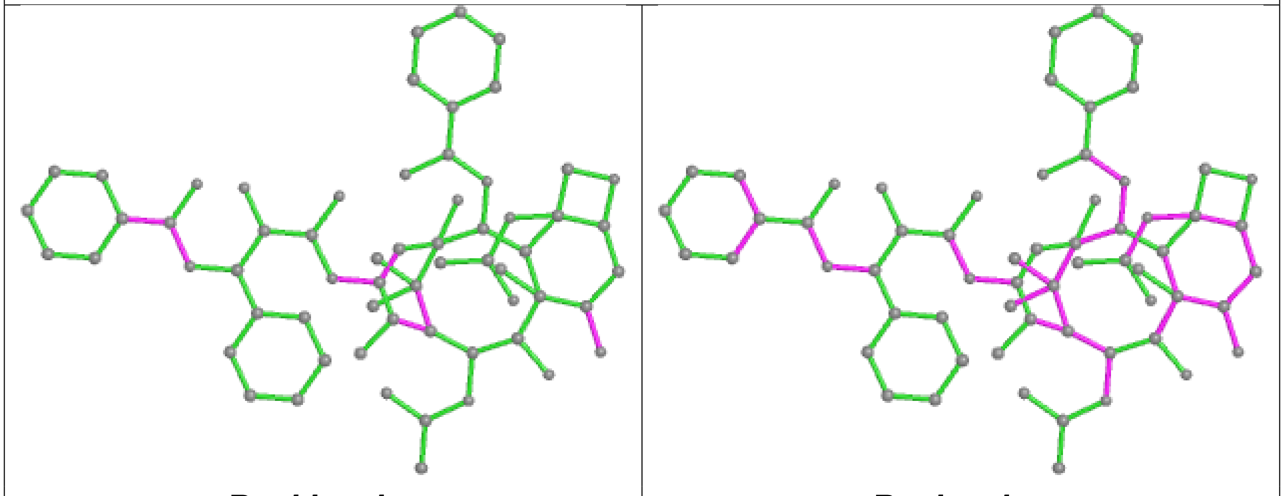


Bond lengths **Bond angles**

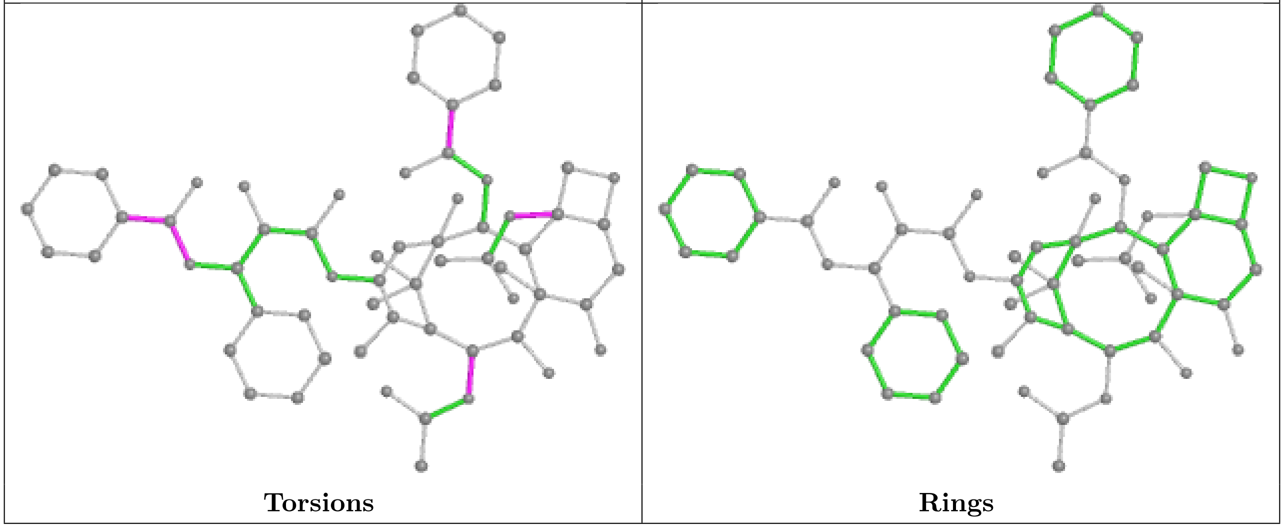


Torsions **Rings**

Ligand TA1 h 601

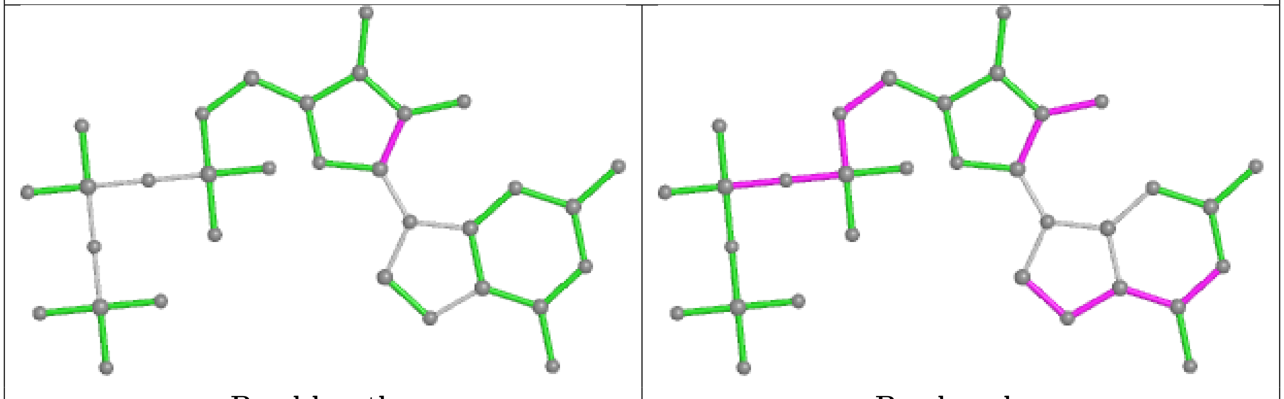


Bond lengths **Bond angles**

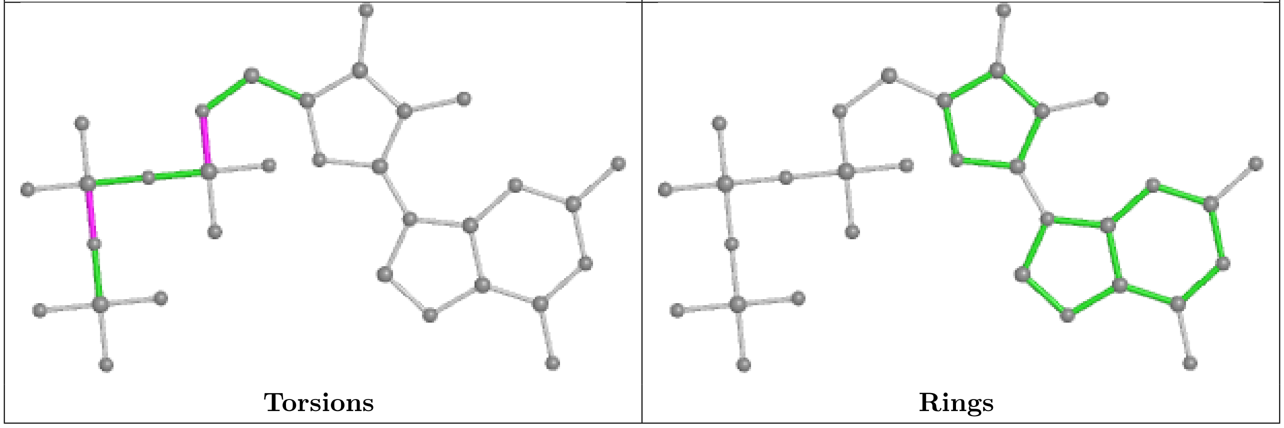


Torsions **Rings**

Ligand GTP Y 502

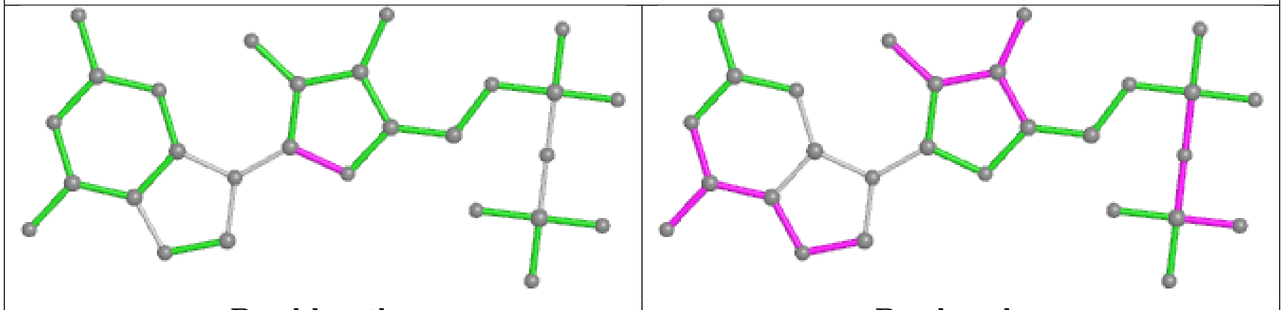


Bond lengths Bond angles

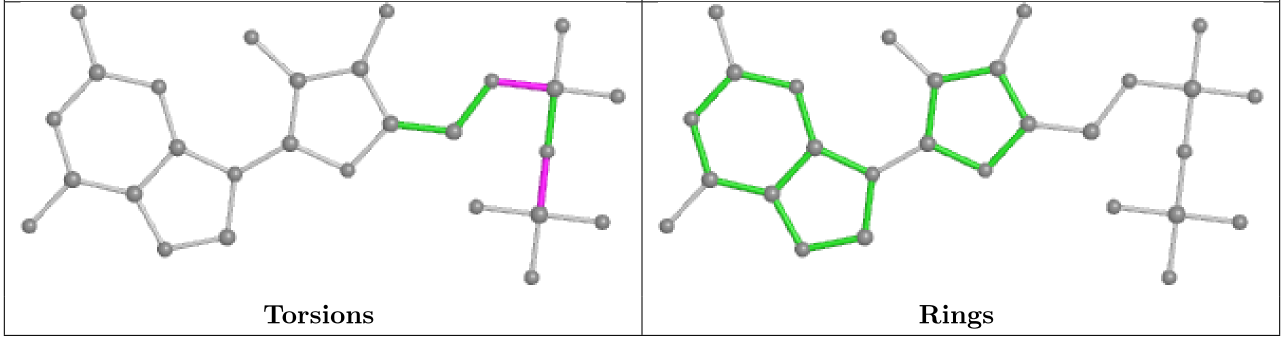


Torsions Rings

Ligand GDP l 602

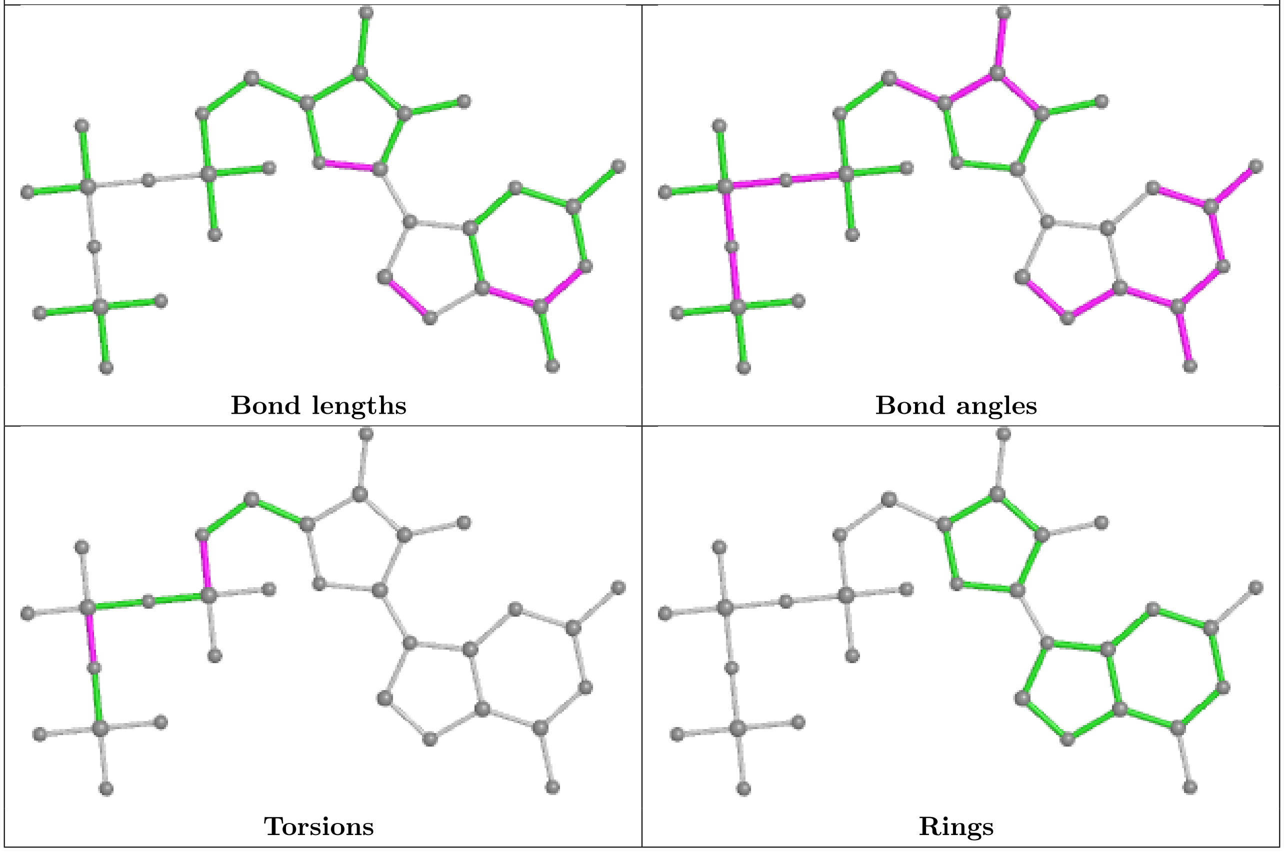


Bond lengths Bond angles



Torsions Rings

Ligand GTP S 502



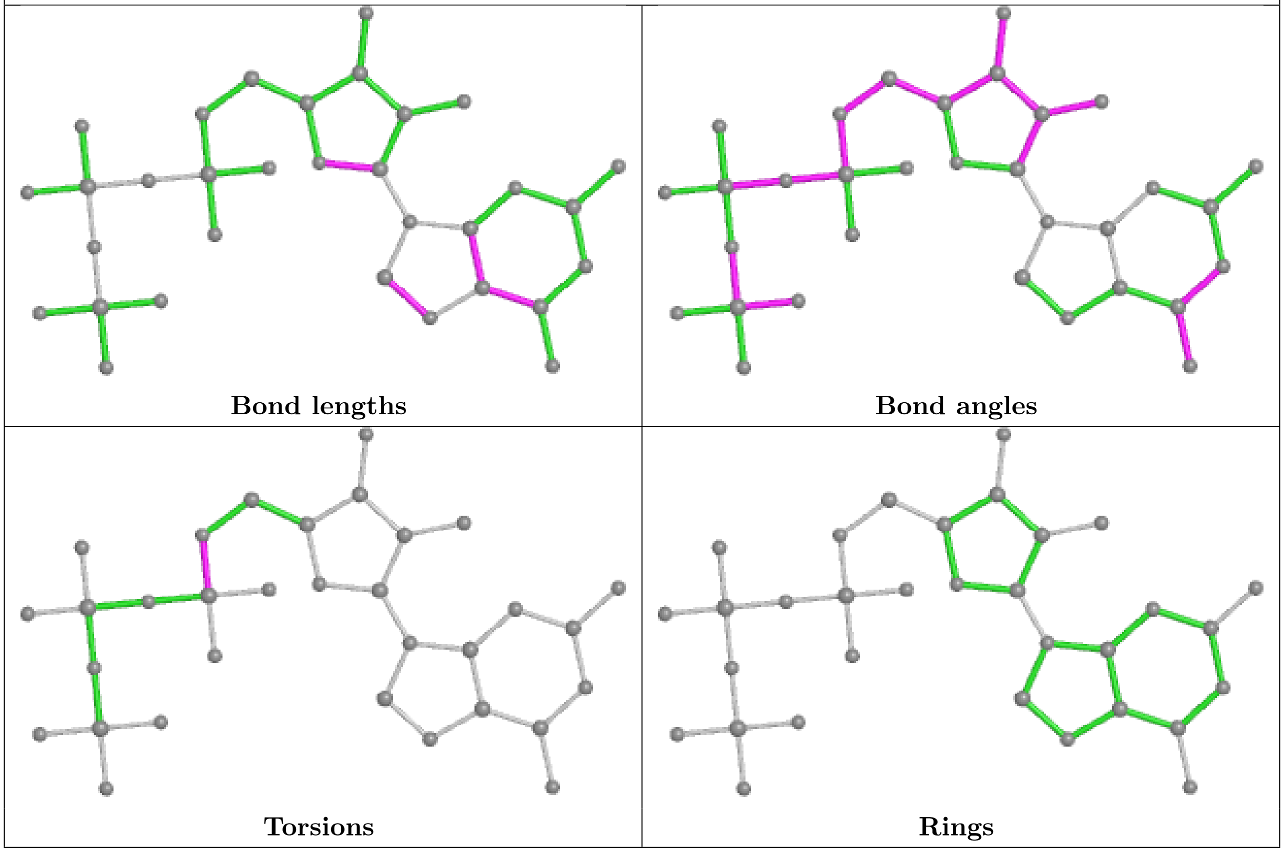
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP V 502



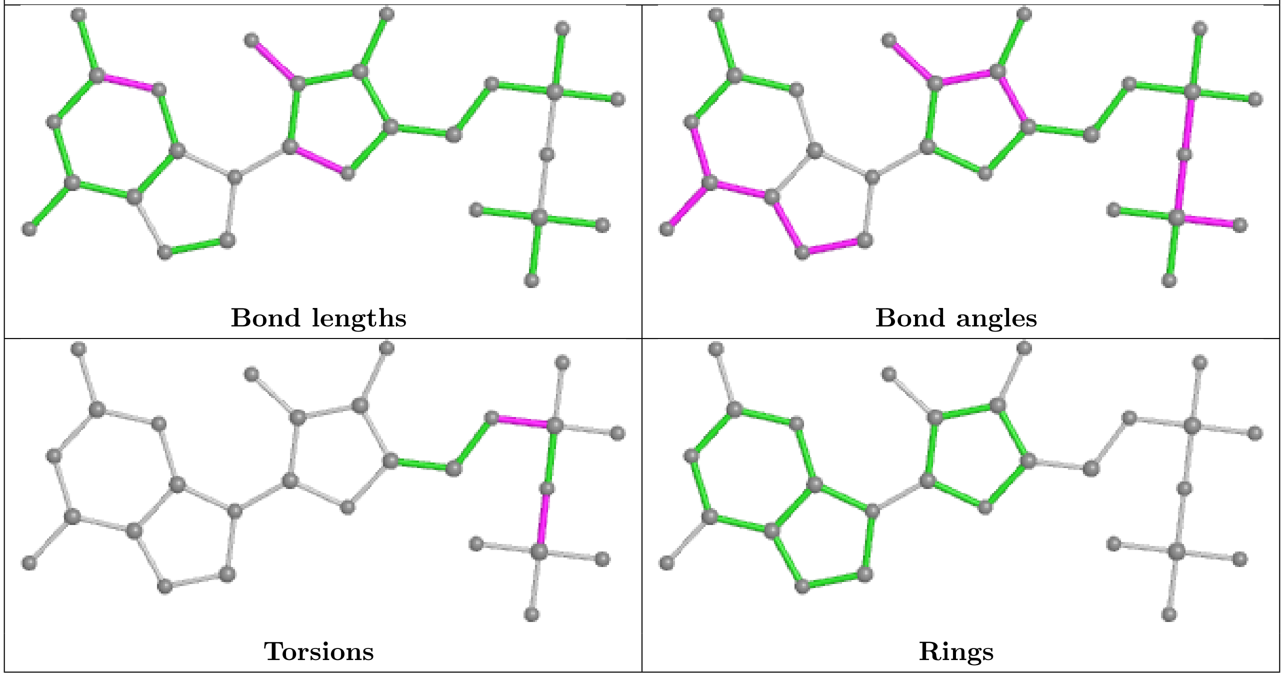
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP m 602



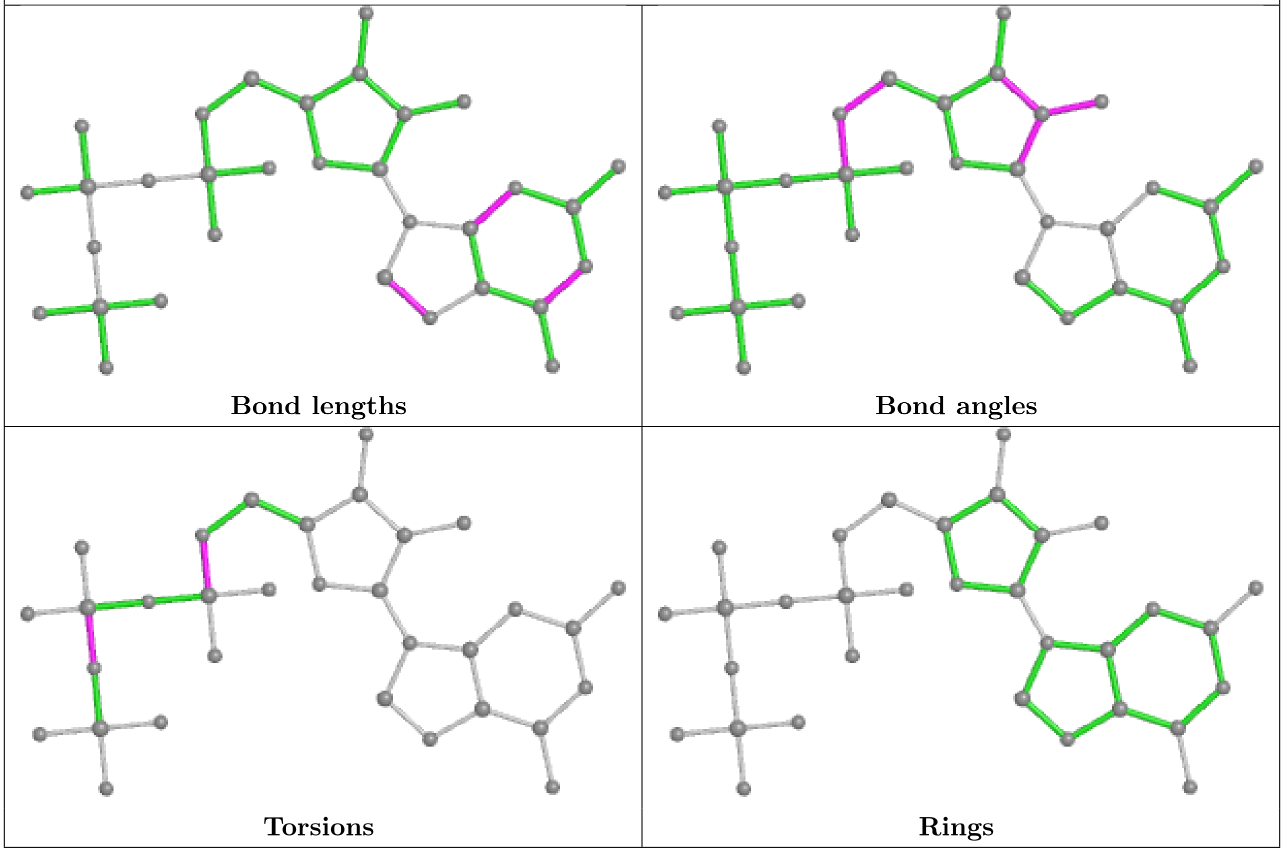
Bond lengths

Bond angles

Torsions

Rings

Ligand GTP N 502



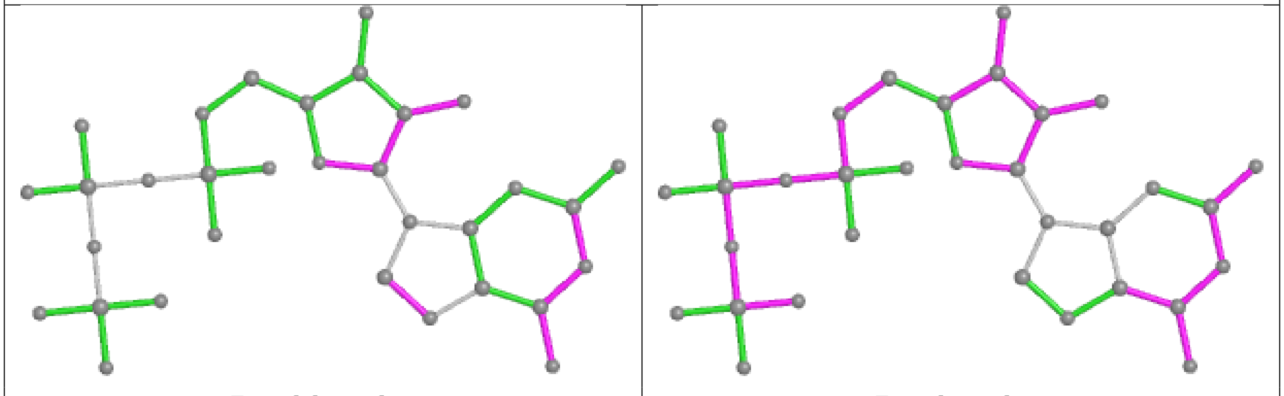
Bond lengths

Bond angles

Torsions

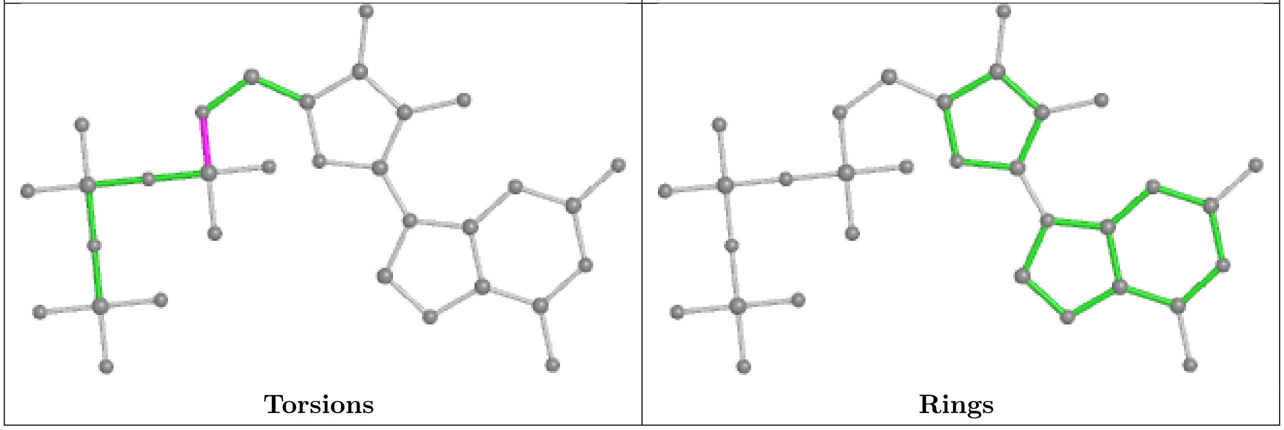
Rings

Ligand GTP U 502



Bond lengths

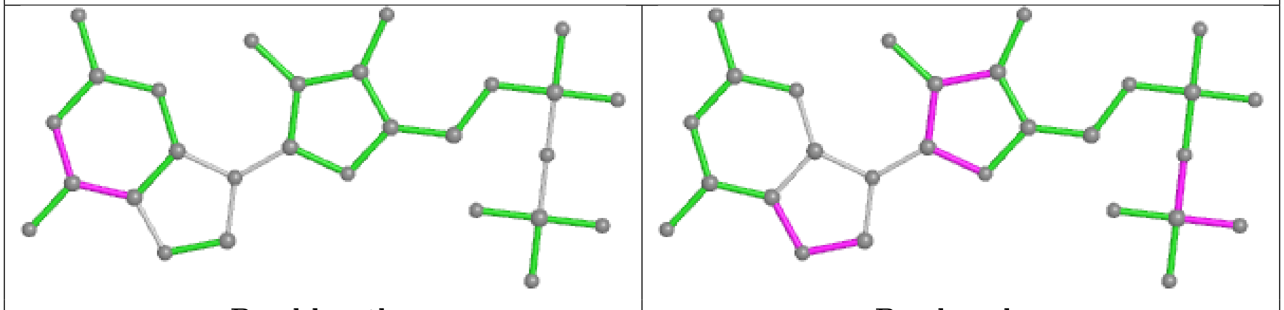
Bond angles



Torsions

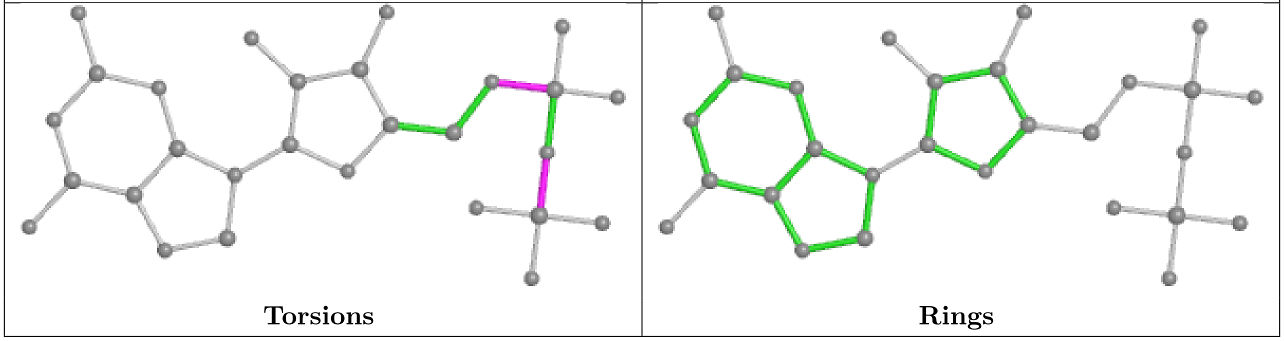
Rings

Ligand GDP a 602



Bond lengths

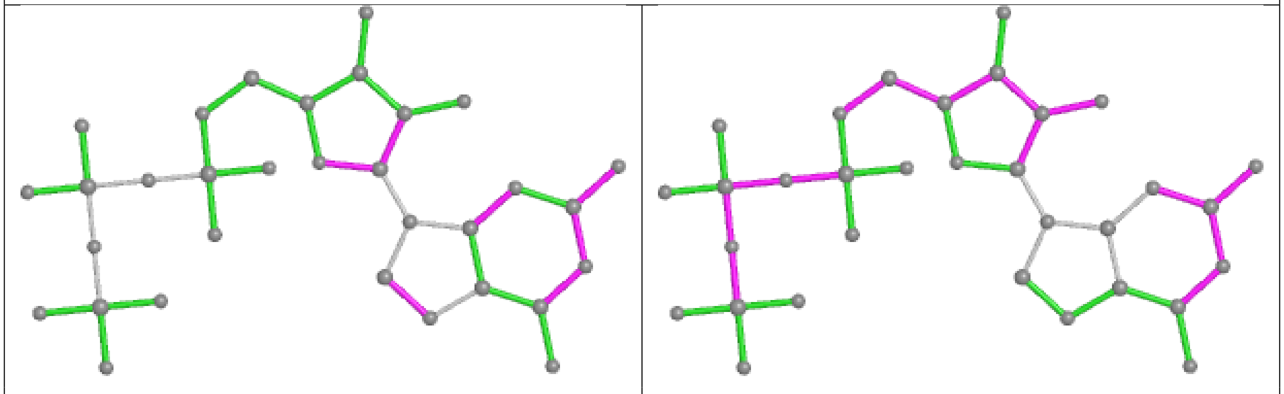
Bond angles



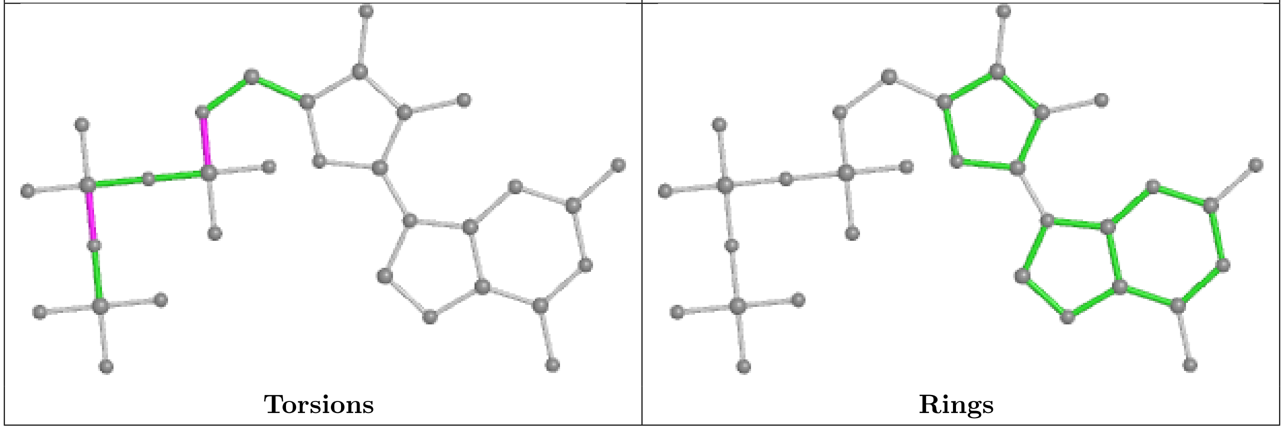
Torsions

Rings

Ligand GTP W 502

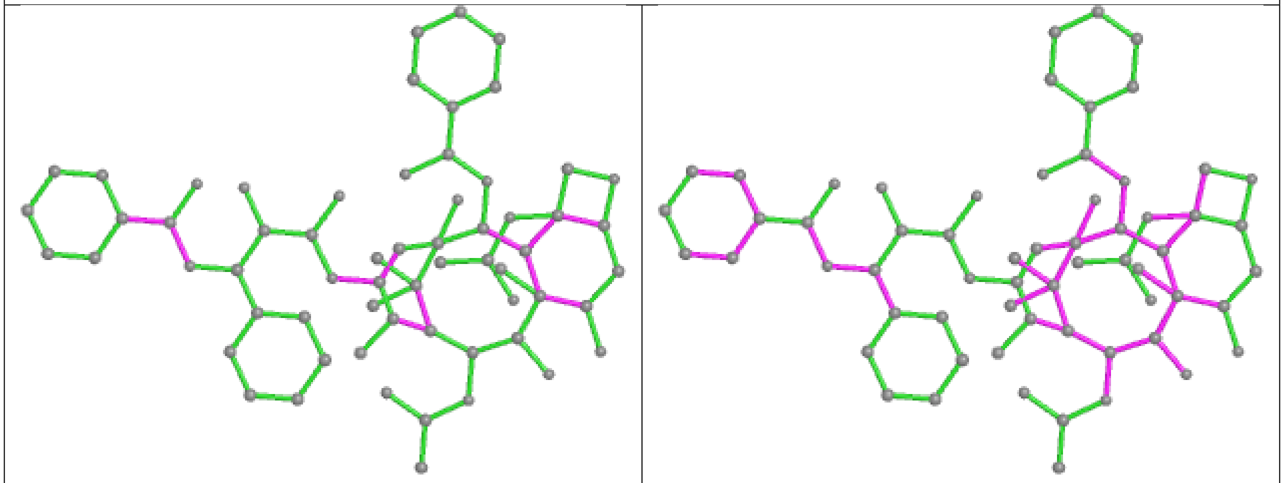


Bond lengths **Bond angles**



Torsions **Rings**

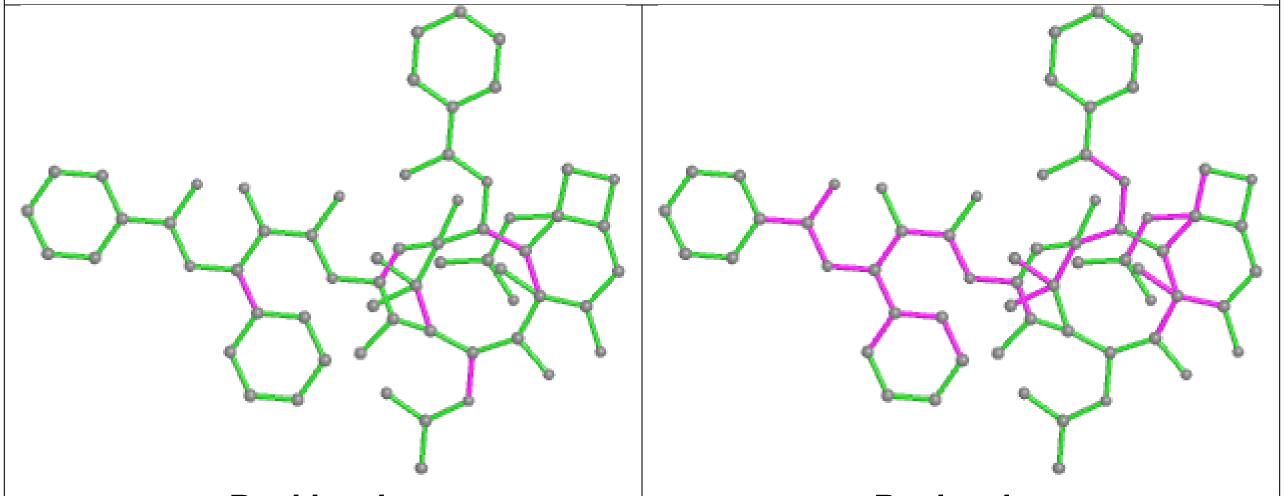
Ligand TA1 f 601



Bond lengths **Bond angles**

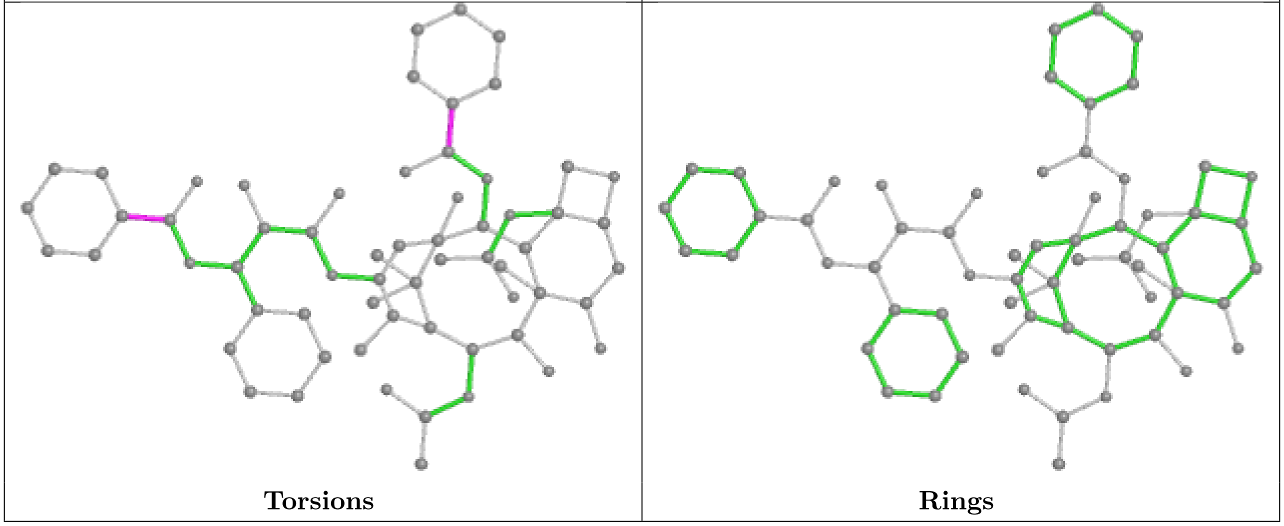
Torsions **Rings**

Ligand TA1 e 601



Bond lengths

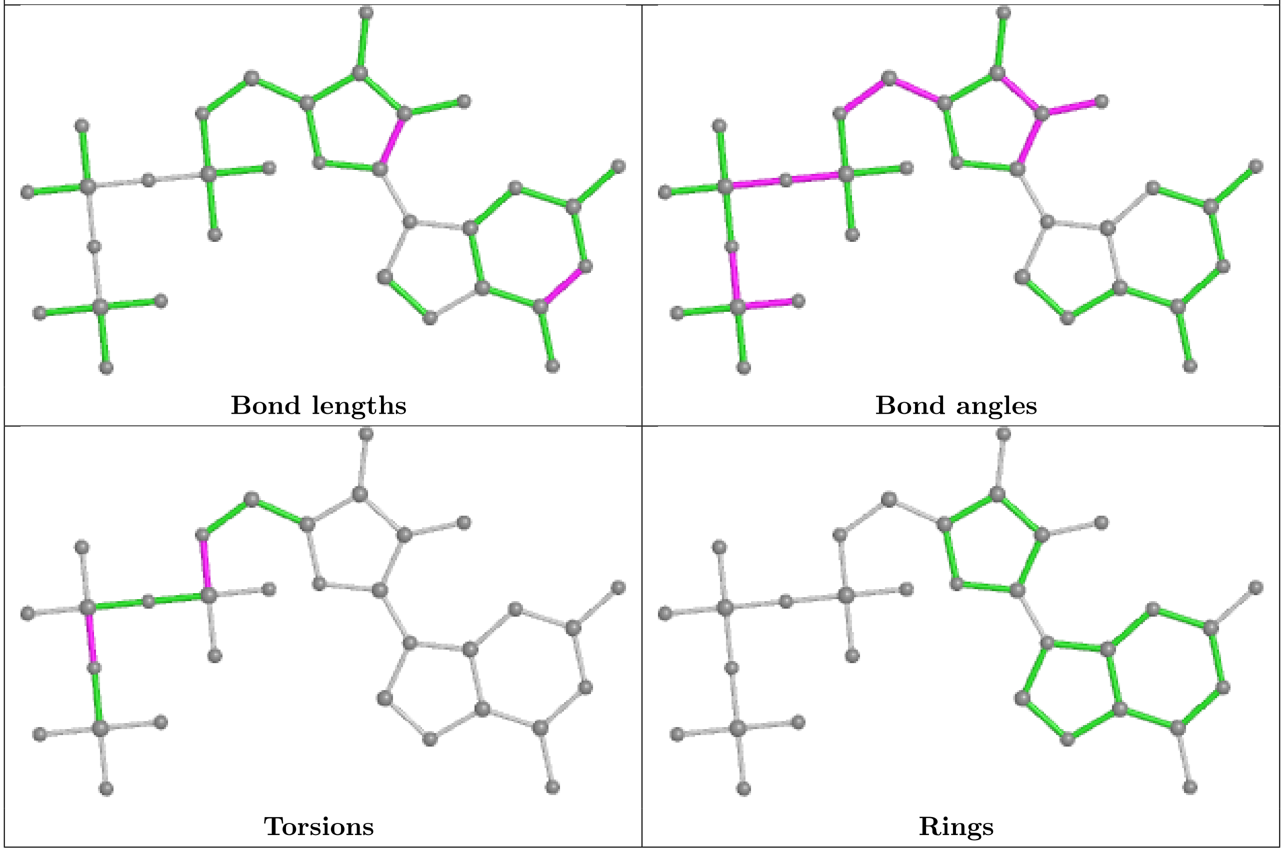
Bond angles



Torsions

Rings

Ligand GTP X 502



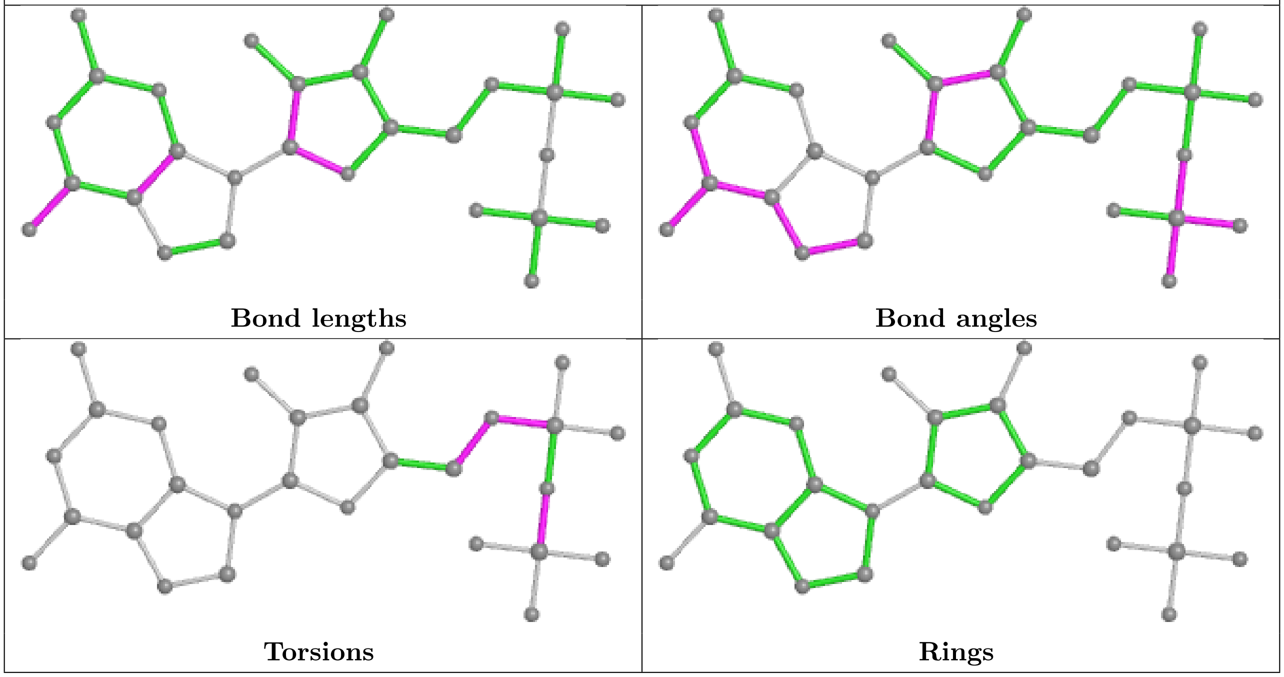
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP b 602



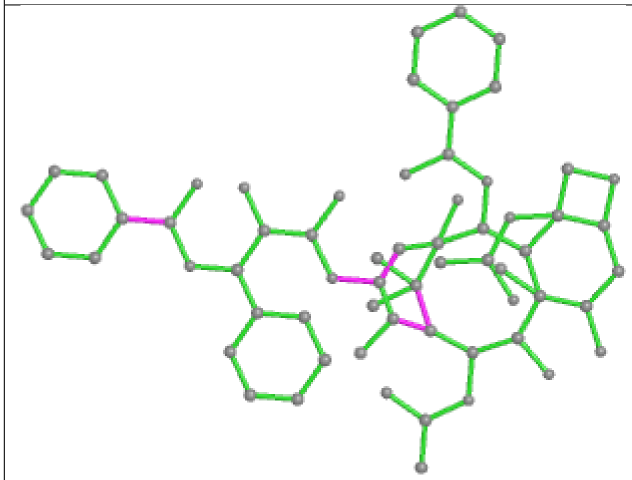
Bond lengths

Bond angles

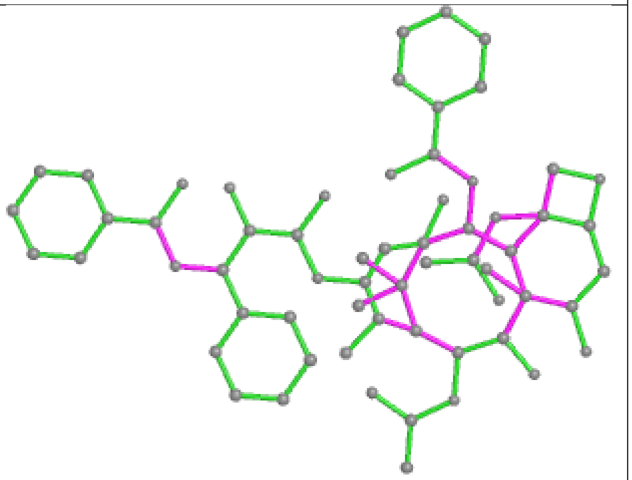
Torsions

Rings

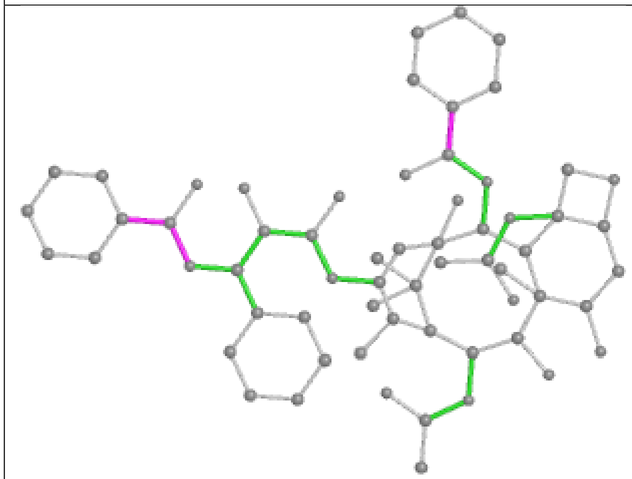
Ligand TA1 l 601



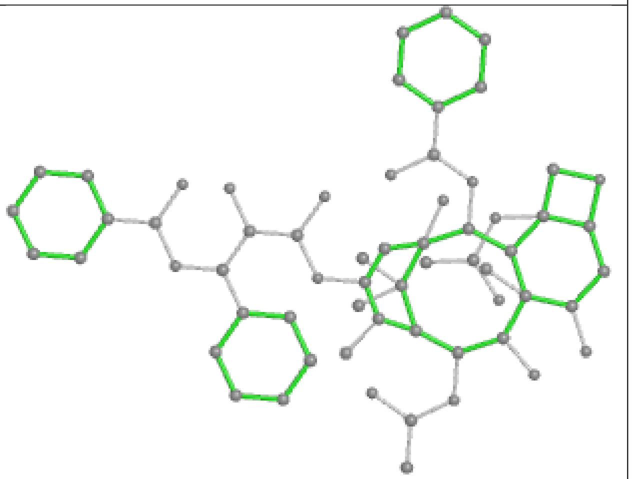
Bond lengths



Bond angles

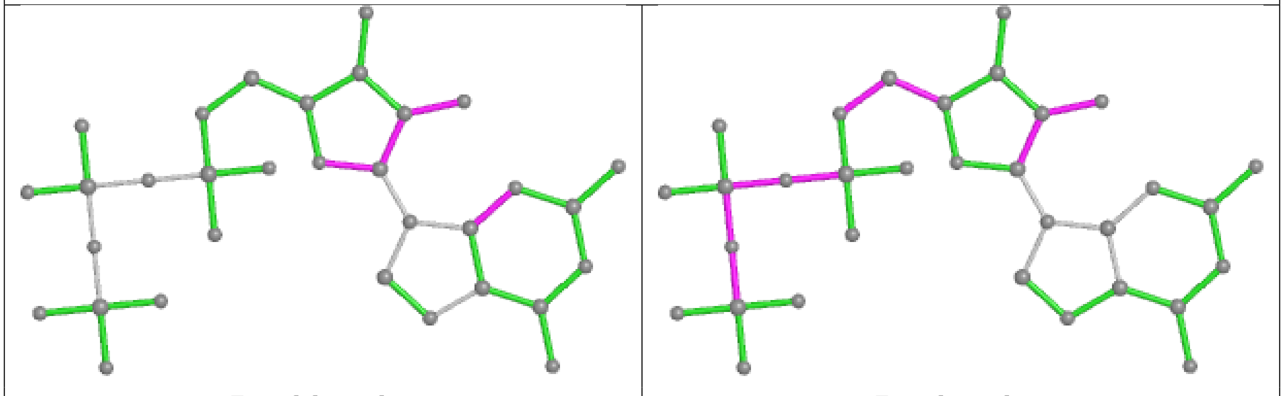


Torsions



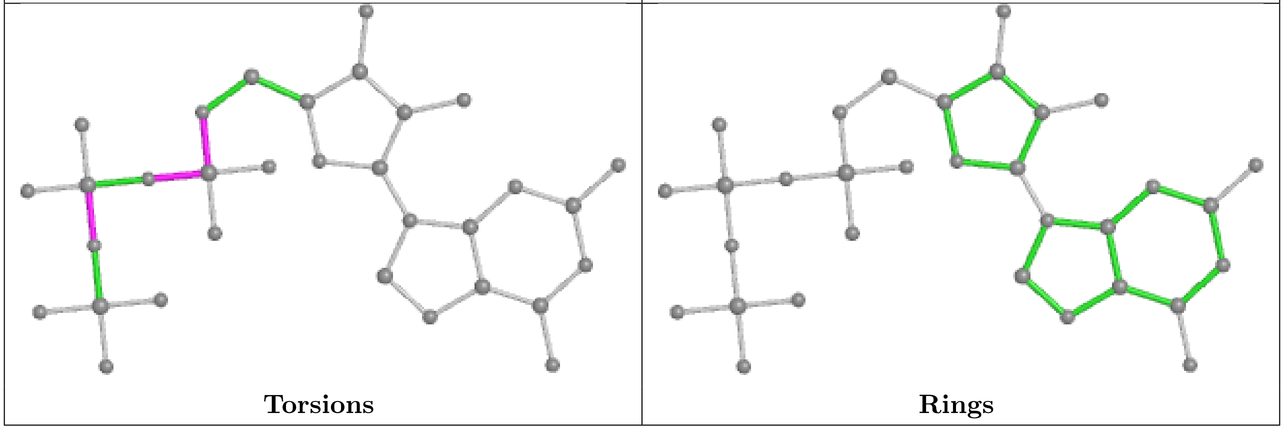
Rings

Ligand GTP Z 502



Bond lengths

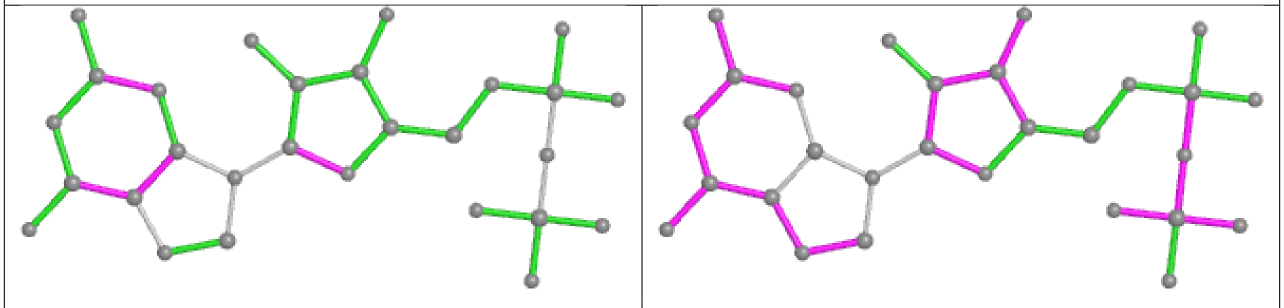
Bond angles



Torsions

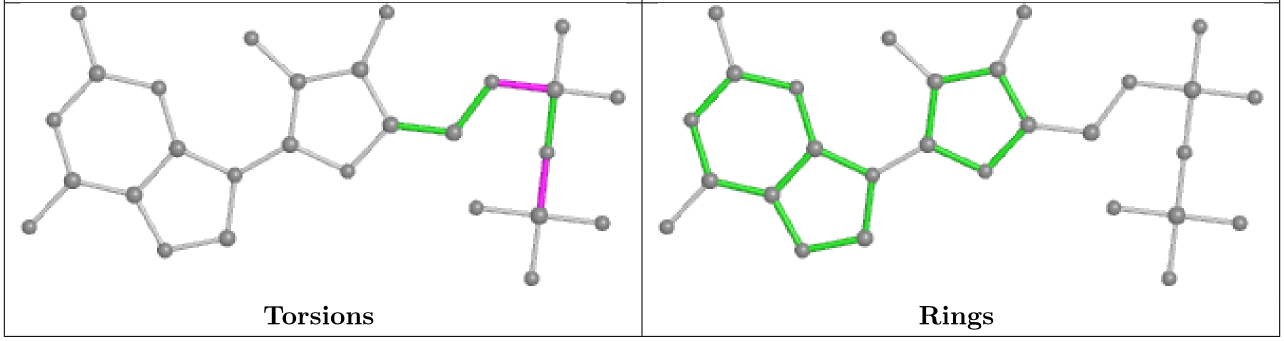
Rings

Ligand GDP g 602



Bond lengths

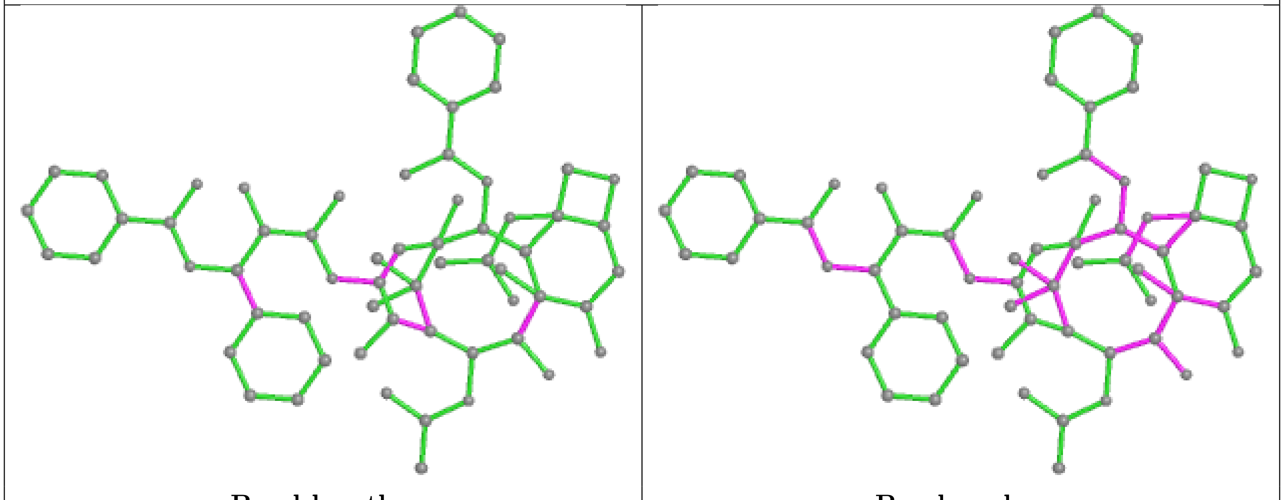
Bond angles



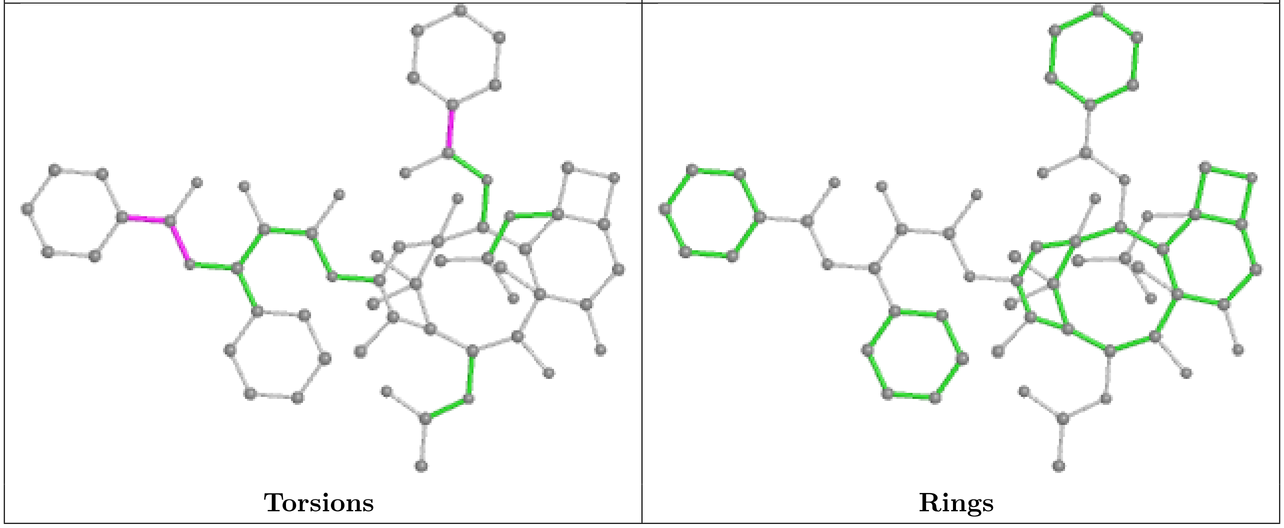
Torsions

Rings

Ligand TA1 b 601

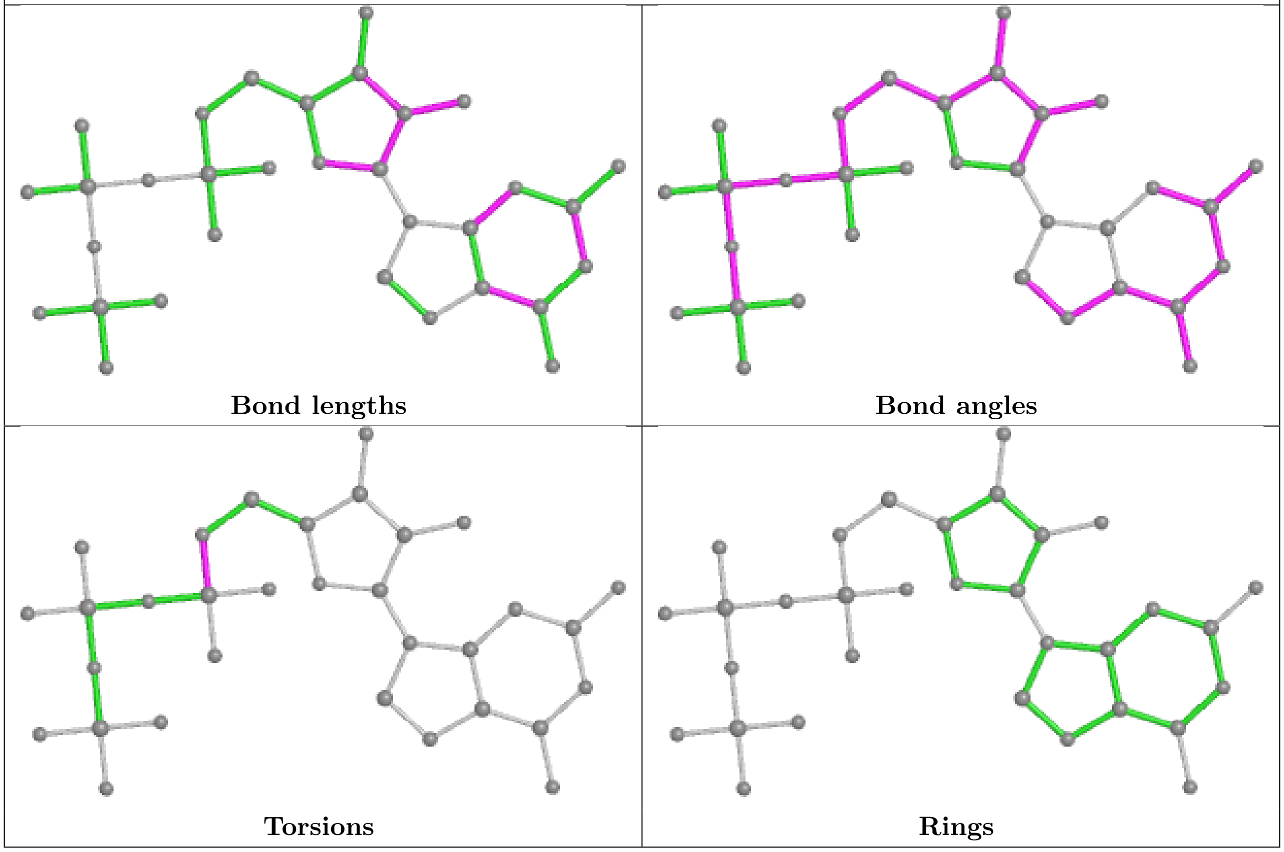


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GTP T 502



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	R	1
1	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	43:GLY	C	44:GLY	N	1.98
1	e	294:PHE	C	295:ASP	N	1.83

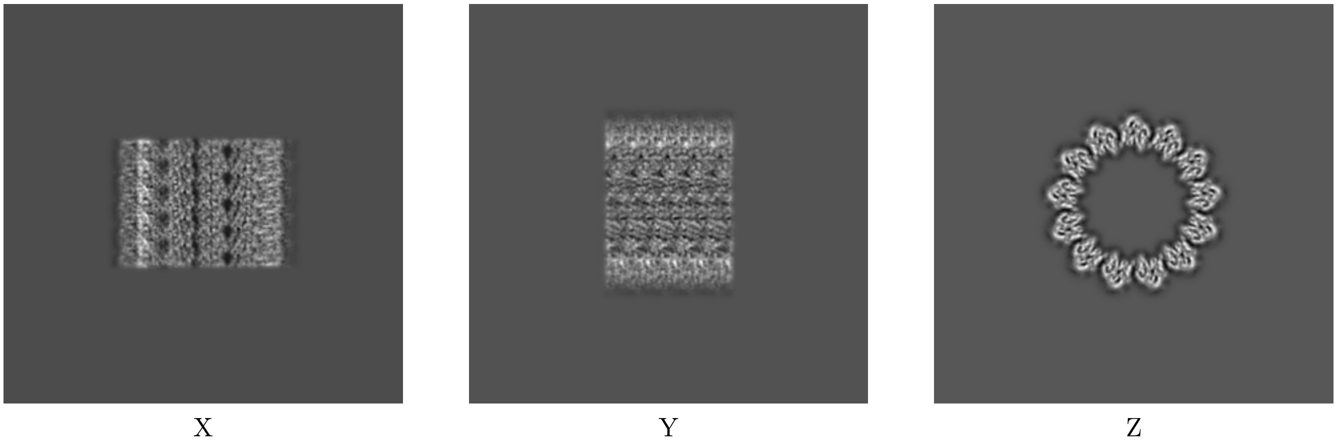
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16435. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

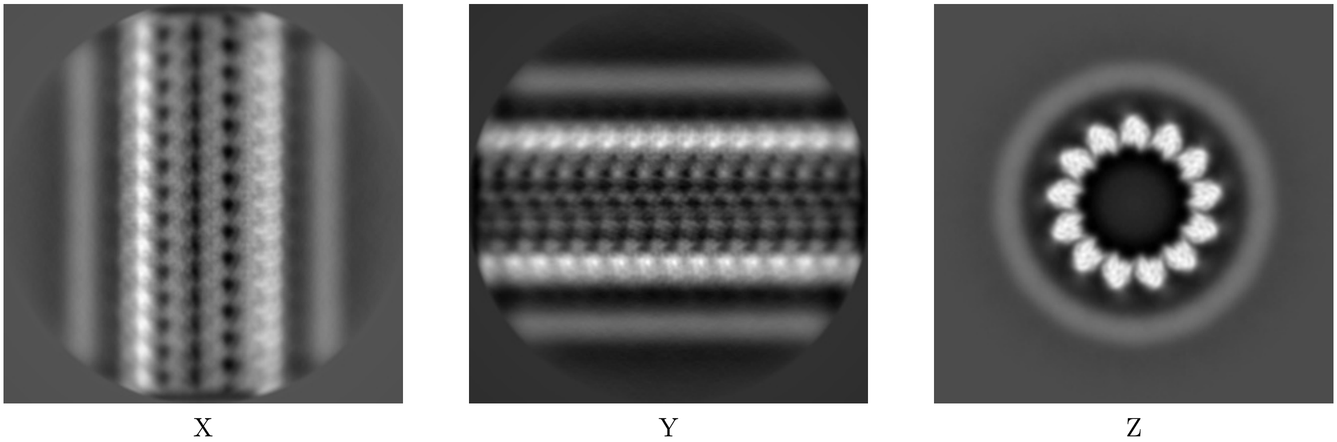
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

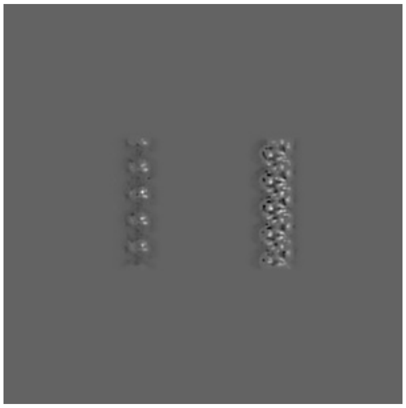


X Y Z

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

6.2 Central slices

6.2.1 Primary map

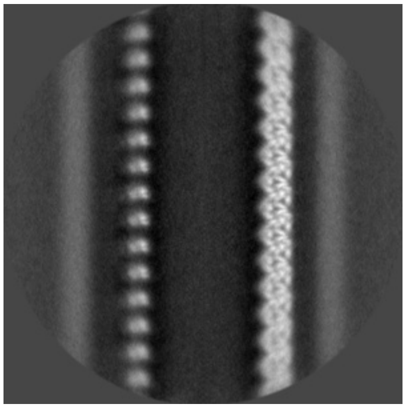


X Index: 160

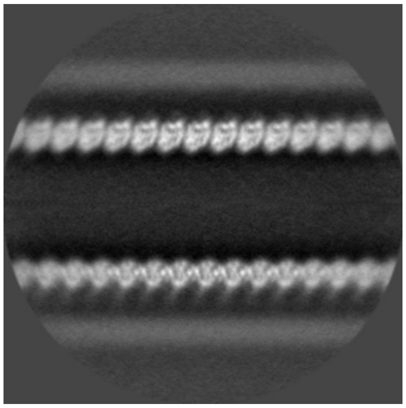
Y Index: 160

Z Index: 160

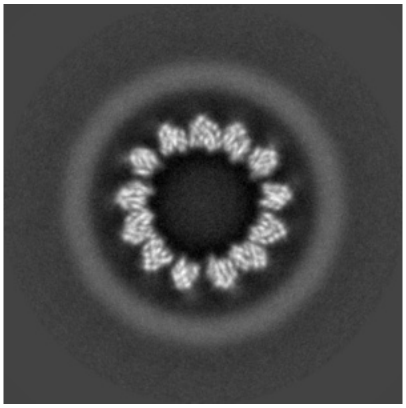
6.2.2 Raw map



X Index: 160



Y Index: 160

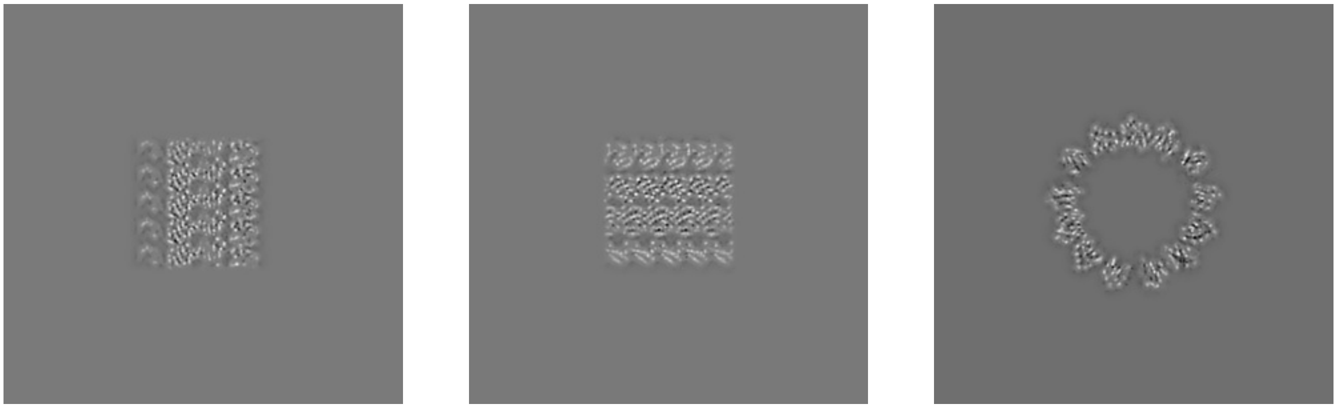


Z Index: 160

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

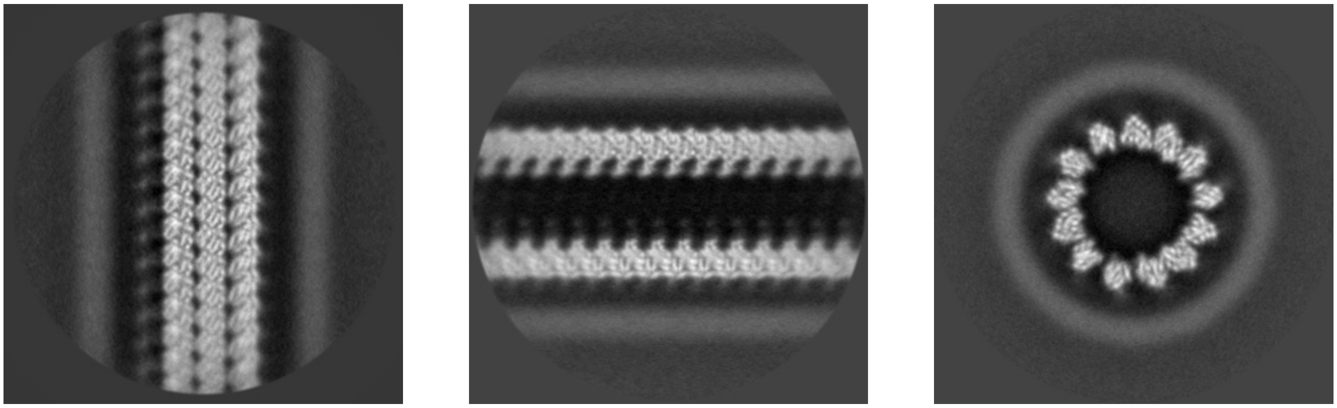
6.3 Largest variance slices ⓘ

6.3.1 Primary map



X Index: 111 Y Index: 109 Z Index: 159

6.3.2 Raw map

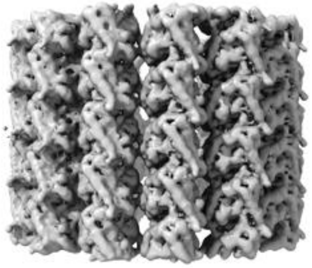


X Index: 213 Y Index: 196 Z Index: 141

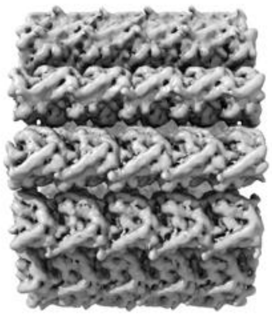
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

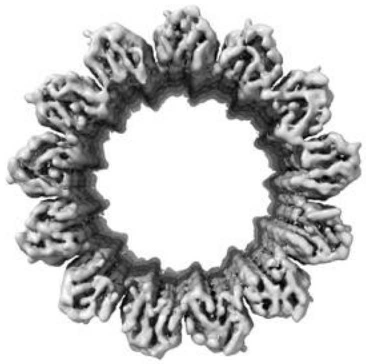
6.4.1 Primary map



X



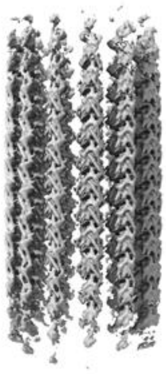
Y



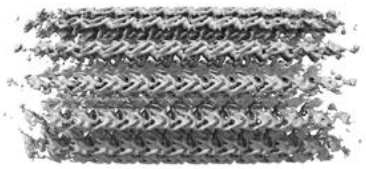
Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y

Z

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

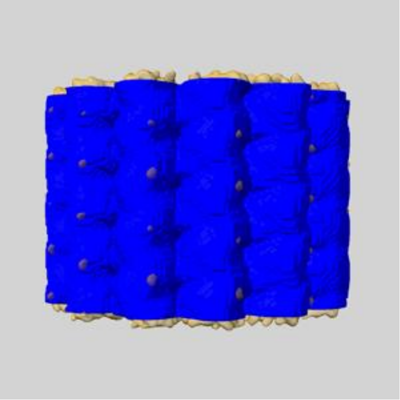
6.5 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

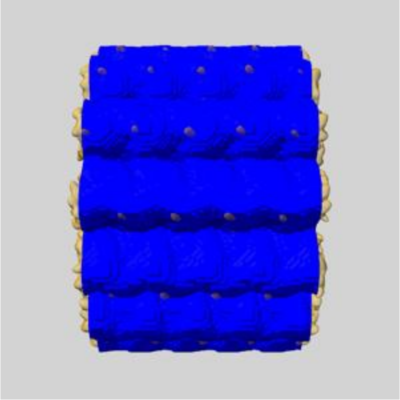
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

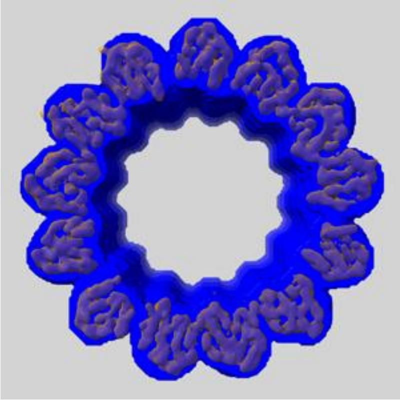
6.5.1 emd_16435_msk_1.map ⓘ



X



Y

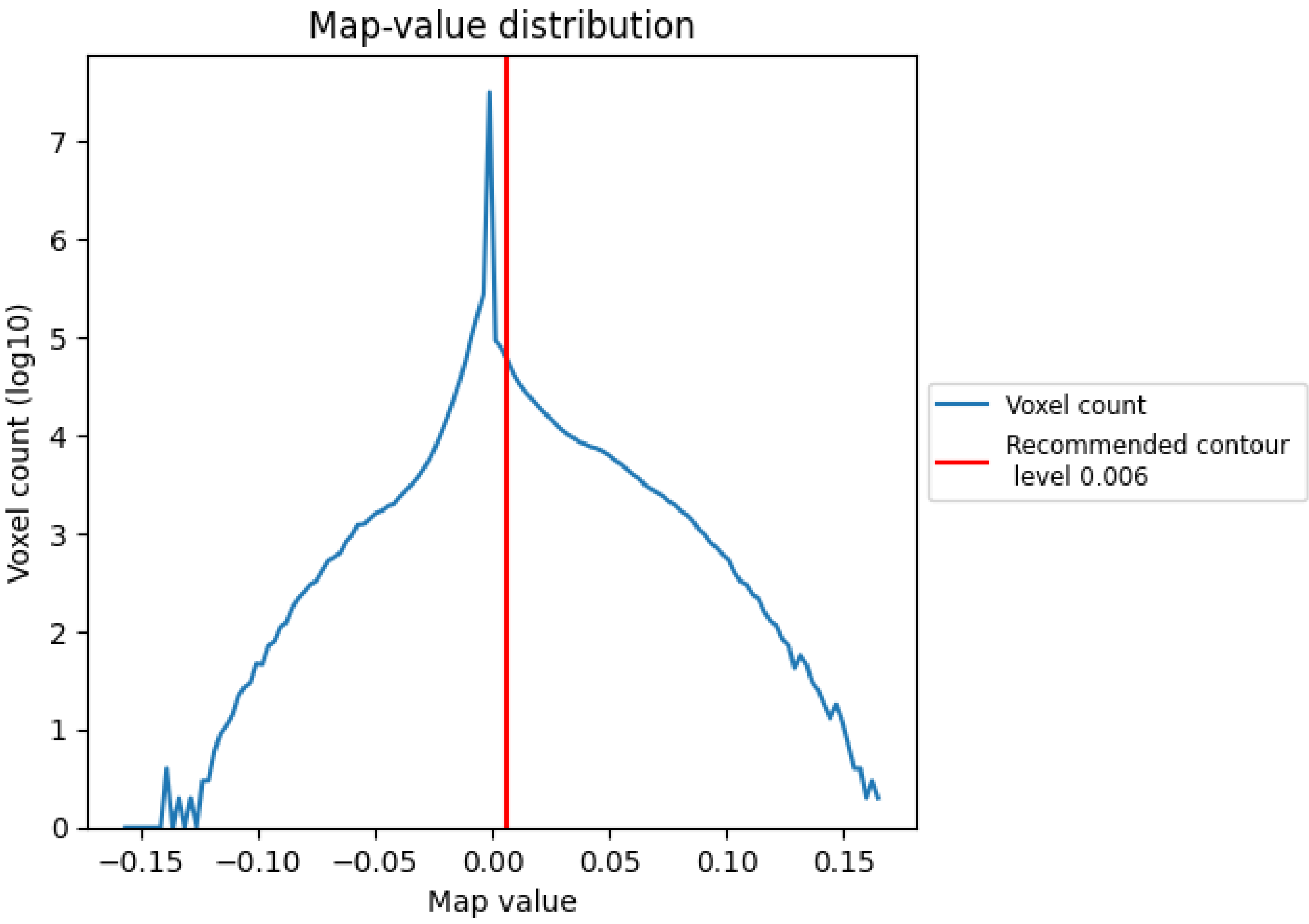


Z

7 Map analysis ⓘ

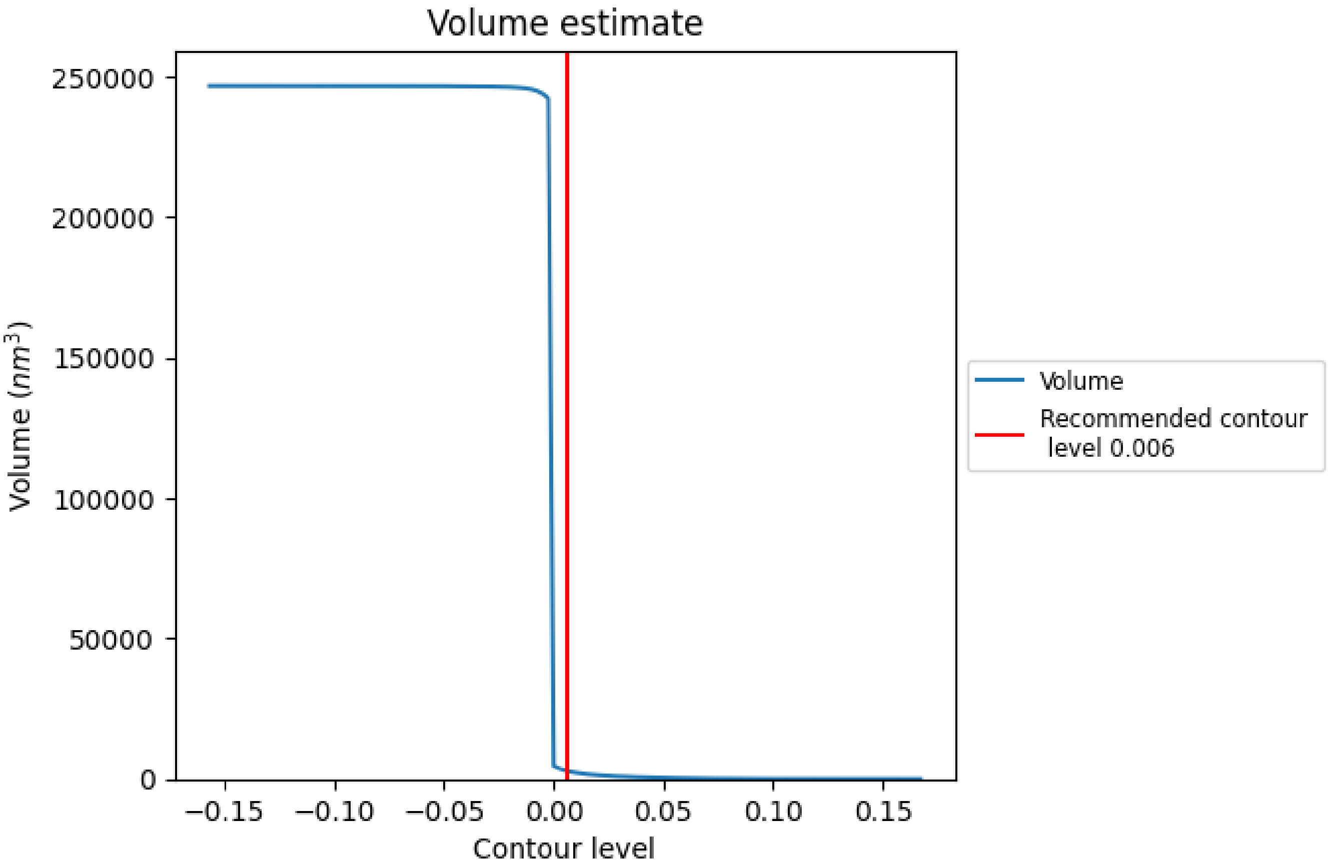
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

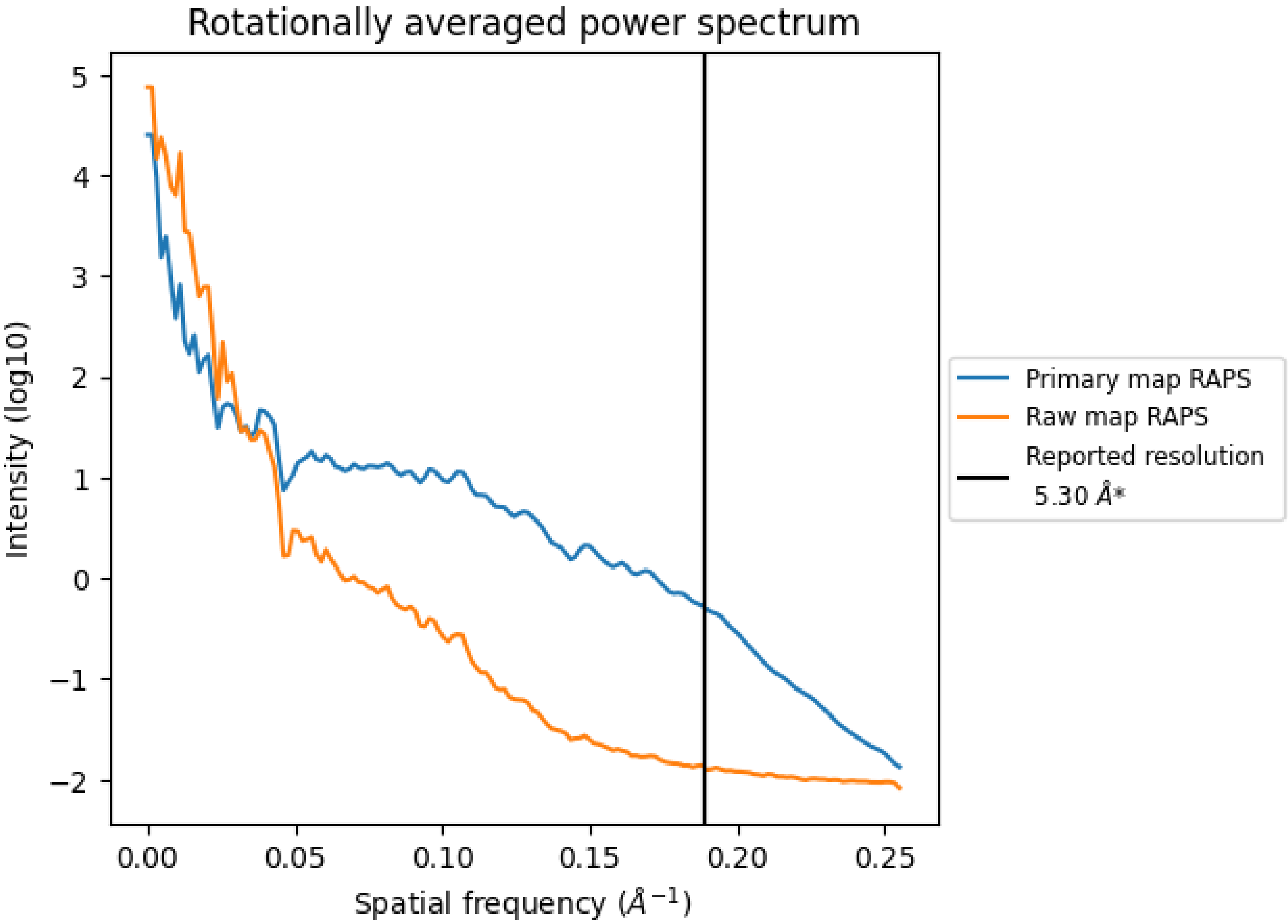
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2953 nm^3; this corresponds to an approximate mass of 2668 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

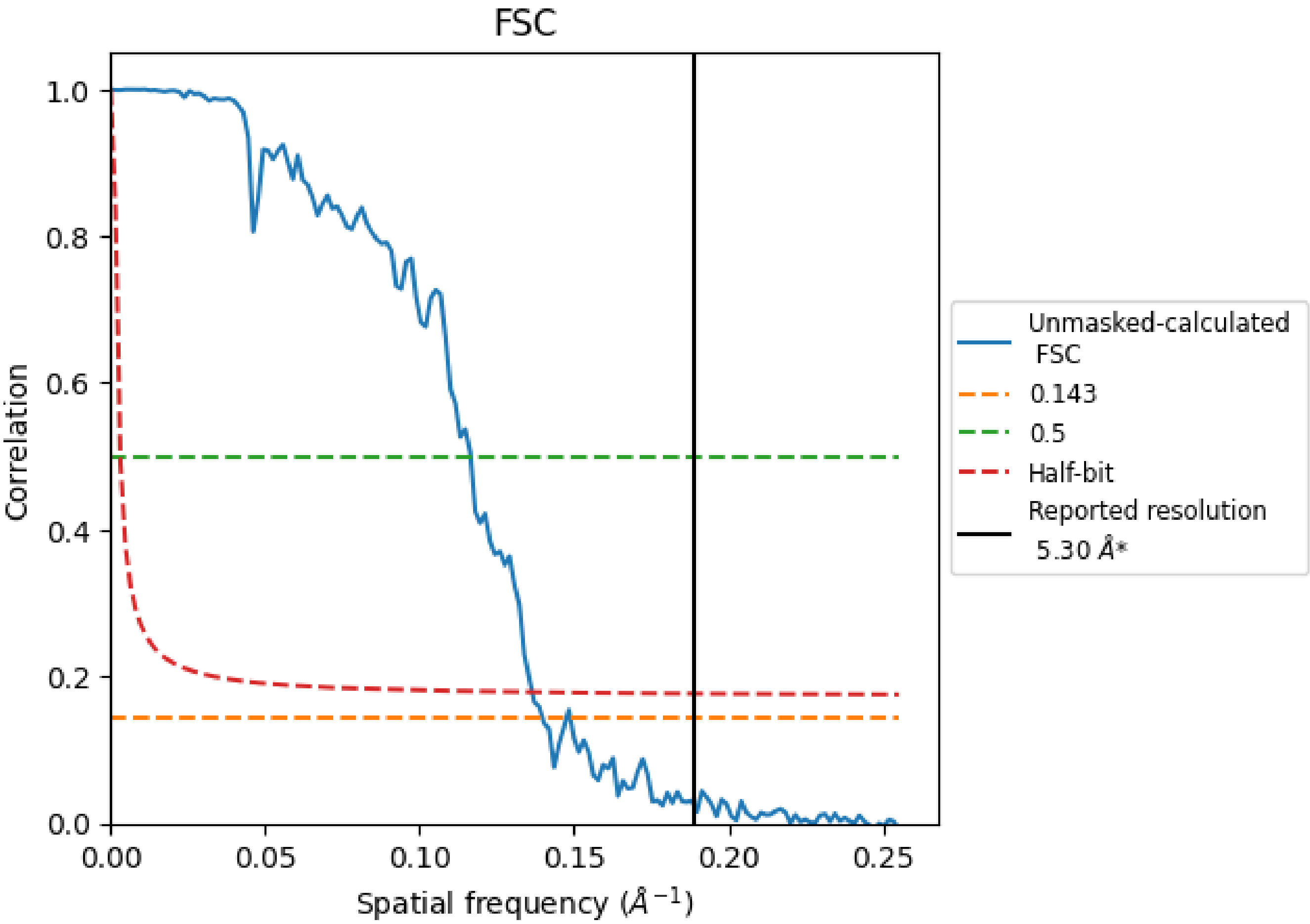


*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.189 Å^{-1}

8.2 Resolution estimates ⓘ

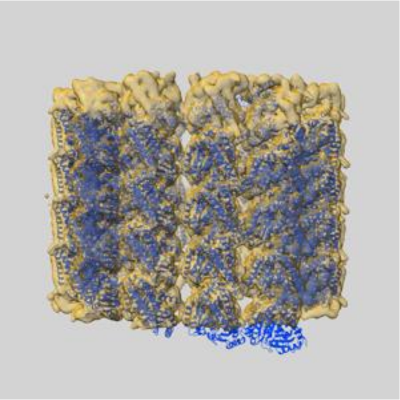
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.15	8.58	7.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 5.3 by more than 10 %

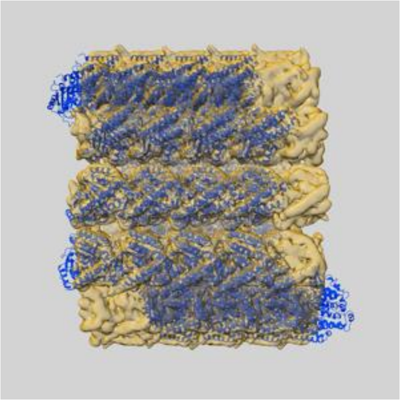
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-16435 and PDB model 8C5C. Per-residue inclusion information can be found in section 3 on page 12.

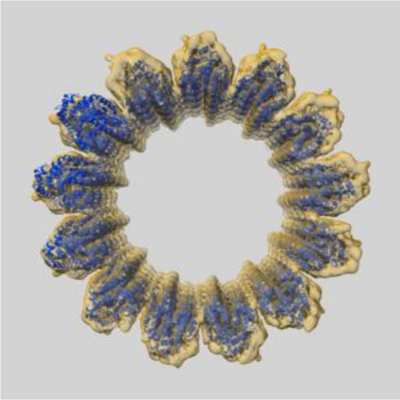
9.1 Map-model overlay (i)



X



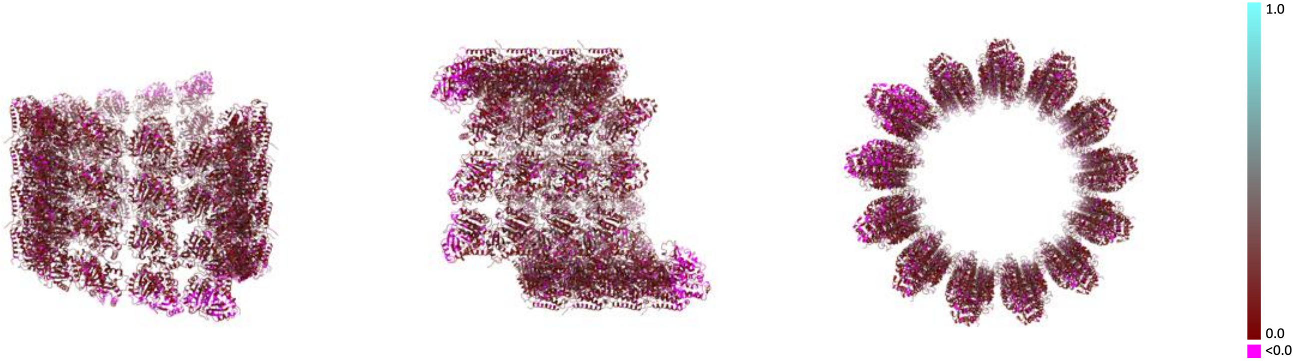
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

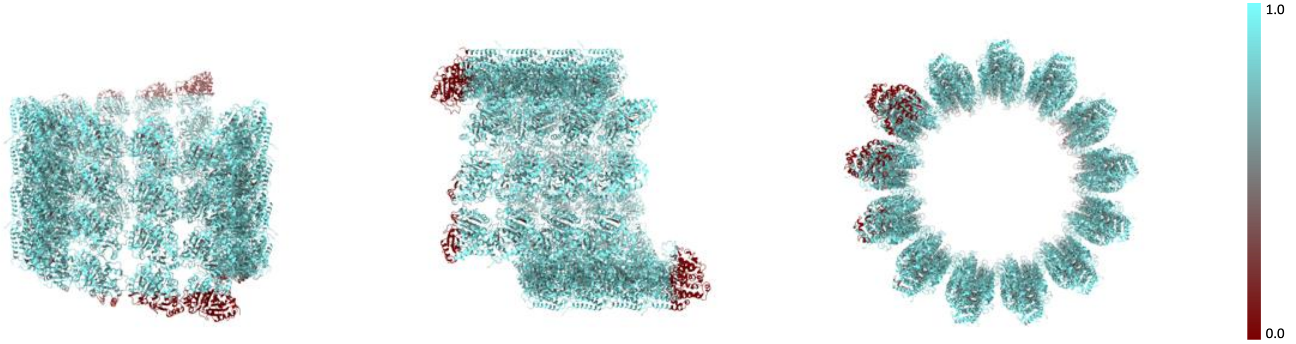
9.2 Q-score mapped to coordinate model



X Y Z

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.

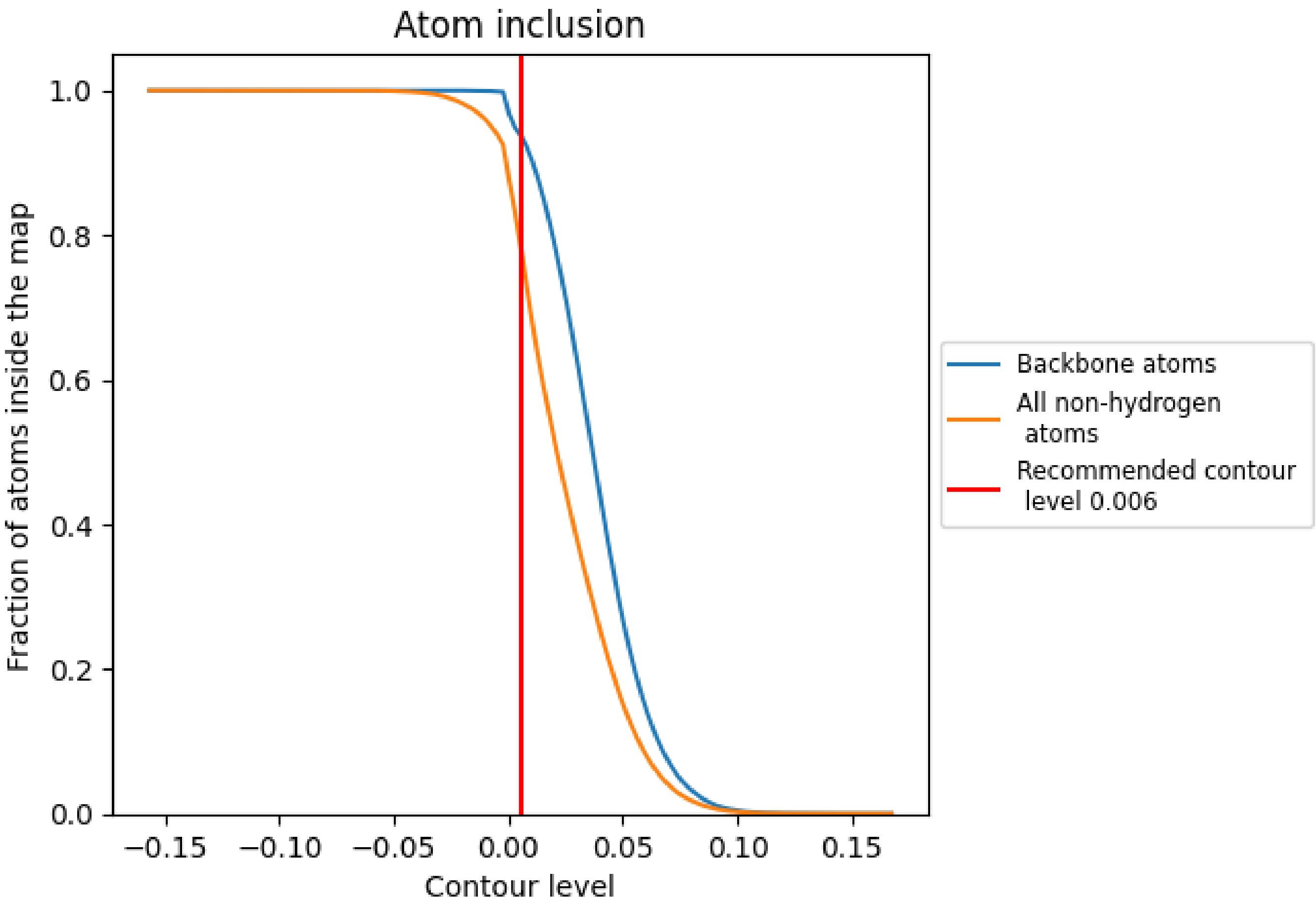
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 77% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7715	0.1530
A	0.5245	0.0860
B	0.3217	0.0470
C	0.8084	0.1670
D	0.8125	0.1620
E	0.8105	0.1620
F	0.8057	0.1670
G	0.8143	0.1680
H	0.8043	0.1630
I	0.8093	0.1650
J	0.8066	0.1640
K	0.8031	0.1550
L	0.7954	0.1470
M	0.7052	0.1290
N	0.8173	0.1740
O	0.8155	0.1730
P	0.8100	0.1600
Q	0.8135	0.1630
R	0.8094	0.1650
S	0.8120	0.1610
T	0.8117	0.1650
U	0.8146	0.1680
V	0.8111	0.1690
W	0.8129	0.1680
X	0.8152	0.1710
Y	0.8129	0.1730
Z	0.8243	0.1750
a	0.8183	0.1650
b	0.8081	0.1580
c	0.8119	0.1690
d	0.8083	0.1700
e	0.8028	0.1680
f	0.8148	0.1720
g	0.8172	0.1730
h	0.8133	0.1750

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	🟦 0.8086	🟥 0.1700
j	🟦 0.8139	🟥 0.1740
k	🟦 0.8151	🟥 0.1740
l	🟦 0.8110	🟥 0.1700
m	🟦 0.8195	🟥 0.1750
n	🟦 0.8134	🟥 0.1670
o	🟦 0.8025	🟥 0.1670
p	⬛ 0.5876	🟥 0.0790
q	🟦 0.7548	🟥 0.1220
r	🟦 0.8071	🟥 0.1470
s	🟫 0.3065	🟥 0.0360
t	⬛ 0.5121	🟥 0.0650
u	🟦 0.7098	🟥 0.1120
v	🟦 0.8013	🟥 0.1460
w	🟦 0.8170	🟥 0.1540
x	🟦 0.8086	🟥 0.1590
y	🟦 0.8092	🟥 0.1630
z	🟦 0.8013	🟥 0.1680