



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:06 PM UTC

PDB ID : 7RS5 / pdb_00007rs5
EMDB ID : EMD-24666
Title : Cryo-EM structure of Kip3 (AMPPNP) bound to Taxol-Stabilized Microtubules
Authors : Hernandez-Lopez, R.A.; Leschziner, A.E.; Arellano-Santoyo, H.; Pellman, D.; Stokasimov, E.; Wang, R.Y.-R.
Deposited on : 2021-08-10
Resolution : 3.90 Å (reported)
Based on initial models : 3JAT, 4FRZ

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

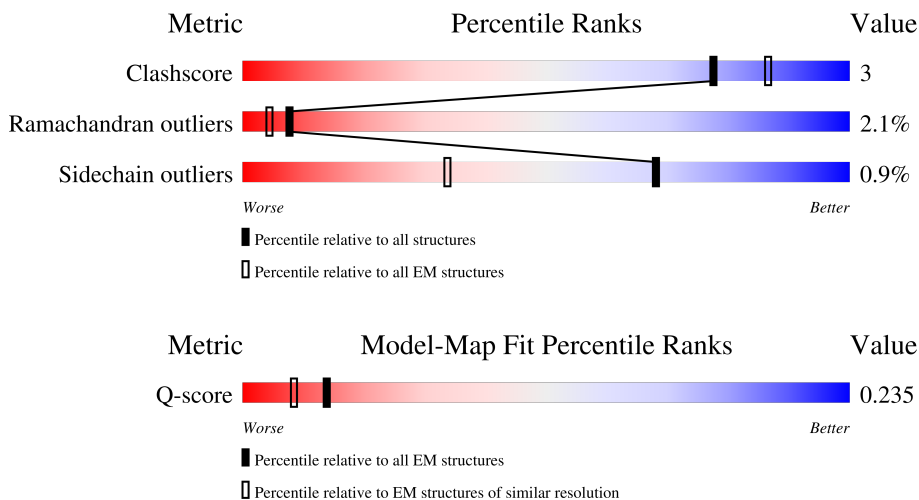
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 Å.

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



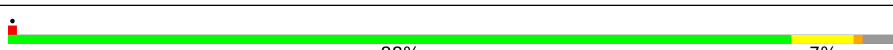
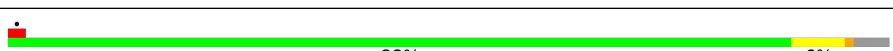
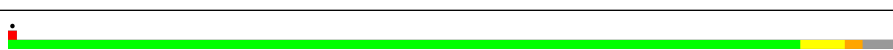
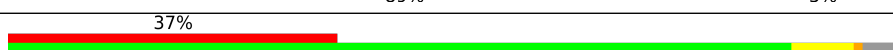
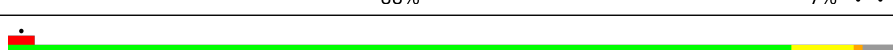
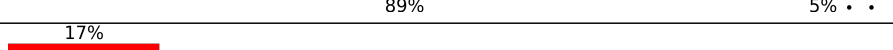
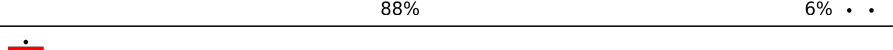
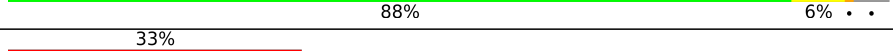
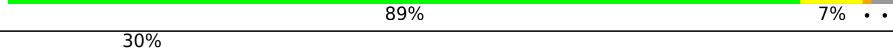
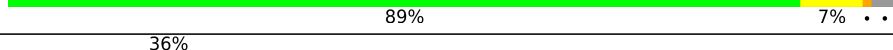
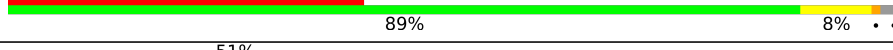
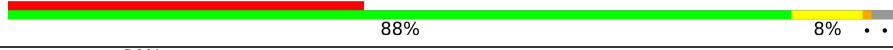
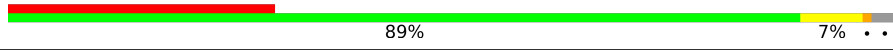
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
1	E	451	

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Mol	Chain	Length	Quality of chain
1	G	451	
1	I	451	
1	L	451	
1	N	451	
1	P	451	
1	R	451	
2	B	445	
2	D	445	
2	F	445	
2	H	445	
2	J	445	
2	M	445	
2	O	445	
2	Q	445	
2	S	445	
3	K	355	
3	a	355	
3	b	355	
3	c	355	
3	d	355	
3	e	355	
3	f	355	
3	g	355	
3	h	355	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 169884 atoms, of which 83763 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	C	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	E	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	G	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	I	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	L	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	N	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	P	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		
1	R	427	Total	C	H	N	O	S	0	0
			6594	2118	3251	569	635	21		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550
C	265	GLY	ALA	conflict	UNP P02550
E	265	GLY	ALA	conflict	UNP P02550
G	265	GLY	ALA	conflict	UNP P02550
I	265	GLY	ALA	conflict	UNP P02550
L	265	GLY	ALA	conflict	UNP P02550
N	265	GLY	ALA	conflict	UNP P02550
P	265	GLY	ALA	conflict	UNP P02550
R	265	GLY	ALA	conflict	UNP P02550

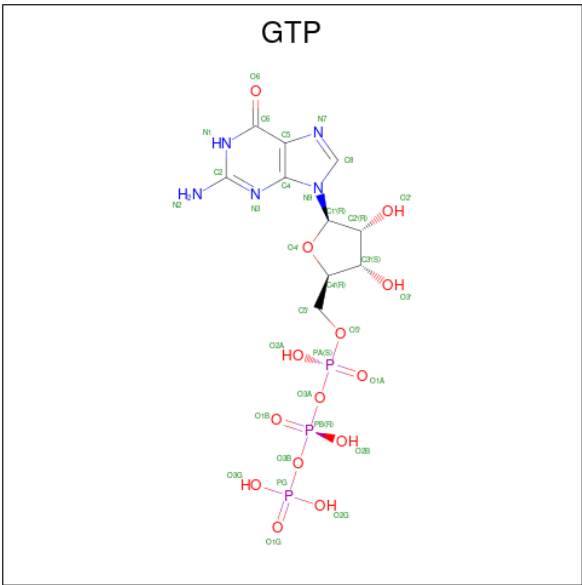
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	D	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	F	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	H	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	J	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	M	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	O	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	Q	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		
2	S	426	Total	C	H	N	O	S	0	0
			6581	2105	3230	575	646	25		

- Molecule 3 is a protein called yeast kinesin-8/ Kip3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	a	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	b	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	c	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	d	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	e	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	f	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	g	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		
3	h	346	Total	C	H	N	O	S	0	0
			5458	1692	2738	490	525	13		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	C	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	E	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	G	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	I	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	L	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	N	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	P	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	R	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

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

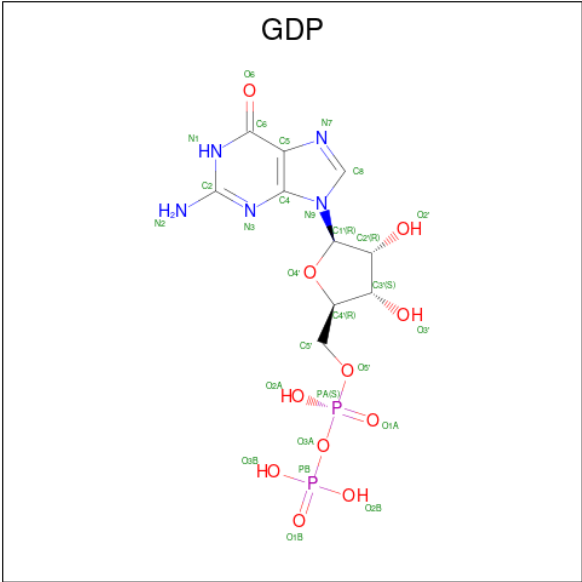
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	K	1	Total	Mg	0
			1	1	

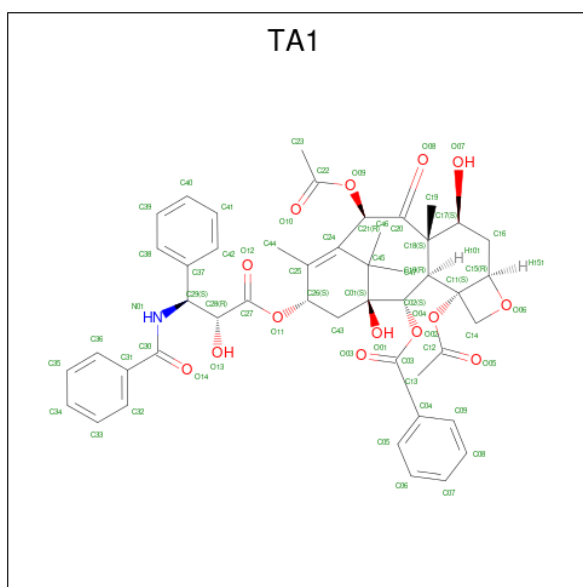
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Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total 1	Mg 1	0
5	a	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0
5	b	1	Total 1	Mg 1	0
5	G	1	Total 1	Mg 1	0
5	c	1	Total 1	Mg 1	0
5	I	1	Total 1	Mg 1	0
5	d	1	Total 1	Mg 1	0
5	L	1	Total 1	Mg 1	0
5	e	1	Total 1	Mg 1	0
5	N	1	Total 1	Mg 1	0
5	f	1	Total 1	Mg 1	0
5	P	1	Total 1	Mg 1	0
5	g	1	Total 1	Mg 1	0
5	R	1	Total 1	Mg 1	0
5	h	1	Total 1	Mg 1	0

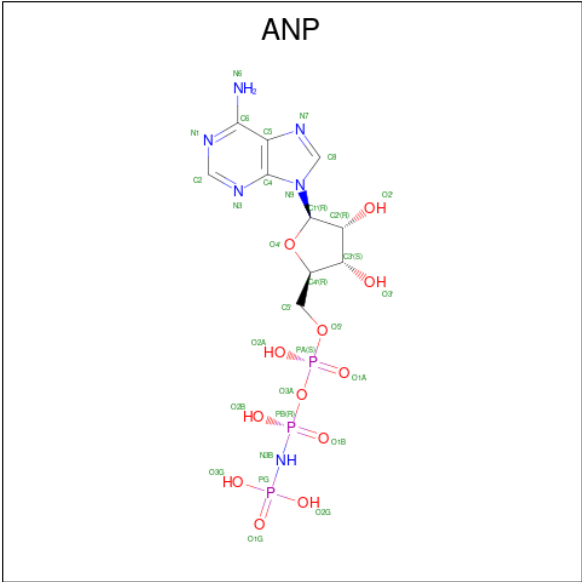
- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	D	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	F	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	H	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	J	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	M	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	O	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	Q	1	Total	C	H	N	O	0
			113	47	51	1	14	
7	S	1	Total	C	H	N	O	0
			113	47	51	1	14	

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

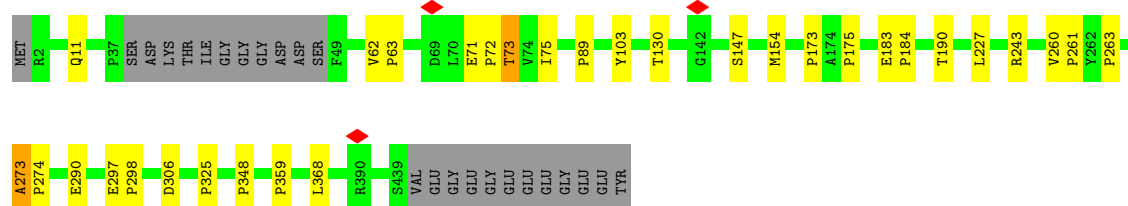


3 Residue-property plots

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

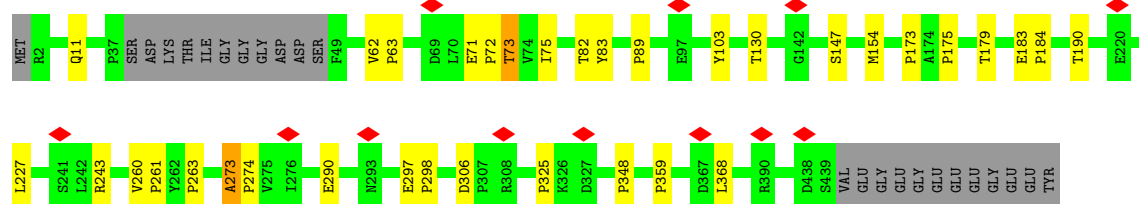
- Molecule 1: Tubulin alpha-1A chain

Chain A: 



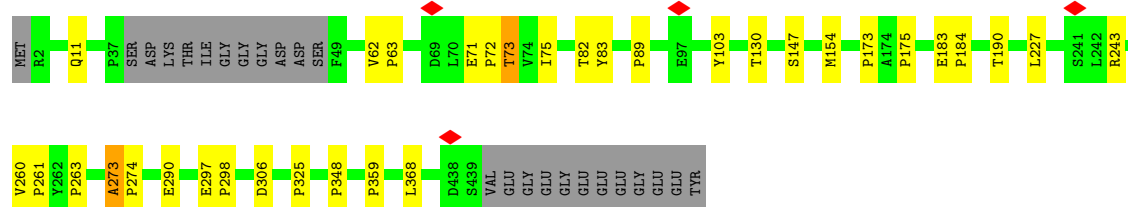
- Molecule 1: Tubulin alpha-1A chain

Chain C: 



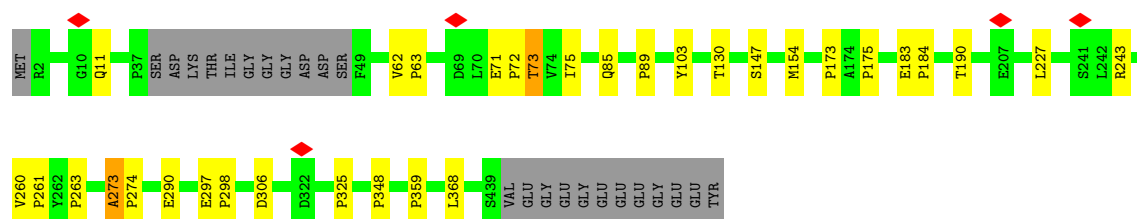
- Molecule 1: Tubulin alpha-1A chain

Chain E: 

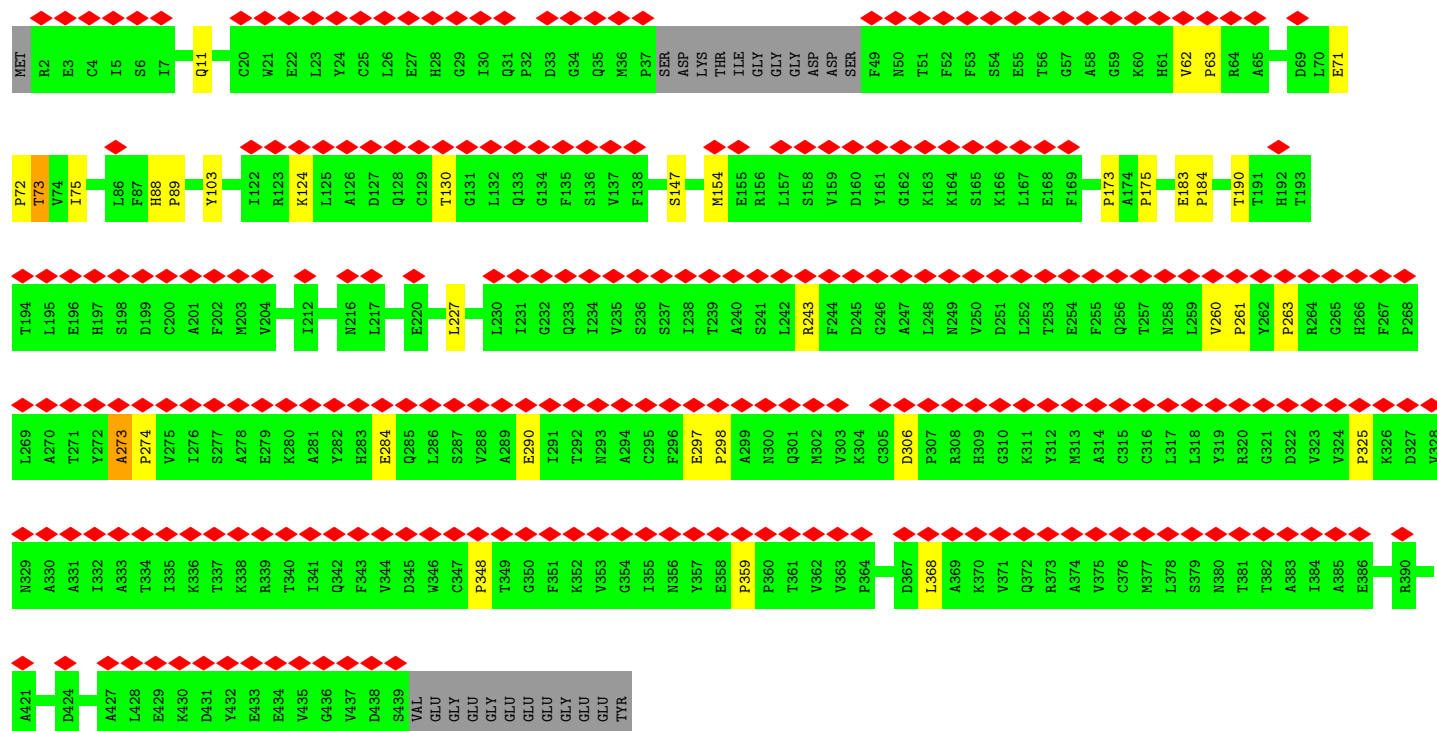
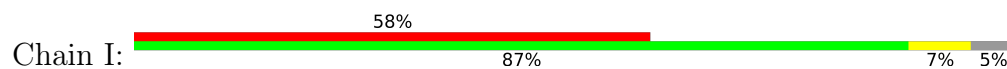


- Molecule 1: Tubulin alpha-1A chain

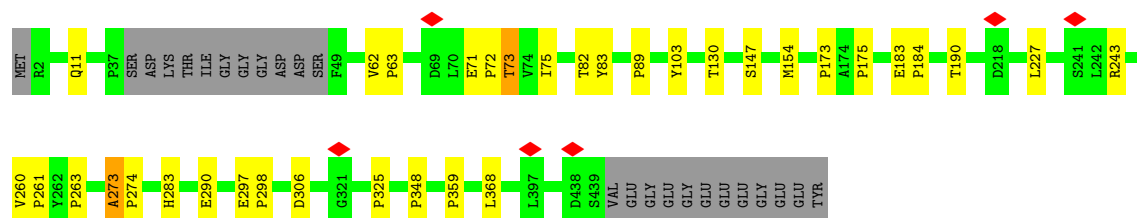
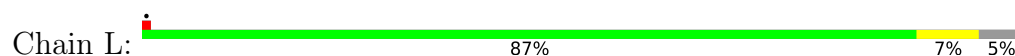
Chain G: 



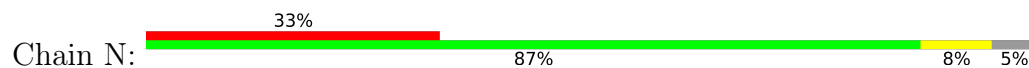
• Molecule 1: Tubulin alpha-1A chain

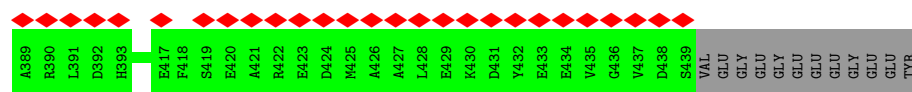


• Molecule 1: Tubulin alpha-1A chain

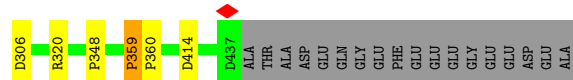
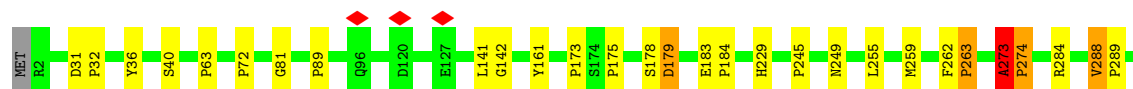
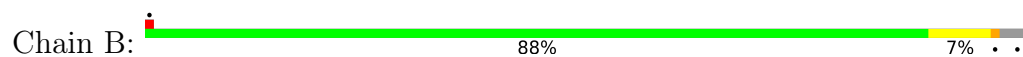


• Molecule 1: Tubulin alpha-1A chain

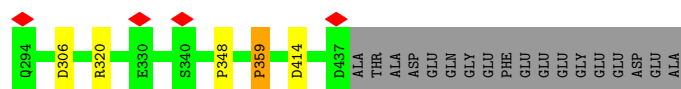
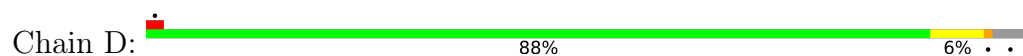




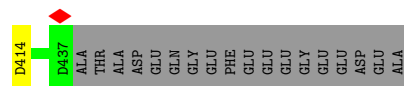
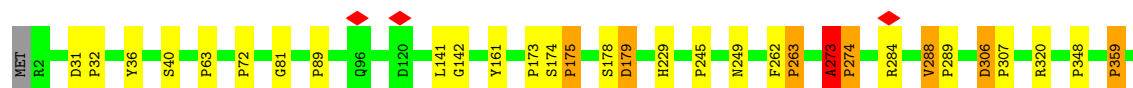
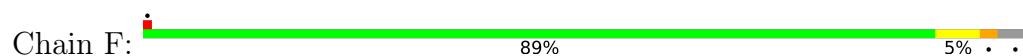
- Molecule 2: Tubulin beta chain



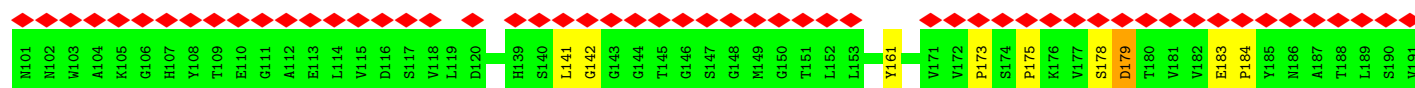
- Molecule 2: Tubulin beta chain

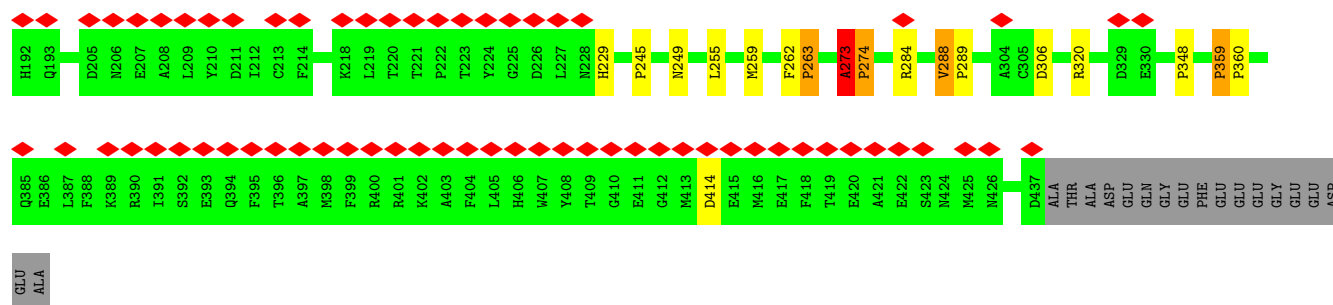


- Molecule 2: Tubulin beta chain

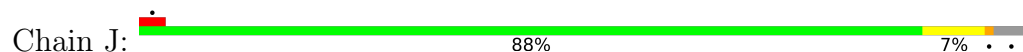


- Molecule 2: Tubulin beta chain

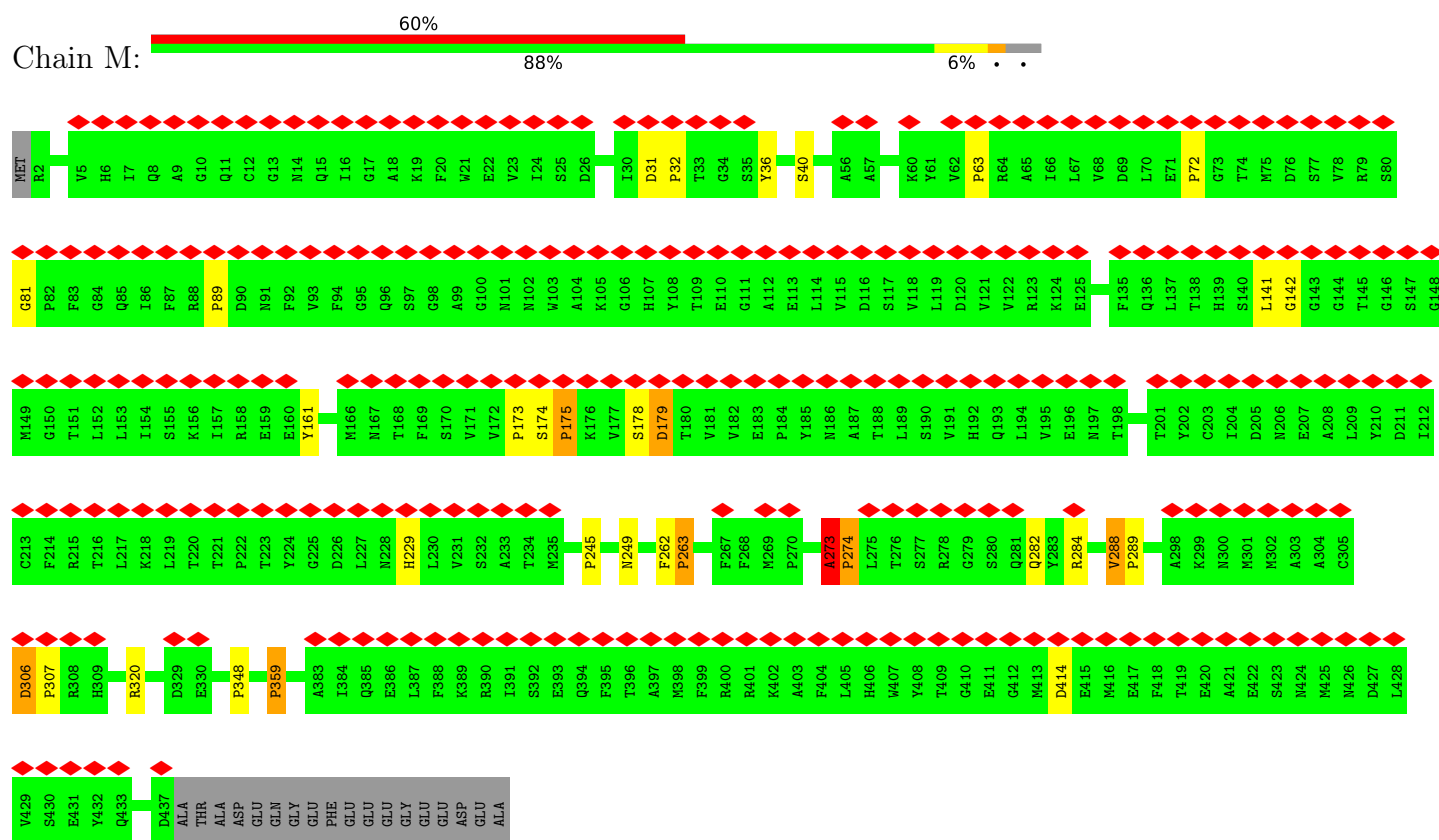




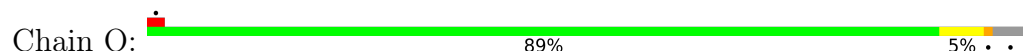
- Molecule 2: Tubulin beta chain

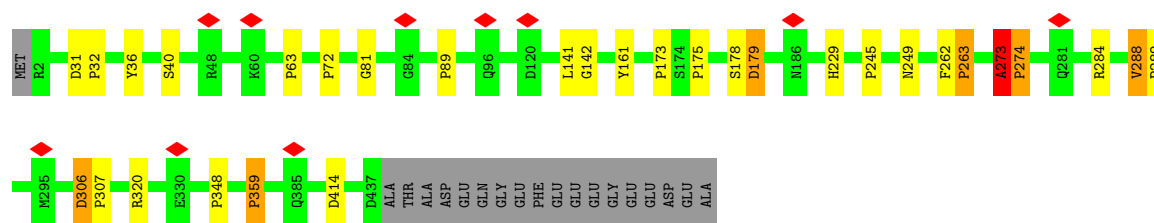


- Molecule 2: Tubulin beta chain

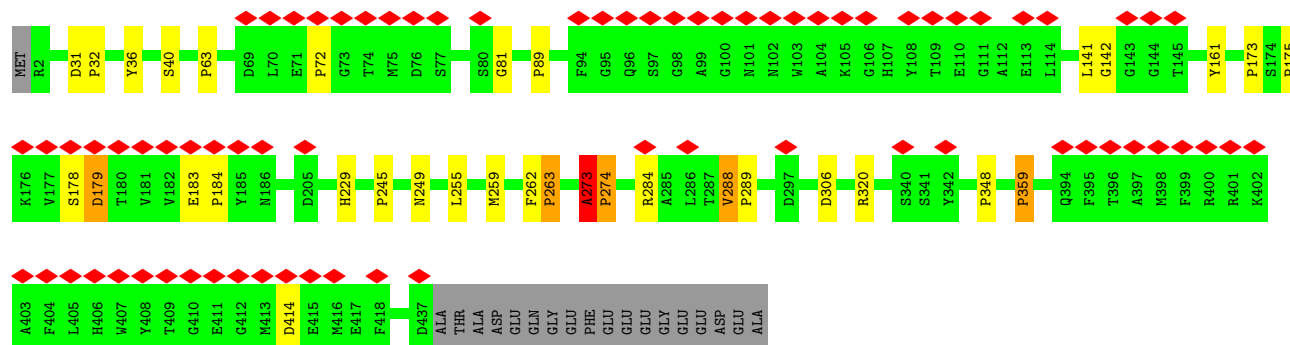
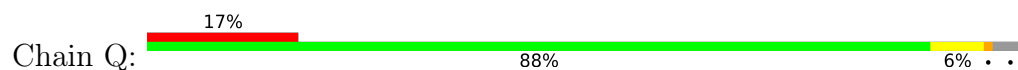


- Molecule 2: Tubulin beta chain

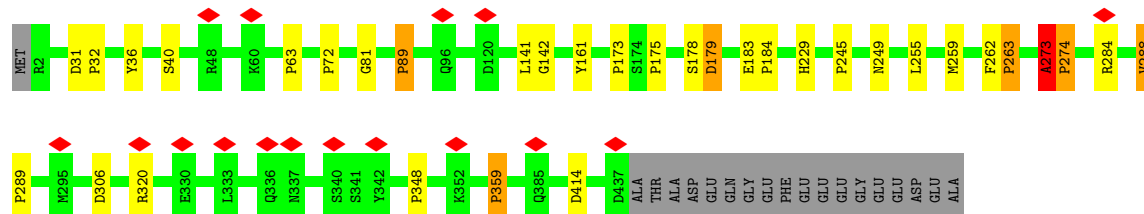
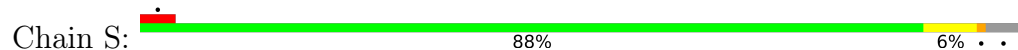




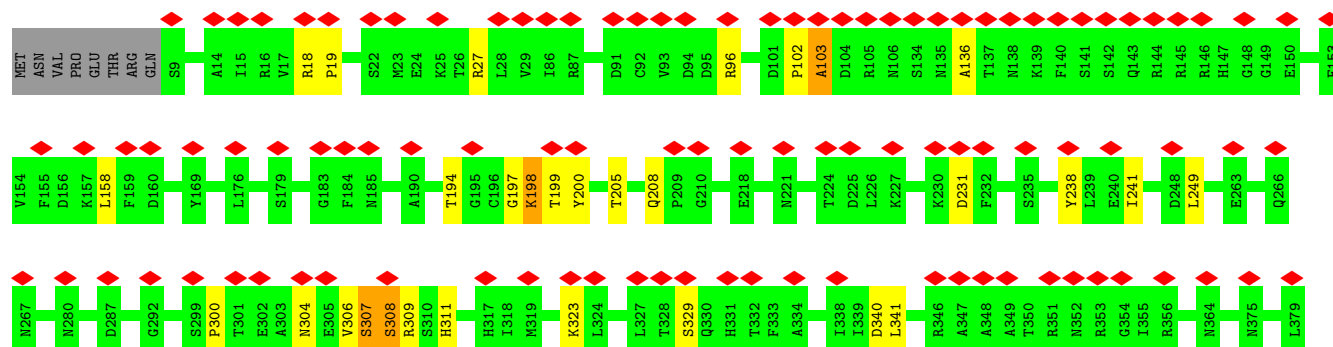
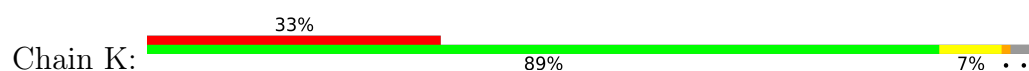
- Molecule 2: Tubulin beta chain

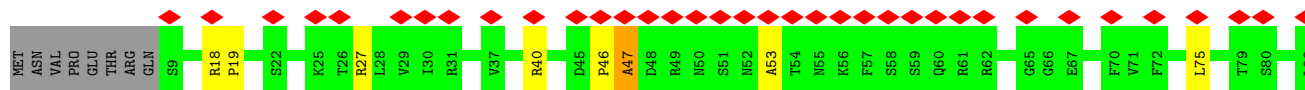


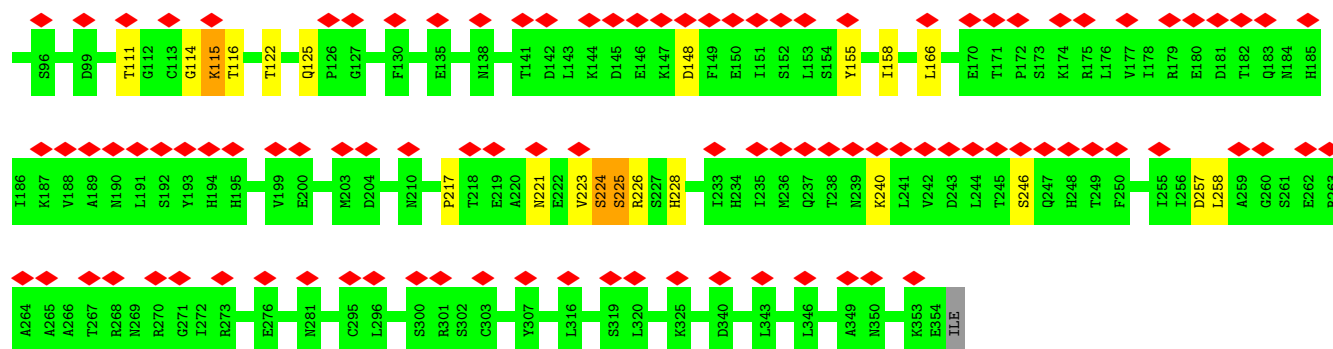
- Molecule 2: Tubulin beta chain



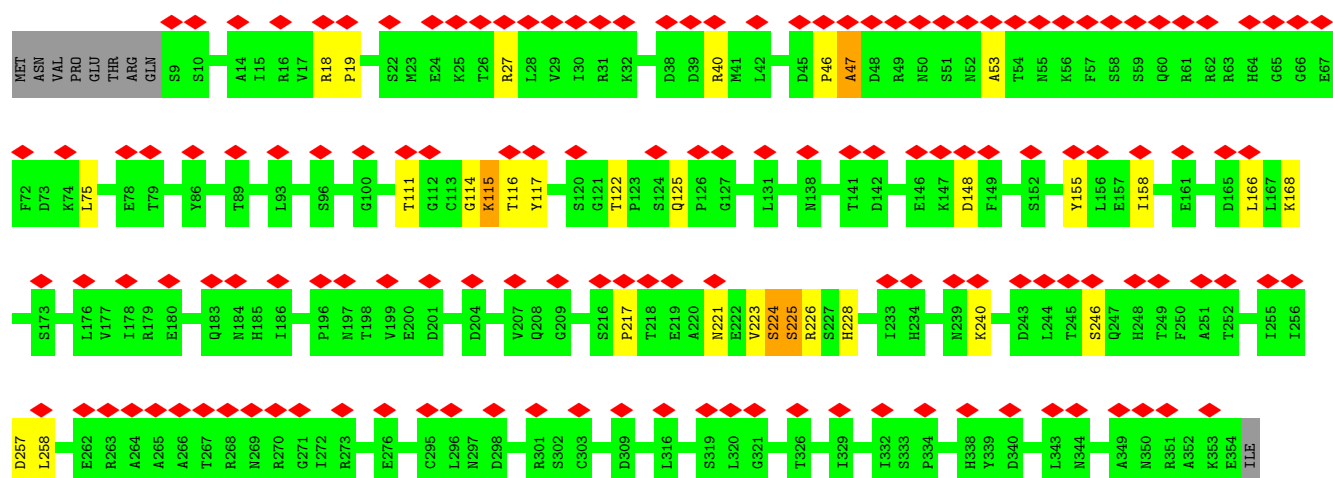
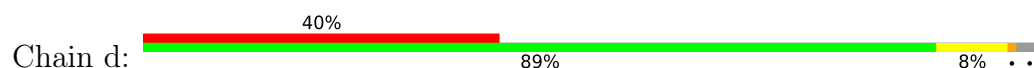
- Molecule 3: yeast kinesin-8/ Kip3



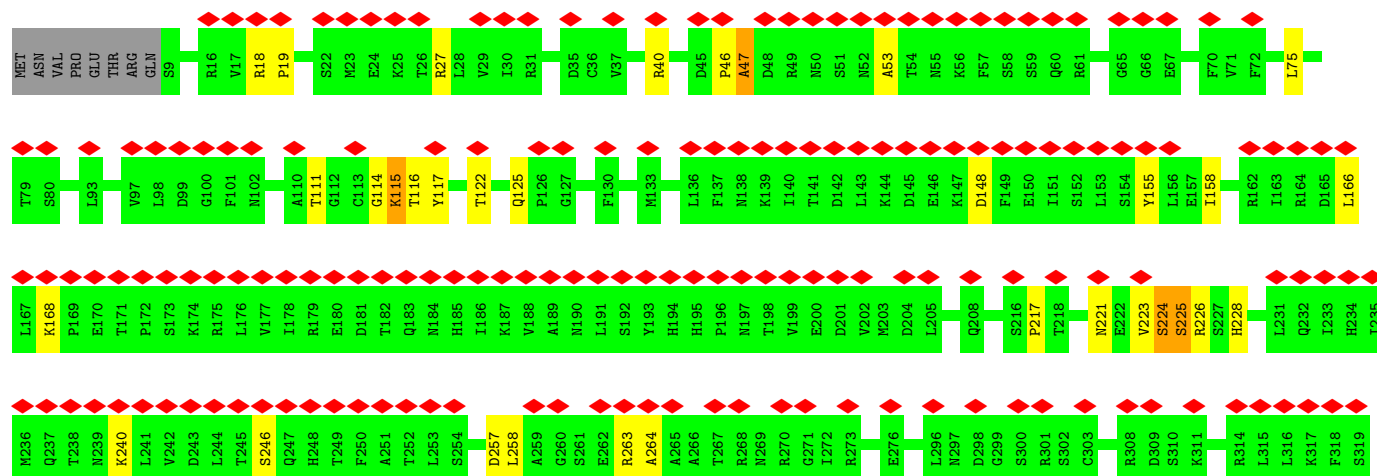
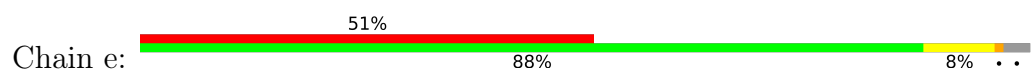


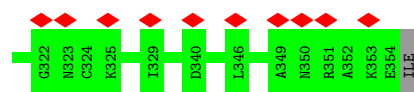


• Molecule 3: yeast kinesin-8/ Kip3

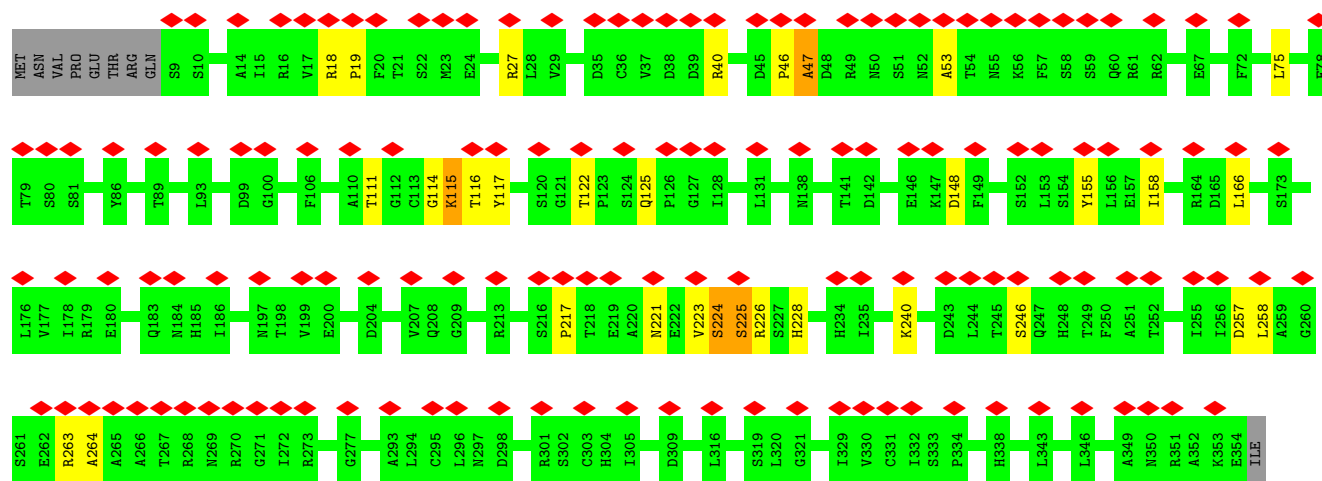
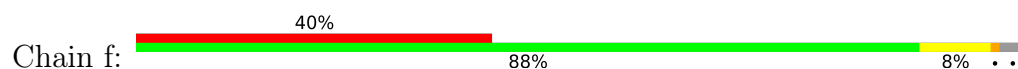


• Molecule 3: yeast kinesin-8/ Kip3

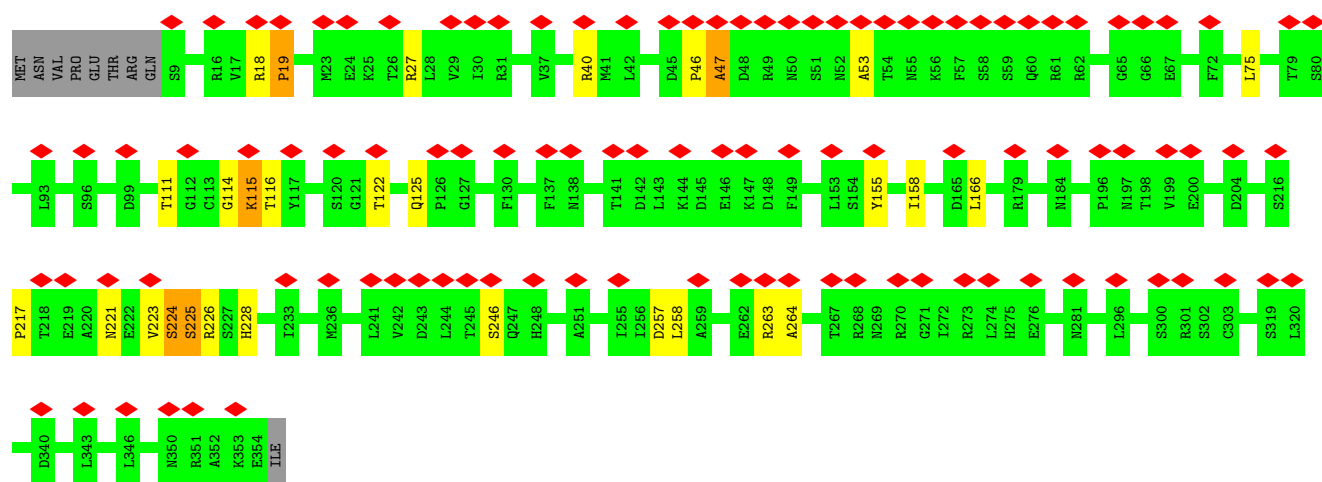
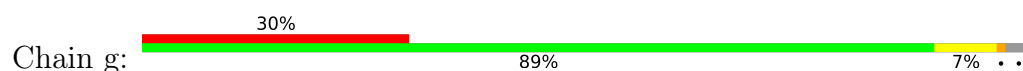




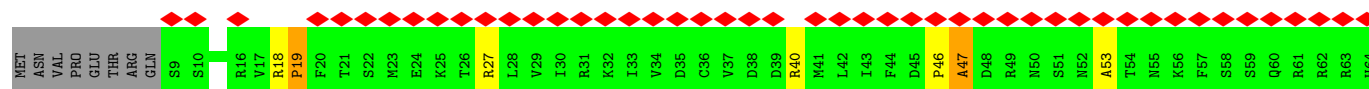
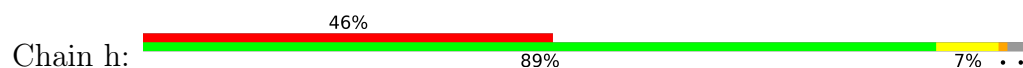
• Molecule 3: yeast kinesin-8/ Kip3

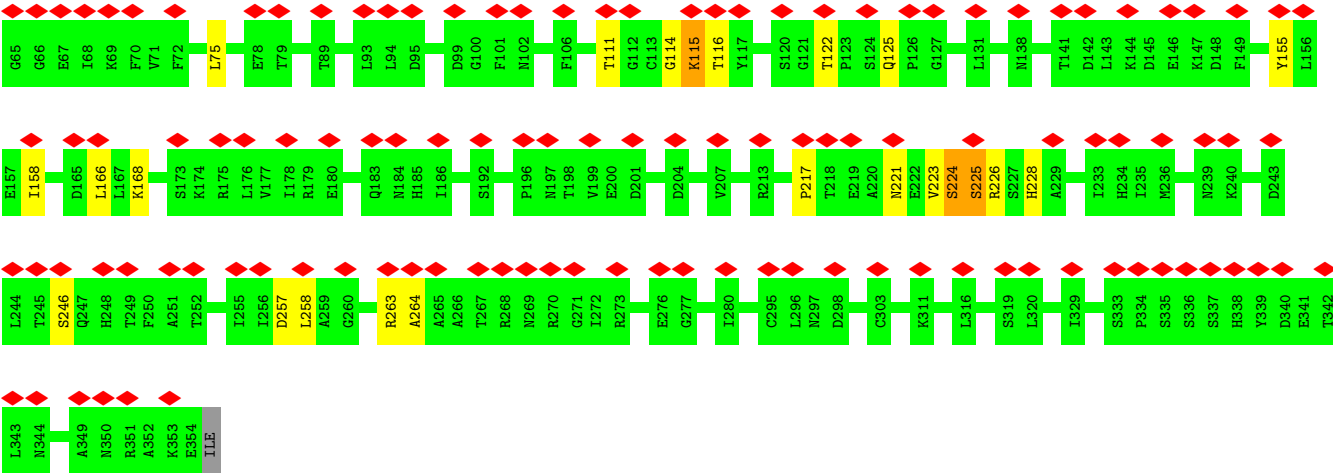


• Molecule 3: yeast kinesin-8/ Kip3



• Molecule 3: yeast kinesin-8/ Kip3





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.76°, rise=8.55 Å, axial sym=C14	Depositor
Number of segments used	14934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) was estimated using CTFFIND4 [(Rohou and Grigorieff, 2015) CTFFIND4: Fast and accurate] with a 500 um step search. A second CTFFIND run with a 100 um step search was carried out to refine the initial defocus values. Micrographs whose estimated resolution was lower than 8 Angstrom with 0.8 confidence were excluded.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.936	Depositor
Minimum map value	-9.617	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.408	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ANP, TA1, MG, 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	0.69	0/3420	0.85	10/4643 (0.2%)
1	C	0.69	0/3420	0.85	10/4643 (0.2%)
1	E	0.69	0/3420	0.85	10/4643 (0.2%)
1	G	0.69	0/3420	0.85	10/4643 (0.2%)
1	I	0.69	0/3420	0.85	10/4643 (0.2%)
1	L	0.69	0/3420	0.85	10/4643 (0.2%)
1	N	0.69	0/3420	0.85	10/4643 (0.2%)
1	P	0.69	0/3420	0.85	10/4643 (0.2%)
1	R	0.69	0/3420	0.85	10/4643 (0.2%)
2	B	0.69	0/3426	0.84	10/4642 (0.2%)
2	D	0.69	0/3426	0.84	10/4642 (0.2%)
2	F	0.69	0/3426	0.84	10/4642 (0.2%)
2	H	0.69	0/3426	0.84	10/4642 (0.2%)
2	J	0.69	0/3426	0.84	10/4642 (0.2%)
2	M	0.69	0/3426	0.84	10/4642 (0.2%)
2	O	0.69	0/3426	0.84	10/4642 (0.2%)
2	Q	0.69	0/3426	0.84	10/4642 (0.2%)
2	S	0.69	0/3426	0.84	10/4642 (0.2%)
3	K	0.68	0/2762	0.82	5/3733 (0.1%)
3	a	0.68	0/2762	0.82	5/3733 (0.1%)
3	b	0.68	0/2762	0.82	5/3733 (0.1%)
3	c	0.68	0/2762	0.82	5/3733 (0.1%)
3	d	0.68	0/2762	0.82	7/3733 (0.2%)
3	e	0.68	0/2762	0.82	7/3733 (0.2%)
3	f	0.68	0/2762	0.82	5/3733 (0.1%)
3	g	0.68	0/2762	0.82	5/3733 (0.1%)
3	h	0.68	0/2762	0.82	7/3733 (0.2%)
All	All	0.69	0/86472	0.84	231/117162 (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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	M	0	1
2	O	0	1
2	Q	0	1
2	S	0	1
All	All	0	9

There are no bond length outliers.

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	359	PRO	CA-C-N	9.97	130.05	119.78
1	E	359	PRO	C-N-CA	9.97	130.05	119.78
1	R	359	PRO	CA-C-N	9.94	130.01	119.78
1	R	359	PRO	C-N-CA	9.94	130.01	119.78
1	G	359	PRO	CA-C-N	9.91	129.99	119.78
1	G	359	PRO	C-N-CA	9.91	129.99	119.78
1	I	359	PRO	CA-C-N	9.90	129.98	119.78
1	I	359	PRO	C-N-CA	9.90	129.98	119.78
1	L	359	PRO	CA-C-N	9.89	129.97	119.78
1	L	359	PRO	C-N-CA	9.89	129.97	119.78
1	C	359	PRO	CA-C-N	9.89	129.96	119.78
1	C	359	PRO	C-N-CA	9.89	129.96	119.78
1	N	359	PRO	CA-C-N	9.88	129.96	119.78
1	N	359	PRO	C-N-CA	9.88	129.96	119.78
1	P	359	PRO	CA-C-N	9.88	129.96	119.78
1	P	359	PRO	C-N-CA	9.88	129.96	119.78
1	A	359	PRO	CA-C-N	9.86	129.93	119.78
1	A	359	PRO	C-N-CA	9.86	129.93	119.78
2	M	359	PRO	CA-C-N	7.35	127.80	119.93
2	M	359	PRO	C-N-CA	7.35	127.80	119.93
2	D	359	PRO	CA-C-N	7.35	127.80	119.93
2	D	359	PRO	C-N-CA	7.35	127.80	119.93
2	F	359	PRO	CA-C-N	7.32	127.76	119.93
2	F	359	PRO	C-N-CA	7.32	127.76	119.93
2	O	359	PRO	CA-C-N	7.31	127.76	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	359	PRO	C-N-CA	7.31	127.76	119.93
2	Q	359	PRO	CA-C-N	7.31	127.75	119.93
2	Q	359	PRO	C-N-CA	7.31	127.75	119.93
2	B	359	PRO	CA-C-N	7.31	127.75	119.93
2	B	359	PRO	C-N-CA	7.31	127.75	119.93
2	J	359	PRO	CA-C-N	7.30	127.74	119.93
2	J	359	PRO	C-N-CA	7.30	127.74	119.93
2	H	359	PRO	CA-C-N	7.30	127.74	119.93
2	H	359	PRO	C-N-CA	7.30	127.74	119.93
2	S	359	PRO	CA-C-N	7.23	127.66	119.93
2	S	359	PRO	C-N-CA	7.23	127.66	119.93
2	H	306	ASP	CA-C-N	6.80	128.34	119.84
2	H	306	ASP	C-N-CA	6.80	128.34	119.84
2	F	306	ASP	CA-C-N	6.79	128.33	119.84
2	F	306	ASP	C-N-CA	6.79	128.33	119.84
2	S	306	ASP	CA-C-N	6.76	128.30	119.84
2	S	306	ASP	C-N-CA	6.76	128.30	119.84
2	B	306	ASP	CA-C-N	6.76	128.29	119.84
2	B	306	ASP	C-N-CA	6.76	128.29	119.84
2	Q	306	ASP	CA-C-N	6.75	128.28	119.84
2	Q	306	ASP	C-N-CA	6.75	128.28	119.84
2	J	306	ASP	CA-C-N	6.73	128.25	119.84
2	J	306	ASP	C-N-CA	6.73	128.25	119.84
2	D	306	ASP	CA-C-N	6.70	128.22	119.84
2	D	306	ASP	C-N-CA	6.70	128.22	119.84
2	O	306	ASP	CA-C-N	6.70	128.22	119.84
2	O	306	ASP	C-N-CA	6.70	128.22	119.84
2	M	306	ASP	CA-C-N	6.68	128.19	119.84
2	M	306	ASP	C-N-CA	6.68	128.19	119.84
1	I	306	ASP	CA-C-N	6.66	128.16	119.84
1	I	306	ASP	C-N-CA	6.66	128.16	119.84
1	N	306	ASP	CA-C-N	6.66	128.16	119.84
1	N	306	ASP	C-N-CA	6.66	128.16	119.84
1	C	306	ASP	CA-C-N	6.65	128.15	119.84
1	C	306	ASP	C-N-CA	6.65	128.15	119.84
1	G	306	ASP	CA-C-N	6.64	128.14	119.84
1	G	306	ASP	C-N-CA	6.64	128.14	119.84
1	P	306	ASP	CA-C-N	6.63	128.12	119.84
1	P	306	ASP	C-N-CA	6.63	128.12	119.84
1	R	306	ASP	CA-C-N	6.61	128.10	119.84
1	R	306	ASP	C-N-CA	6.61	128.10	119.84
1	L	306	ASP	CA-C-N	6.61	128.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	306	ASP	C-N-CA	6.61	128.10	119.84
1	A	306	ASP	CA-C-N	6.59	128.08	119.84
1	A	306	ASP	C-N-CA	6.59	128.08	119.84
1	E	306	ASP	CA-C-N	6.56	128.04	119.84
1	E	306	ASP	C-N-CA	6.56	128.04	119.84
3	f	125	GLN	CA-C-N	6.26	126.45	120.31
3	f	125	GLN	C-N-CA	6.26	126.45	120.31
3	a	125	GLN	CA-C-N	6.25	126.44	120.31
3	a	125	GLN	C-N-CA	6.25	126.44	120.31
3	g	125	GLN	CA-C-N	6.25	126.43	120.31
3	g	125	GLN	C-N-CA	6.25	126.43	120.31
3	b	125	GLN	CA-C-N	6.24	126.42	120.31
3	b	125	GLN	C-N-CA	6.24	126.42	120.31
3	d	125	GLN	CA-C-N	6.24	126.42	120.31
3	d	125	GLN	C-N-CA	6.24	126.42	120.31
3	a	122	THR	CA-C-N	6.23	127.62	119.84
3	a	122	THR	C-N-CA	6.23	127.62	119.84
3	e	125	GLN	CA-C-N	6.23	126.41	120.31
3	e	125	GLN	C-N-CA	6.23	126.41	120.31
3	c	125	GLN	CA-C-N	6.22	126.41	120.31
3	c	125	GLN	C-N-CA	6.22	126.41	120.31
3	h	125	GLN	CA-C-N	6.21	126.39	120.31
3	h	125	GLN	C-N-CA	6.21	126.39	120.31
3	K	208	GLN	CA-C-N	6.19	126.38	120.31
3	K	208	GLN	C-N-CA	6.19	126.38	120.31
3	h	122	THR	CA-C-N	6.17	127.55	119.84
3	h	122	THR	C-N-CA	6.17	127.55	119.84
3	g	122	THR	CA-C-N	6.17	127.55	119.84
3	g	122	THR	C-N-CA	6.17	127.55	119.84
3	e	122	THR	CA-C-N	6.16	127.55	119.84
3	e	122	THR	C-N-CA	6.16	127.55	119.84
3	K	205	THR	CA-C-N	6.16	127.54	119.84
3	K	205	THR	C-N-CA	6.16	127.54	119.84
3	b	122	THR	CA-C-N	6.16	127.54	119.84
3	b	122	THR	C-N-CA	6.16	127.54	119.84
3	f	122	THR	CA-C-N	6.14	127.51	119.84
3	f	122	THR	C-N-CA	6.14	127.51	119.84
3	c	122	THR	CA-C-N	6.12	127.50	119.84
3	c	122	THR	C-N-CA	6.12	127.50	119.84
3	d	122	THR	CA-C-N	6.09	127.45	119.84
3	d	122	THR	C-N-CA	6.09	127.45	119.84
1	I	62	VAL	CA-C-N	6.02	125.96	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	62	VAL	C-N-CA	6.02	125.96	119.76
2	Q	161	TYR	CA-C-N	6.00	125.68	119.56
2	Q	161	TYR	C-N-CA	6.00	125.68	119.56
1	P	62	VAL	CA-C-N	5.99	125.93	119.76
1	P	62	VAL	C-N-CA	5.99	125.93	119.76
1	G	62	VAL	CA-C-N	5.99	125.93	119.76
1	G	62	VAL	C-N-CA	5.99	125.93	119.76
2	H	161	TYR	CA-C-N	5.98	125.66	119.56
2	H	161	TYR	C-N-CA	5.98	125.66	119.56
2	O	161	TYR	CA-C-N	5.97	125.66	119.56
2	O	161	TYR	C-N-CA	5.97	125.66	119.56
2	S	161	TYR	CA-C-N	5.97	125.65	119.56
2	S	161	TYR	C-N-CA	5.97	125.65	119.56
2	F	161	TYR	CA-C-N	5.97	125.65	119.56
2	F	161	TYR	C-N-CA	5.97	125.65	119.56
2	B	161	TYR	CA-C-N	5.96	125.64	119.56
2	B	161	TYR	C-N-CA	5.96	125.64	119.56
2	D	161	TYR	CA-C-N	5.95	125.63	119.56
2	D	161	TYR	C-N-CA	5.95	125.63	119.56
2	J	161	TYR	CA-C-N	5.94	125.62	119.56
2	J	161	TYR	C-N-CA	5.94	125.62	119.56
1	N	62	VAL	CA-C-N	5.94	125.88	119.76
1	N	62	VAL	C-N-CA	5.94	125.88	119.76
2	M	161	TYR	CA-C-N	5.93	125.61	119.56
2	M	161	TYR	C-N-CA	5.93	125.61	119.56
2	Q	288	VAL	CA-C-N	5.88	127.18	119.84
2	Q	288	VAL	C-N-CA	5.88	127.18	119.84
2	M	288	VAL	CA-C-N	5.87	127.18	119.84
2	M	288	VAL	C-N-CA	5.87	127.18	119.84
2	S	288	VAL	CA-C-N	5.85	127.16	119.84
2	S	288	VAL	C-N-CA	5.85	127.16	119.84
2	O	288	VAL	CA-C-N	5.85	127.15	119.84
2	O	288	VAL	C-N-CA	5.85	127.15	119.84
2	B	288	VAL	CA-C-N	5.84	127.14	119.84
2	B	288	VAL	C-N-CA	5.84	127.14	119.84
2	J	288	VAL	CA-C-N	5.84	127.14	119.84
2	J	288	VAL	C-N-CA	5.84	127.14	119.84
2	D	288	VAL	CA-C-N	5.84	127.14	119.84
2	D	288	VAL	C-N-CA	5.84	127.14	119.84
2	F	288	VAL	CA-C-N	5.83	127.13	119.84
2	F	288	VAL	C-N-CA	5.83	127.13	119.84
2	H	288	VAL	CA-C-N	5.82	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	288	VAL	C-N-CA	5.82	127.12	119.84
1	C	297	GLU	CA-C-N	5.78	127.06	119.84
1	C	297	GLU	C-N-CA	5.78	127.06	119.84
1	P	297	GLU	CA-C-N	5.77	127.06	119.84
1	P	297	GLU	C-N-CA	5.77	127.06	119.84
1	L	297	GLU	CA-C-N	5.76	127.04	119.84
1	L	297	GLU	C-N-CA	5.76	127.04	119.84
1	A	297	GLU	CA-C-N	5.75	127.02	119.84
1	A	297	GLU	C-N-CA	5.75	127.02	119.84
1	E	297	GLU	CA-C-N	5.74	127.02	119.84
1	E	297	GLU	C-N-CA	5.74	127.02	119.84
1	I	297	GLU	CA-C-N	5.74	127.01	119.84
1	I	297	GLU	C-N-CA	5.74	127.01	119.84
1	C	62	VAL	CA-C-N	5.73	126.02	119.83
1	C	62	VAL	C-N-CA	5.73	126.02	119.83
1	R	297	GLU	CA-C-N	5.71	126.98	119.84
1	R	297	GLU	C-N-CA	5.71	126.98	119.84
1	G	297	GLU	CA-C-N	5.71	126.97	119.84
1	G	297	GLU	C-N-CA	5.71	126.97	119.84
1	N	297	GLU	CA-C-N	5.70	126.97	119.84
1	N	297	GLU	C-N-CA	5.70	126.97	119.84
1	E	62	VAL	CA-C-N	5.70	125.98	119.83
1	E	62	VAL	C-N-CA	5.70	125.98	119.83
1	R	62	VAL	CA-C-N	5.68	125.96	119.83
1	R	62	VAL	C-N-CA	5.68	125.96	119.83
1	L	62	VAL	CA-C-N	5.68	125.96	119.83
1	L	62	VAL	C-N-CA	5.68	125.96	119.83
1	A	62	VAL	CA-C-N	5.67	125.95	119.83
1	A	62	VAL	C-N-CA	5.67	125.95	119.83
2	F	81	GLY	CA-C-N	5.60	126.84	119.84
2	F	81	GLY	C-N-CA	5.60	126.84	119.84
2	O	81	GLY	CA-C-N	5.58	126.81	119.84
2	O	81	GLY	C-N-CA	5.58	126.81	119.84
1	C	71	GLU	CA-C-N	5.55	125.90	119.47
1	C	71	GLU	C-N-CA	5.55	125.90	119.47
2	D	81	GLY	CA-C-N	5.55	126.77	119.84
2	D	81	GLY	C-N-CA	5.55	126.77	119.84
1	E	71	GLU	CA-C-N	5.54	125.89	119.47
1	E	71	GLU	C-N-CA	5.54	125.89	119.47
2	B	81	GLY	CA-C-N	5.53	126.76	119.84
2	B	81	GLY	C-N-CA	5.53	126.76	119.84
1	I	71	GLU	CA-C-N	5.53	125.89	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	71	GLU	C-N-CA	5.53	125.89	119.47
2	Q	81	GLY	CA-C-N	5.52	126.73	119.84
2	Q	81	GLY	C-N-CA	5.52	126.73	119.84
1	G	71	GLU	CA-C-N	5.51	125.86	119.47
1	G	71	GLU	C-N-CA	5.51	125.86	119.47
1	R	71	GLU	CA-C-N	5.50	125.86	119.47
1	R	71	GLU	C-N-CA	5.50	125.86	119.47
2	H	81	GLY	CA-C-N	5.50	126.71	119.84
2	H	81	GLY	C-N-CA	5.50	126.71	119.84
2	S	81	GLY	CA-C-N	5.49	126.71	119.84
2	S	81	GLY	C-N-CA	5.49	126.71	119.84
1	P	71	GLU	CA-C-N	5.49	125.84	119.47
1	P	71	GLU	C-N-CA	5.49	125.84	119.47
2	J	81	GLY	CA-C-N	5.49	126.70	119.84
2	J	81	GLY	C-N-CA	5.49	126.70	119.84
2	M	81	GLY	CA-C-N	5.48	126.69	119.84
2	M	81	GLY	C-N-CA	5.48	126.69	119.84
1	N	71	GLU	CA-C-N	5.47	125.82	119.47
1	N	71	GLU	C-N-CA	5.47	125.82	119.47
1	L	71	GLU	CA-C-N	5.46	125.81	119.47
1	L	71	GLU	C-N-CA	5.46	125.81	119.47
1	A	71	GLU	CA-C-N	5.45	125.79	119.47
1	A	71	GLU	C-N-CA	5.45	125.79	119.47
3	d	115	LYS	N-CA-C	-5.14	103.74	110.53
3	a	115	LYS	N-CA-C	-5.12	103.77	110.53
3	c	115	LYS	N-CA-C	-5.12	103.77	110.53
3	e	115	LYS	N-CA-C	-5.12	103.77	110.53
3	b	115	LYS	N-CA-C	-5.12	103.78	110.53
3	f	115	LYS	N-CA-C	-5.09	103.81	110.53
3	g	115	LYS	N-CA-C	-5.07	103.83	110.53
3	K	198	LYS	N-CA-C	-5.07	103.84	110.53
3	h	115	LYS	N-CA-C	-5.07	103.84	110.53
3	d	168	LYS	CA-C-N	5.05	125.12	119.87
3	d	168	LYS	C-N-CA	5.05	125.12	119.87
3	e	168	LYS	CA-C-N	5.01	125.08	119.87
3	e	168	LYS	C-N-CA	5.01	125.08	119.87
3	h	168	LYS	CA-C-N	5.01	125.08	119.87
3	h	168	LYS	C-N-CA	5.01	125.08	119.87

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	ALA	Peptide
2	D	273	ALA	Peptide
2	F	273	ALA	Peptide
2	H	273	ALA	Peptide
2	J	273	ALA	Peptide
2	M	273	ALA	Peptide
2	O	273	ALA	Peptide
2	Q	273	ALA	Peptide
2	S	273	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3343	3251	3249	12	0
1	C	3343	3251	3249	14	0
1	E	3343	3251	3249	13	0
1	G	3343	3251	3249	13	0
1	I	3343	3251	3249	16	0
1	L	3343	3251	3249	14	0
1	N	3343	3251	3249	16	0
1	P	3343	3251	3249	14	0
1	R	3343	3251	3249	15	0
2	B	3351	3230	3229	20	0
2	D	3351	3230	3229	19	0
2	F	3351	3230	3229	19	0
2	H	3351	3230	3229	21	0
2	J	3351	3230	3229	20	0
2	M	3351	3230	3229	20	0
2	O	3351	3230	3229	18	0
2	Q	3351	3230	3229	19	0
2	S	3351	3230	3229	20	0
3	K	2720	2738	2735	18	0
3	a	2720	2738	2735	19	0
3	b	2720	2738	2735	20	0
3	c	2720	2738	2735	18	0
3	d	2720	2738	2735	18	0
3	e	2720	2738	2735	20	0
3	f	2720	2738	2735	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	g	2720	2738	2735	19	0
3	h	2720	2738	2735	19	0
4	A	32	12	12	1	0
4	C	32	12	12	2	0
4	E	32	12	12	1	0
4	G	32	12	12	1	0
4	I	32	12	12	1	0
4	L	32	12	12	1	0
4	N	32	12	12	1	0
4	P	32	12	12	2	0
4	R	32	12	12	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
5	R	1	0	0	0	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
5	c	1	0	0	0	0
5	d	1	0	0	0	0
5	e	1	0	0	0	0
5	f	1	0	0	0	0
5	g	1	0	0	0	0
5	h	1	0	0	0	0
6	B	28	12	12	0	0
6	D	28	12	12	0	0
6	F	28	12	12	0	0
6	H	28	12	12	0	0
6	J	28	12	12	0	0
6	M	28	12	12	0	0
6	O	28	12	12	0	0
6	Q	28	12	12	0	0
6	S	28	12	12	0	0
7	B	62	51	51	3	0
7	D	62	51	51	3	0
7	F	62	51	51	3	0
7	H	62	51	51	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	62	51	51	3	0
7	M	62	51	51	3	0
7	O	62	51	51	3	0
7	Q	62	51	51	3	0
7	S	62	51	51	3	0
8	K	31	13	13	3	0
8	a	31	13	13	4	0
8	b	31	13	13	3	0
8	c	31	13	13	3	0
8	d	31	13	13	3	0
8	e	31	13	13	3	0
8	f	31	13	13	3	0
8	g	31	13	13	4	0
8	h	31	13	13	4	0
All	All	86121	83763	83709	494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (494) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:290:GLU:OE1	1:R:290:GLU:N	2.17	0.78
1:C:290:GLU:OE1	1:C:290:GLU:N	2.17	0.77
1:P:290:GLU:N	1:P:290:GLU:OE1	2.17	0.77
1:A:290:GLU:OE1	1:A:290:GLU:N	2.17	0.77
1:I:290:GLU:N	1:I:290:GLU:OE1	2.17	0.77
1:G:290:GLU:N	1:G:290:GLU:OE1	2.17	0.77
1:N:290:GLU:N	1:N:290:GLU:OE1	2.17	0.77
1:E:290:GLU:N	1:E:290:GLU:OE1	2.17	0.76
1:L:290:GLU:N	1:L:290:GLU:OE1	2.17	0.76
1:C:11:GLN:N	4:C:501:GTP:O2B	2.28	0.67
1:G:11:GLN:N	4:G:501:GTP:O2B	2.28	0.67
1:A:11:GLN:N	4:A:501:GTP:O2B	2.28	0.67
3:b:226:ARG:O	3:b:226:ARG:HG2	1.95	0.67
3:f:226:ARG:O	3:f:226:ARG:HG2	1.95	0.67
1:P:11:GLN:N	4:P:501:GTP:O2B	2.28	0.67
1:R:11:GLN:N	4:R:501:GTP:O2B	2.28	0.67
3:K:309:ARG:HG2	3:K:309:ARG:O	1.95	0.67
1:I:11:GLN:N	4:I:501:GTP:O2B	2.28	0.67
3:e:226:ARG:HG2	3:e:226:ARG:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:226:ARG:O	3:d:226:ARG:HG2	1.95	0.67
1:N:11:GLN:N	4:N:501:GTP:O2B	2.28	0.67
1:E:11:GLN:N	4:E:501:GTP:O2B	2.28	0.67
3:c:226:ARG:O	3:c:226:ARG:HG2	1.95	0.67
1:L:11:GLN:N	4:L:501:GTP:O2B	2.28	0.67
3:a:226:ARG:O	3:a:226:ARG:HG2	1.95	0.66
3:h:226:ARG:O	3:h:226:ARG:HG2	1.95	0.66
3:g:226:ARG:O	3:g:226:ARG:HG2	1.95	0.66
7:F:502:TA1:H261	7:F:502:TA1:H463	1.80	0.64
7:O:502:TA1:H463	7:O:502:TA1:H261	1.80	0.64
7:M:502:TA1:H463	7:M:502:TA1:H261	1.80	0.64
7:Q:502:TA1:H463	7:Q:502:TA1:H261	1.80	0.64
7:D:502:TA1:H261	7:D:502:TA1:H463	1.80	0.63
7:H:502:TA1:H463	7:H:502:TA1:H261	1.80	0.63
7:B:502:TA1:H463	7:B:502:TA1:H261	1.80	0.63
7:J:502:TA1:H463	7:J:502:TA1:H261	1.80	0.63
7:S:502:TA1:H463	7:S:502:TA1:H261	1.80	0.63
2:D:141:LEU:HG	2:D:141:LEU:O	2.00	0.62
2:Q:141:LEU:O	2:Q:141:LEU:HG	2.00	0.62
2:S:141:LEU:O	2:S:141:LEU:HG	2.00	0.62
2:M:141:LEU:HG	2:M:141:LEU:O	2.00	0.62
2:F:141:LEU:HG	2:F:141:LEU:O	2.00	0.61
2:J:141:LEU:O	2:J:141:LEU:HG	2.00	0.61
2:O:141:LEU:O	2:O:141:LEU:HG	2.00	0.61
2:B:141:LEU:O	2:B:141:LEU:HG	2.00	0.61
2:H:141:LEU:O	2:H:141:LEU:HG	2.00	0.61
1:I:88:HIS:CD2	1:N:283:HIS:HB3	2.36	0.61
2:B:284:ARG:NE	2:B:284:ARG:HA	2.17	0.59
3:f:115:LYS:HZ1	3:f:258:LEU:H	1.51	0.59
2:D:284:ARG:NE	2:D:284:ARG:HA	2.17	0.58
3:K:198:LYS:HZ1	3:K:341:LEU:H	1.51	0.58
3:b:115:LYS:HZ1	3:b:258:LEU:H	1.51	0.58
2:J:284:ARG:HA	2:J:284:ARG:NE	2.17	0.58
2:Q:284:ARG:HA	2:Q:284:ARG:NE	2.17	0.58
2:S:284:ARG:NE	2:S:284:ARG:HA	2.18	0.58
3:K:197:GLY:HA2	8:K:501:ANP:O2A	2.03	0.58
2:H:284:ARG:HA	2:H:284:ARG:NE	2.17	0.58
3:d:115:LYS:HZ1	3:d:258:LEU:H	1.52	0.58
3:f:114:GLY:HA2	8:f:401:ANP:O2A	2.03	0.58
3:b:114:GLY:HA2	8:b:401:ANP:O2A	2.03	0.58
3:c:114:GLY:HA2	8:c:401:ANP:O2A	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:115:LYS:HZ1	3:c:258:LEU:H	1.52	0.58
3:d:114:GLY:HA2	8:d:401:ANP:O2A	2.03	0.58
2:M:284:ARG:HA	2:M:284:ARG:NE	2.17	0.58
3:e:114:GLY:HA2	8:e:401:ANP:O2A	2.03	0.58
2:F:284:ARG:HA	2:F:284:ARG:NE	2.17	0.58
2:O:284:ARG:HA	2:O:284:ARG:NE	2.17	0.58
3:a:115:LYS:HZ1	3:a:258:LEU:H	1.52	0.58
3:g:115:LYS:HZ1	3:g:258:LEU:H	1.53	0.57
3:h:115:LYS:HZ1	3:h:258:LEU:H	1.53	0.57
3:e:115:LYS:HZ1	3:e:258:LEU:H	1.51	0.57
3:h:114:GLY:HA2	8:h:401:ANP:O2A	2.03	0.57
3:a:114:GLY:HA2	8:a:401:ANP:O2A	2.03	0.56
3:g:114:GLY:HA2	8:g:401:ANP:O2A	2.03	0.56
3:a:46:PRO:O	3:a:47:ALA:HB3	2.08	0.54
3:K:102:PRO:O	3:K:103:ALA:HB3	2.08	0.54
1:G:183:GLU:N	1:G:184:PRO:CD	2.71	0.54
3:g:46:PRO:O	3:g:47:ALA:HB3	2.08	0.54
3:h:46:PRO:O	3:h:47:ALA:HB3	2.08	0.54
1:A:183:GLU:N	1:A:184:PRO:CD	2.71	0.54
1:I:183:GLU:N	1:I:184:PRO:CD	2.71	0.54
3:d:46:PRO:O	3:d:47:ALA:HB3	2.08	0.54
3:c:46:PRO:O	3:c:47:ALA:HB3	2.08	0.54
3:f:46:PRO:O	3:f:47:ALA:HB3	2.08	0.53
1:N:183:GLU:N	1:N:184:PRO:CD	2.71	0.53
1:E:183:GLU:N	1:E:184:PRO:CD	2.71	0.53
3:b:46:PRO:O	3:b:47:ALA:HB3	2.08	0.53
3:e:46:PRO:O	3:e:47:ALA:HB3	2.08	0.53
1:P:183:GLU:N	1:P:184:PRO:CD	2.71	0.53
1:C:183:GLU:N	1:C:184:PRO:CD	2.71	0.53
1:L:183:GLU:N	1:L:184:PRO:CD	2.71	0.52
1:R:183:GLU:N	1:R:184:PRO:CD	2.71	0.52
1:A:103:TYR:C	1:A:103:TYR:CD2	2.88	0.52
1:G:103:TYR:C	1:G:103:TYR:CD2	2.88	0.52
1:P:103:TYR:C	1:P:103:TYR:CD2	2.88	0.52
1:C:103:TYR:C	1:C:103:TYR:CD2	2.88	0.52
1:E:103:TYR:C	1:E:103:TYR:CD2	2.88	0.52
1:L:103:TYR:CD2	1:L:103:TYR:C	2.88	0.52
1:N:103:TYR:C	1:N:103:TYR:CD2	2.88	0.52
1:I:103:TYR:C	1:I:103:TYR:CD2	2.88	0.52
1:R:103:TYR:C	1:R:103:TYR:CD2	2.88	0.52
3:K:198:LYS:O	3:K:199:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:115:LYS:O	3:b:116:THR:HB	2.11	0.51
1:I:147:SER:OG	1:I:190:THR:OG1	2.25	0.51
3:e:115:LYS:O	3:e:116:THR:HB	2.11	0.51
3:c:115:LYS:O	3:c:116:THR:HB	2.11	0.51
3:f:115:LYS:O	3:f:116:THR:HB	2.11	0.51
1:G:147:SER:OG	1:G:190:THR:OG1	2.25	0.51
3:d:115:LYS:O	3:d:116:THR:HB	2.11	0.51
3:g:115:LYS:O	3:g:116:THR:HB	2.11	0.51
3:h:115:LYS:O	3:h:116:THR:HB	2.11	0.51
3:a:115:LYS:O	3:a:116:THR:HB	2.11	0.51
1:L:147:SER:OG	1:L:190:THR:OG1	2.25	0.51
1:N:147:SER:OG	1:N:190:THR:OG1	2.25	0.51
1:E:147:SER:OG	1:E:190:THR:OG1	2.25	0.51
1:A:147:SER:OG	1:A:190:THR:OG1	2.25	0.50
1:R:147:SER:OG	1:R:190:THR:OG1	2.25	0.50
1:P:147:SER:OG	1:P:190:THR:OG1	2.25	0.50
1:C:147:SER:OG	1:C:190:THR:OG1	2.25	0.50
3:g:115:LYS:NZ	3:g:257:ASP:OD1	2.45	0.49
3:a:115:LYS:NZ	3:a:257:ASP:OD1	2.45	0.49
1:E:273:ALA:N	1:E:274:PRO:CD	2.76	0.49
1:L:273:ALA:N	1:L:274:PRO:CD	2.76	0.49
3:h:115:LYS:NZ	3:h:257:ASP:OD1	2.46	0.49
1:N:273:ALA:N	1:N:274:PRO:CD	2.76	0.49
1:R:273:ALA:N	1:R:274:PRO:CD	2.76	0.49
3:e:115:LYS:NZ	3:e:257:ASP:OD1	2.45	0.49
3:b:115:LYS:NZ	3:b:257:ASP:OD1	2.45	0.49
1:G:154:MET:HA	1:G:154:MET:HE2	1.94	0.49
1:G:273:ALA:N	1:G:274:PRO:CD	2.76	0.49
3:f:115:LYS:NZ	3:f:257:ASP:OD1	2.46	0.49
1:P:179:THR:HG1	4:P:501:GTP:HO3'	1.57	0.49
1:C:179:THR:HG1	4:C:501:GTP:HO3'	1.57	0.48
2:D:249:ASN:C	2:D:249:ASN:OD1	2.56	0.48
1:P:154:MET:HE2	1:P:154:MET:HA	1.94	0.48
1:C:273:ALA:N	1:C:274:PRO:CD	2.76	0.48
1:P:273:ALA:N	1:P:274:PRO:CD	2.76	0.48
2:Q:249:ASN:OD1	2:Q:249:ASN:C	2.56	0.48
2:S:249:ASN:C	2:S:249:ASN:OD1	2.56	0.48
1:A:273:ALA:N	1:A:274:PRO:CD	2.76	0.48
3:K:198:LYS:NZ	3:K:340:ASP:OD1	2.45	0.48
1:C:154:MET:HE2	1:C:154:MET:HA	1.94	0.48
1:A:154:MET:HE2	1:A:154:MET:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:MET:HE2	1:I:154:MET:HA	1.94	0.48
1:I:273:ALA:N	1:I:274:PRO:CD	2.76	0.48
1:R:154:MET:HE2	1:R:154:MET:HA	1.94	0.48
1:R:179:THR:HG1	4:R:501:GTP:HO3'	1.57	0.48
3:c:115:LYS:NZ	3:c:257:ASP:OD1	2.46	0.48
3:d:115:LYS:NZ	3:d:257:ASP:OD1	2.45	0.48
2:H:249:ASN:OD1	2:H:249:ASN:C	2.56	0.48
2:J:249:ASN:OD1	2:J:249:ASN:C	2.56	0.48
1:L:154:MET:HA	1:L:154:MET:HE2	1.94	0.48
1:E:154:MET:HA	1:E:154:MET:HE2	1.94	0.48
1:I:124:LYS:NZ	1:N:284:GLU:OE1	2.36	0.48
2:B:249:ASN:C	2:B:249:ASN:OD1	2.56	0.48
2:D:36:TYR:OH	2:D:40:SER:O	2.32	0.48
2:Q:36:TYR:OH	2:Q:40:SER:O	2.32	0.48
2:S:36:TYR:OH	2:S:40:SER:O	2.32	0.48
2:J:179:ASP:OD1	2:J:179:ASP:O	2.32	0.48
1:N:154:MET:HE2	1:N:154:MET:HA	1.94	0.48
2:H:36:TYR:OH	2:H:40:SER:O	2.32	0.47
2:H:179:ASP:OD1	2:H:179:ASP:O	2.32	0.47
2:B:273:ALA:O	2:B:274:PRO:C	2.57	0.47
2:B:288:VAL:N	2:B:289:PRO:HD2	2.30	0.47
2:D:179:ASP:OD1	2:D:179:ASP:O	2.32	0.47
2:J:36:TYR:OH	2:J:40:SER:O	2.32	0.47
2:J:288:VAL:N	2:J:289:PRO:HD2	2.30	0.47
2:Q:179:ASP:O	2:Q:179:ASP:OD1	2.32	0.47
2:S:179:ASP:OD1	2:S:179:ASP:O	2.32	0.47
2:B:36:TYR:OH	2:B:40:SER:O	2.31	0.47
2:B:179:ASP:OD1	2:B:179:ASP:O	2.32	0.47
2:F:179:ASP:OD1	2:F:179:ASP:O	2.32	0.47
2:H:288:VAL:N	2:H:289:PRO:HD2	2.30	0.47
2:J:273:ALA:O	2:J:274:PRO:C	2.57	0.47
2:O:179:ASP:OD1	2:O:179:ASP:O	2.32	0.47
2:D:273:ALA:O	2:D:274:PRO:C	2.57	0.47
2:H:273:ALA:O	2:H:274:PRO:C	2.57	0.47
2:M:36:TYR:OH	2:M:40:SER:O	2.31	0.47
2:M:179:ASP:OD1	2:M:179:ASP:O	2.32	0.47
2:M:273:ALA:O	2:M:274:PRO:C	2.57	0.47
2:Q:273:ALA:O	2:Q:274:PRO:C	2.57	0.47
2:F:36:TYR:OH	2:F:40:SER:O	2.31	0.47
2:F:273:ALA:O	2:F:274:PRO:C	2.57	0.47
2:O:36:TYR:OH	2:O:40:SER:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:414:ASP:OD1	2:Q:414:ASP:C	2.58	0.47
2:S:273:ALA:O	2:S:274:PRO:C	2.57	0.47
2:D:414:ASP:C	2:D:414:ASP:OD1	2.58	0.47
2:O:273:ALA:O	2:O:274:PRO:C	2.57	0.47
1:I:88:HIS:CD2	1:N:283:HIS:CB	2.98	0.47
2:S:414:ASP:OD1	2:S:414:ASP:C	2.58	0.47
1:L:72:PRO:O	1:L:73:THR:C	2.58	0.47
2:O:249:ASN:OD1	2:O:249:ASN:C	2.56	0.47
1:E:72:PRO:O	1:E:73:THR:C	2.58	0.47
2:H:60:LYS:HD3	2:M:282:GLN:O	2.15	0.47
1:N:72:PRO:O	1:N:73:THR:C	2.58	0.47
2:Q:288:VAL:N	2:Q:289:PRO:HD2	2.29	0.47
2:S:288:VAL:N	2:S:289:PRO:HD2	2.29	0.46
2:D:288:VAL:N	2:D:289:PRO:HD2	2.30	0.46
2:F:249:ASN:C	2:F:249:ASN:OD1	2.56	0.46
2:M:288:VAL:N	2:M:289:PRO:HD2	2.30	0.46
2:M:249:ASN:OD1	2:M:249:ASN:C	2.56	0.46
2:F:288:VAL:N	2:F:289:PRO:HD2	2.30	0.46
3:c:27:ARG:O	3:c:27:ARG:HG3	2.16	0.46
3:d:27:ARG:O	3:d:27:ARG:HG3	2.15	0.46
1:R:72:PRO:O	1:R:73:THR:C	2.58	0.46
1:C:72:PRO:O	1:C:73:THR:C	2.58	0.46
2:O:288:VAL:N	2:O:289:PRO:HD2	2.30	0.46
1:P:72:PRO:O	1:P:73:THR:C	2.58	0.46
7:F:502:TA1:H463	7:F:502:TA1:C26	2.46	0.46
7:O:502:TA1:H463	7:O:502:TA1:C26	2.46	0.46
3:K:27:ARG:O	3:K:27:ARG:HG3	2.15	0.46
2:H:414:ASP:OD1	2:H:414:ASP:C	2.58	0.46
2:J:178:SER:O	2:J:179:ASP:HB2	2.17	0.45
7:M:502:TA1:H463	7:M:502:TA1:C26	2.46	0.45
1:A:72:PRO:O	1:A:73:THR:C	2.58	0.45
2:B:178:SER:O	2:B:179:ASP:HB2	2.17	0.45
3:a:27:ARG:O	3:a:27:ARG:HG3	2.15	0.45
2:H:178:SER:O	2:H:179:ASP:HB2	2.17	0.45
2:D:178:SER:O	2:D:179:ASP:HB2	2.16	0.45
2:J:414:ASP:OD1	2:J:414:ASP:C	2.58	0.45
2:Q:178:SER:O	2:Q:179:ASP:HB2	2.17	0.45
1:G:72:PRO:O	1:G:73:THR:C	2.58	0.45
3:g:27:ARG:O	3:g:27:ARG:HG3	2.16	0.45
2:B:414:ASP:OD1	2:B:414:ASP:C	2.58	0.45
3:e:27:ARG:O	3:e:27:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:178:SER:O	2:S:179:ASP:HB2	2.17	0.45
3:h:27:ARG:O	3:h:27:ARG:HG3	2.16	0.45
7:B:502:TA1:H463	7:B:502:TA1:C26	2.46	0.45
1:I:72:PRO:O	1:I:73:THR:C	2.58	0.45
2:O:178:SER:O	2:O:179:ASP:HB2	2.17	0.45
2:B:288:VAL:N	2:B:289:PRO:CD	2.80	0.45
2:F:320:ARG:HB3	2:F:359:PRO:HA	1.99	0.45
2:H:288:VAL:N	2:H:289:PRO:CD	2.80	0.45
7:H:502:TA1:H463	7:H:502:TA1:C26	2.46	0.45
2:J:288:VAL:N	2:J:289:PRO:CD	2.80	0.45
7:J:502:TA1:H463	7:J:502:TA1:C26	2.46	0.45
2:M:320:ARG:HB3	2:M:359:PRO:HA	1.99	0.45
2:O:320:ARG:HB3	2:O:359:PRO:HA	1.99	0.45
3:c:46:PRO:O	3:c:47:ALA:CB	2.65	0.45
3:K:102:PRO:O	3:K:103:ALA:CB	2.65	0.45
2:F:178:SER:O	2:F:179:ASP:HB2	2.17	0.45
2:M:178:SER:O	2:M:179:ASP:HB2	2.17	0.45
2:B:320:ARG:HB3	2:B:359:PRO:HA	1.99	0.45
3:d:46:PRO:O	3:d:47:ALA:CB	2.65	0.45
2:Q:229:HIS:CD2	2:Q:229:HIS:C	2.94	0.45
3:f:27:ARG:O	3:f:27:ARG:HG3	2.15	0.44
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.99	0.44
2:D:229:HIS:C	2:D:229:HIS:CD2	2.94	0.44
1:I:284:GLU:HB2	1:R:88:HIS:HE2	1.82	0.44
2:S:229:HIS:C	2:S:229:HIS:CD2	2.94	0.44
3:K:304:ASN:O	3:K:307:SER:HB2	2.17	0.44
3:b:27:ARG:O	3:b:27:ARG:HG3	2.16	0.44
2:H:320:ARG:HB3	2:H:359:PRO:HA	1.99	0.44
2:M:288:VAL:N	2:M:289:PRO:CD	2.80	0.44
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.99	0.44
2:F:288:VAL:N	2:F:289:PRO:CD	2.80	0.44
2:H:229:HIS:C	2:H:229:HIS:CD2	2.94	0.44
2:H:288:VAL:HB	2:H:289:PRO:HD3	2.00	0.44
3:d:221:ASN:O	3:d:224:SER:HB2	2.18	0.44
3:f:46:PRO:O	3:f:47:ALA:CB	2.65	0.44
2:Q:288:VAL:HB	2:Q:289:PRO:HD3	1.99	0.44
2:S:320:ARG:HB3	2:S:359:PRO:HA	1.99	0.44
2:F:288:VAL:HB	2:F:289:PRO:HD3	1.99	0.44
3:b:46:PRO:O	3:b:47:ALA:CB	2.65	0.44
3:c:221:ASN:O	3:c:224:SER:HB2	2.18	0.44
2:J:229:HIS:C	2:J:229:HIS:CD2	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:288:VAL:HB	2:J:289:PRO:HD3	2.00	0.44
2:J:320:ARG:HB3	2:J:359:PRO:HA	1.99	0.44
2:O:288:VAL:N	2:O:289:PRO:CD	2.80	0.44
2:D:320:ARG:HB3	2:D:359:PRO:HA	1.99	0.44
7:D:502:TA1:H463	7:D:502:TA1:C26	2.46	0.44
2:M:288:VAL:HB	2:M:289:PRO:HD3	2.00	0.44
2:O:229:HIS:CD2	2:O:229:HIS:C	2.94	0.44
2:O:306:ASP:HA	2:O:307:PRO:HD3	1.85	0.44
8:f:401:ANP:O2A	8:f:401:ANP:H8	2.18	0.44
2:Q:288:VAL:N	2:Q:289:PRO:CD	2.80	0.44
8:g:401:ANP:O2A	8:g:401:ANP:H8	2.18	0.44
2:S:288:VAL:HB	2:S:289:PRO:HD3	2.00	0.44
7:S:502:TA1:H463	7:S:502:TA1:C26	2.46	0.44
8:h:401:ANP:O2A	8:h:401:ANP:H8	2.18	0.44
2:D:288:VAL:N	2:D:289:PRO:CD	2.80	0.44
3:e:46:PRO:O	3:e:47:ALA:CB	2.65	0.44
2:O:288:VAL:HB	2:O:289:PRO:HD3	2.00	0.44
2:Q:320:ARG:HB3	2:Q:359:PRO:HA	1.99	0.44
7:Q:502:TA1:H463	7:Q:502:TA1:C26	2.46	0.44
2:S:288:VAL:N	2:S:289:PRO:CD	2.80	0.44
3:h:46:PRO:O	3:h:47:ALA:CB	2.65	0.44
3:a:46:PRO:O	3:a:47:ALA:CB	2.65	0.44
8:a:401:ANP:O2A	8:a:401:ANP:H8	2.18	0.44
2:F:229:HIS:CD2	2:F:229:HIS:C	2.94	0.44
3:b:221:ASN:O	3:b:224:SER:HB2	2.17	0.44
8:b:401:ANP:O2A	8:b:401:ANP:H8	2.18	0.44
8:e:401:ANP:O2A	8:e:401:ANP:H8	2.18	0.44
3:g:221:ASN:O	3:g:224:SER:HB2	2.17	0.44
3:K:231:ASP:OD1	3:K:323:LYS:NZ	2.45	0.44
8:K:501:ANP:O2A	8:K:501:ANP:H8	2.18	0.44
3:c:148:ASP:OD1	3:c:240:LYS:NZ	2.45	0.44
8:d:401:ANP:O2A	8:d:401:ANP:H8	2.18	0.44
2:M:414:ASP:OD1	2:M:414:ASP:C	2.58	0.44
3:e:221:ASN:O	3:e:224:SER:HB2	2.17	0.44
3:g:46:PRO:O	3:g:47:ALA:CB	2.65	0.44
2:B:229:HIS:C	2:B:229:HIS:CD2	2.95	0.43
3:a:221:ASN:O	3:a:224:SER:HB2	2.17	0.43
2:F:31:ASP:C	2:F:31:ASP:OD1	2.61	0.43
2:F:306:ASP:HA	2:F:307:PRO:HD3	1.84	0.43
8:c:401:ANP:O2A	8:c:401:ANP:H8	2.18	0.43
2:M:31:ASP:C	2:M:31:ASP:OD1	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:229:HIS:CD2	2:M:229:HIS:C	2.94	0.43
2:Q:31:ASP:OD1	2:Q:31:ASP:C	2.61	0.43
3:h:221:ASN:O	3:h:224:SER:HB2	2.17	0.43
3:d:148:ASP:OD1	3:d:240:LYS:NZ	2.45	0.43
2:O:31:ASP:OD1	2:O:31:ASP:C	2.61	0.43
3:f:221:ASN:O	3:f:224:SER:HB2	2.17	0.43
2:F:179:ASP:O	2:F:179:ASP:CG	2.62	0.43
2:O:414:ASP:OD1	2:O:414:ASP:C	2.58	0.43
2:F:414:ASP:C	2:F:414:ASP:OD1	2.58	0.43
2:M:179:ASP:O	2:M:179:ASP:CG	2.62	0.43
2:O:179:ASP:O	2:O:179:ASP:CG	2.62	0.43
2:D:179:ASP:O	2:D:179:ASP:CG	2.62	0.43
2:M:306:ASP:HA	2:M:307:PRO:HD3	1.84	0.43
2:S:179:ASP:O	2:S:179:ASP:CG	2.62	0.43
2:Q:179:ASP:O	2:Q:179:ASP:CG	2.62	0.43
1:A:72:PRO:O	1:A:75:ILE:N	2.52	0.43
1:G:72:PRO:O	1:G:75:ILE:N	2.52	0.43
1:I:72:PRO:O	1:I:75:ILE:N	2.52	0.43
1:N:72:PRO:O	1:N:75:ILE:N	2.51	0.43
3:K:198:LYS:NZ	3:K:198:LYS:HB3	2.34	0.42
3:b:148:ASP:OD1	3:b:240:LYS:NZ	2.45	0.42
3:d:115:LYS:NZ	3:d:115:LYS:HB3	2.34	0.42
1:L:243:ARG:HA	1:L:243:ARG:NE	2.34	0.42
3:e:148:ASP:OD1	3:e:240:LYS:NZ	2.45	0.42
3:f:148:ASP:OD1	3:f:240:LYS:NZ	2.45	0.42
1:A:243:ARG:HA	1:A:243:ARG:NE	2.34	0.42
1:E:243:ARG:HA	1:E:243:ARG:NE	2.34	0.42
2:H:31:ASP:OD1	2:H:31:ASP:C	2.61	0.42
1:I:243:ARG:HA	1:I:243:ARG:NE	2.34	0.42
1:L:72:PRO:O	1:L:75:ILE:N	2.52	0.42
2:B:31:ASP:OD1	2:B:31:ASP:C	2.61	0.42
1:E:72:PRO:O	1:E:75:ILE:N	2.52	0.42
2:H:179:ASP:O	2:H:179:ASP:CG	2.62	0.42
3:c:115:LYS:NZ	3:c:115:LYS:HB3	2.34	0.42
2:J:31:ASP:OD1	2:J:31:ASP:C	2.61	0.42
1:N:243:ARG:HA	1:N:243:ARG:NE	2.34	0.42
2:S:31:ASP:OD1	2:S:31:ASP:C	2.61	0.42
2:D:31:ASP:OD1	2:D:31:ASP:C	2.61	0.42
1:G:243:ARG:HA	1:G:243:ARG:NE	2.34	0.42
3:g:115:LYS:NZ	3:g:115:LYS:HB3	2.34	0.42
2:B:179:ASP:O	2:B:179:ASP:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:PRO:O	1:P:75:ILE:N	2.52	0.42
1:C:72:PRO:O	1:C:75:ILE:N	2.52	0.42
2:D:229:HIS:NE2	7:D:502:TA1:O14	2.52	0.42
3:e:40:ARG:HA	3:e:75:LEU:HB3	2.02	0.42
2:Q:229:HIS:NE2	7:Q:502:TA1:O14	2.52	0.42
3:h:115:LYS:NZ	3:h:115:LYS:HB3	2.34	0.42
1:C:243:ARG:NE	1:C:243:ARG:HA	2.34	0.42
3:a:115:LYS:NZ	3:a:115:LYS:HB3	2.34	0.42
3:b:40:ARG:HA	3:b:75:LEU:HB3	2.02	0.42
3:b:226:ARG:O	3:b:226:ARG:CG	2.62	0.42
2:J:179:ASP:O	2:J:179:ASP:CG	2.62	0.42
3:f:40:ARG:HA	3:f:75:LEU:HB3	2.02	0.42
1:P:243:ARG:HA	1:P:243:ARG:NE	2.34	0.42
1:R:72:PRO:O	1:R:75:ILE:N	2.52	0.42
2:S:229:HIS:NE2	7:S:502:TA1:O14	2.53	0.42
3:K:96:ARG:HA	3:K:158:LEU:HB3	2.02	0.42
3:c:40:ARG:HA	3:c:75:LEU:HB3	2.02	0.42
1:R:243:ARG:NE	1:R:243:ARG:HA	2.35	0.42
3:h:115:LYS:HB3	3:h:115:LYS:HZ3	1.85	0.42
3:c:114:GLY:CA	8:c:401:ANP:O2A	2.68	0.42
3:e:226:ARG:O	3:e:226:ARG:CG	2.62	0.42
3:g:115:LYS:HB3	3:g:115:LYS:HZ3	1.85	0.42
3:K:197:GLY:CA	8:K:501:ANP:O2A	2.68	0.42
3:b:115:LYS:NZ	3:b:115:LYS:HB3	2.34	0.42
3:f:226:ARG:O	3:f:226:ARG:CG	2.62	0.42
2:B:229:HIS:NE2	7:B:502:TA1:O14	2.52	0.41
2:J:229:HIS:NE2	7:J:502:TA1:O14	2.52	0.41
3:d:40:ARG:HA	3:d:75:LEU:HB3	2.02	0.41
1:L:260:VAL:HA	1:L:261:PRO:HD2	1.94	0.41
3:e:115:LYS:NZ	3:e:115:LYS:HB3	2.34	0.41
3:f:224:SER:O	3:f:225:SER:C	2.63	0.41
3:h:114:GLY:CA	8:h:401:ANP:O2A	2.68	0.41
3:K:306:VAL:O	3:K:307:SER:C	2.64	0.41
3:b:224:SER:O	3:b:225:SER:C	2.64	0.41
2:M:262:PHE:O	2:M:263:PRO:C	2.63	0.41
3:e:224:SER:O	3:e:225:SER:C	2.64	0.41
3:f:114:GLY:CA	8:f:401:ANP:O2A	2.68	0.41
3:a:114:GLY:CA	8:a:401:ANP:O2A	2.68	0.41
3:b:114:GLY:CA	8:b:401:ANP:O2A	2.68	0.41
2:H:229:HIS:NE2	7:H:502:TA1:O14	2.52	0.41
3:c:223:VAL:O	3:c:224:SER:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:262:PHE:O	2:J:263:PRO:C	2.63	0.41
3:d:223:VAL:O	3:d:224:SER:C	2.64	0.41
3:f:115:LYS:NZ	3:f:115:LYS:HB3	2.34	0.41
3:a:40:ARG:HA	3:a:75:LEU:HB3	2.02	0.41
3:a:224:SER:O	3:a:225:SER:C	2.63	0.41
2:F:262:PHE:O	2:F:263:PRO:C	2.63	0.41
2:H:262:PHE:O	2:H:263:PRO:C	2.63	0.41
2:O:262:PHE:O	2:O:263:PRO:C	2.63	0.41
3:g:40:ARG:HA	3:g:75:LEU:HB3	2.02	0.41
3:g:114:GLY:CA	8:g:401:ANP:O2A	2.68	0.41
1:E:260:VAL:HA	1:E:261:PRO:HD2	1.94	0.41
1:G:85:GLN:O	1:L:283:HIS:NE2	2.48	0.41
3:e:114:GLY:CA	8:e:401:ANP:O2A	2.68	0.41
3:g:155:TYR:HB3	3:g:166:LEU:HB3	2.02	0.41
3:g:224:SER:O	3:g:225:SER:C	2.64	0.41
3:h:40:ARG:HA	3:h:75:LEU:HB3	2.02	0.41
2:B:262:PHE:O	2:B:263:PRO:C	2.63	0.41
3:a:155:TYR:HB3	3:a:166:LEU:HB3	2.02	0.41
3:a:158:ILE:HB	3:a:228:HIS:HB2	2.02	0.41
3:a:223:VAL:O	3:a:224:SER:C	2.64	0.41
3:b:155:TYR:HB3	3:b:166:LEU:HB3	2.02	0.41
3:c:155:TYR:HB3	3:c:166:LEU:HB3	2.02	0.41
3:e:155:TYR:HB3	3:e:166:LEU:HB3	2.02	0.41
3:g:158:ILE:HB	3:g:228:HIS:HB2	2.02	0.41
3:g:223:VAL:O	3:g:224:SER:C	2.64	0.41
3:h:155:TYR:HB3	3:h:166:LEU:HB3	2.02	0.41
3:h:224:SER:O	3:h:225:SER:C	2.64	0.41
3:K:307:SER:O	3:K:308:SER:C	2.64	0.41
3:b:158:ILE:HB	3:b:228:HIS:HB2	2.02	0.41
1:G:260:VAL:HA	1:G:261:PRO:HD2	1.94	0.41
1:I:260:VAL:HA	1:I:261:PRO:HD2	1.94	0.41
2:J:283:TYR:CE1	2:S:89:PRO:HD2	2.55	0.41
3:d:224:SER:O	3:d:225:SER:C	2.63	0.41
3:f:155:TYR:HB3	3:f:166:LEU:HB3	2.02	0.41
3:f:158:ILE:HB	3:f:228:HIS:HB2	2.02	0.41
3:h:158:ILE:HB	3:h:228:HIS:HB2	2.02	0.41
3:K:238:TYR:HB3	3:K:249:LEU:HB3	2.02	0.41
3:K:241:ILE:HB	3:K:311:HIS:HB2	2.02	0.41
3:d:155:TYR:HB3	3:d:166:LEU:HB3	2.02	0.41
3:e:158:ILE:HB	3:e:228:HIS:HB2	2.02	0.41
1:N:260:VAL:HA	1:N:261:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:229:HIS:NE2	7:O:502:TA1:O14	2.52	0.41
1:A:260:VAL:HA	1:A:261:PRO:HD2	1.94	0.41
2:D:262:PHE:O	2:D:263:PRO:C	2.63	0.41
2:F:229:HIS:NE2	7:F:502:TA1:O14	2.52	0.41
2:H:183:GLU:N	2:H:184:PRO:HD2	2.36	0.41
3:c:158:ILE:HB	3:c:228:HIS:HB2	2.02	0.41
3:c:224:SER:O	3:c:225:SER:C	2.64	0.41
1:I:227:LEU:C	1:I:227:LEU:HD23	2.46	0.41
3:e:263:ARG:O	3:e:264:ALA:C	2.64	0.41
3:f:223:VAL:O	3:f:224:SER:C	2.64	0.41
2:S:262:PHE:O	2:S:263:PRO:C	2.63	0.41
3:h:223:VAL:O	3:h:224:SER:C	2.64	0.41
2:B:183:GLU:N	2:B:184:PRO:HD2	2.36	0.41
2:B:255:LEU:O	2:B:259:MET:N	2.54	0.41
1:C:227:LEU:C	1:C:227:LEU:HD23	2.46	0.41
2:D:183:GLU:N	2:D:184:PRO:HD2	2.36	0.41
1:G:227:LEU:C	1:G:227:LEU:HD23	2.46	0.41
2:H:359:PRO:HA	2:H:360:PRO:HD3	1.93	0.41
3:d:158:ILE:HB	3:d:228:HIS:HB2	2.02	0.41
2:M:229:HIS:NE2	7:M:502:TA1:O14	2.52	0.41
2:Q:262:PHE:O	2:Q:263:PRO:C	2.63	0.41
1:R:227:LEU:C	1:R:227:LEU:HD23	2.46	0.41
2:S:183:GLU:N	2:S:184:PRO:HD2	2.36	0.41
1:C:82:THR:O	1:C:83:TYR:HB2	2.21	0.40
1:C:260:VAL:HA	1:C:261:PRO:HD2	1.94	0.40
3:a:19:PRO:HD3	8:a:401:ANP:C6	2.51	0.40
1:E:227:LEU:HD23	1:E:227:LEU:C	2.46	0.40
3:b:117:TYR:CD2	3:b:117:TYR:C	2.99	0.40
3:b:223:VAL:O	3:b:224:SER:C	2.64	0.40
3:b:263:ARG:O	3:b:264:ALA:C	2.65	0.40
2:H:255:LEU:O	2:H:259:MET:N	2.54	0.40
3:f:117:TYR:CD2	3:f:117:TYR:C	2.99	0.40
3:f:263:ARG:O	3:f:264:ALA:C	2.64	0.40
1:P:227:LEU:C	1:P:227:LEU:HD23	2.46	0.40
1:P:260:VAL:HA	1:P:261:PRO:HD2	1.94	0.40
3:g:19:PRO:HD3	8:g:401:ANP:C6	2.51	0.40
3:h:19:PRO:HD3	8:h:401:ANP:C6	2.51	0.40
1:A:227:LEU:C	1:A:227:LEU:HD23	2.46	0.40
3:a:115:LYS:HB3	3:a:115:LYS:HZ3	1.87	0.40
3:a:263:ARG:O	3:a:264:ALA:C	2.64	0.40
2:J:255:LEU:O	2:J:259:MET:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:223:VAL:O	3:e:224:SER:C	2.64	0.40
3:g:263:ARG:O	3:g:264:ALA:C	2.64	0.40
2:S:255:LEU:O	2:S:259:MET:N	2.54	0.40
3:h:263:ARG:O	3:h:264:ALA:C	2.64	0.40
2:B:359:PRO:HA	2:B:360:PRO:HD3	1.93	0.40
3:K:200:TYR:CD2	3:K:200:TYR:C	2.99	0.40
2:D:255:LEU:O	2:D:259:MET:N	2.54	0.40
2:F:174:SER:HA	2:F:175:PRO:HD3	1.96	0.40
3:d:114:GLY:CA	8:d:401:ANP:O2A	2.68	0.40
3:e:117:TYR:CD2	3:e:117:TYR:C	2.99	0.40
1:N:227:LEU:HD23	1:N:227:LEU:C	2.46	0.40
2:Q:255:LEU:O	2:Q:259:MET:N	2.54	0.40
1:R:82:THR:O	1:R:83:TYR:HB2	2.22	0.40
1:R:260:VAL:HA	1:R:261:PRO:HD2	1.94	0.40
1:E:82:THR:O	1:E:83:TYR:HB2	2.22	0.40
2:J:183:GLU:N	2:J:184:PRO:HD2	2.36	0.40
1:L:227:LEU:HD23	1:L:227:LEU:C	2.46	0.40
2:M:174:SER:HA	2:M:175:PRO:HD3	1.96	0.40
1:P:82:THR:O	1:P:83:TYR:HB2	2.22	0.40
2:Q:183:GLU:N	2:Q:184:PRO:HD2	2.36	0.40
3:c:226:ARG:O	3:c:226:ARG:CG	2.62	0.40
3:d:117:TYR:CD2	3:d:117:TYR:C	2.99	0.40
1:L:82:THR:O	1:L:83:TYR:HB2	2.22	0.40
1:N:82:THR:O	1:N:83:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	E	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	G	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	I	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	L	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	N	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	P	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
1	R	423/451 (94%)	397 (94%)	19 (4%)	7 (2%)	7	35
2	B	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	D	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	F	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	H	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	J	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	M	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	O	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	Q	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
2	S	424/445 (95%)	396 (93%)	18 (4%)	10 (2%)	4	29
3	K	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	a	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	b	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	c	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	d	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	e	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	f	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	g	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
3	h	344/355 (97%)	314 (91%)	22 (6%)	8 (2%)	5	30
All	All	10719/11259 (95%)	9963 (93%)	531 (5%)	225 (2%)	8	31

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	179	ASP
2	B	273	ALA

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Mol	Chain	Res	Type
3	K	18	ARG
3	K	19	PRO
3	K	103	ALA
2	D	179	ASP
2	D	273	ALA
3	a	18	ARG
3	a	19	PRO
3	a	47	ALA
2	F	179	ASP
2	F	273	ALA
3	b	18	ARG
3	b	19	PRO
3	b	47	ALA
2	H	179	ASP
2	H	273	ALA
3	c	18	ARG
3	c	19	PRO
3	c	47	ALA
2	J	179	ASP
2	J	273	ALA
3	d	18	ARG
3	d	19	PRO
3	d	47	ALA
2	M	179	ASP
2	M	273	ALA
3	e	18	ARG
3	e	19	PRO
3	e	47	ALA
2	O	179	ASP
2	O	273	ALA
3	f	18	ARG
3	f	19	PRO
3	f	47	ALA
2	Q	179	ASP
2	Q	273	ALA
3	g	18	ARG
3	g	19	PRO
3	g	47	ALA
2	S	179	ASP
2	S	273	ALA
3	h	18	ARG
3	h	19	PRO

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Mol	Chain	Res	Type
3	h	47	ALA
1	A	73	THR
1	A	368	LEU
2	B	173	PRO
3	K	300	PRO
3	K	308	SER
3	K	329	SER
1	C	73	THR
1	C	368	LEU
2	D	173	PRO
3	a	217	PRO
3	a	225	SER
3	a	246	SER
1	E	73	THR
1	E	368	LEU
2	F	173	PRO
3	b	217	PRO
3	b	225	SER
3	b	246	SER
1	G	73	THR
1	G	368	LEU
2	H	63	PRO
2	H	173	PRO
3	c	217	PRO
3	c	225	SER
3	c	246	SER
1	I	73	THR
1	I	368	LEU
2	J	173	PRO
3	d	217	PRO
3	d	225	SER
3	d	246	SER
1	L	73	THR
1	L	368	LEU
2	M	173	PRO
3	e	217	PRO
3	e	225	SER
3	e	246	SER
1	N	73	THR
1	N	368	LEU
2	O	173	PRO
3	f	217	PRO

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Mol	Chain	Res	Type
3	f	225	SER
3	f	246	SER
1	P	73	THR
1	P	368	LEU
2	Q	173	PRO
3	g	217	PRO
3	g	225	SER
3	g	246	SER
1	R	73	THR
1	R	368	LEU
2	S	63	PRO
2	S	173	PRO
3	h	217	PRO
3	h	225	SER
3	h	246	SER
2	B	63	PRO
2	B	274	PRO
3	K	136	ALA
2	D	63	PRO
2	D	274	PRO
3	a	53	ALA
2	F	63	PRO
2	F	274	PRO
3	b	53	ALA
2	H	274	PRO
3	c	53	ALA
2	J	63	PRO
2	J	274	PRO
3	d	53	ALA
2	M	63	PRO
2	M	274	PRO
3	e	53	ALA
2	O	63	PRO
2	O	274	PRO
3	f	53	ALA
2	Q	63	PRO
2	Q	274	PRO
3	g	53	ALA
2	S	274	PRO
3	h	53	ALA
1	A	130	THR
2	B	263	PRO

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Mol	Chain	Res	Type
2	B	348	PRO
1	C	130	THR
2	D	263	PRO
2	D	348	PRO
1	E	130	THR
2	F	263	PRO
2	F	348	PRO
1	G	130	THR
2	H	263	PRO
2	H	348	PRO
1	I	130	THR
2	J	263	PRO
2	J	348	PRO
1	L	130	THR
2	M	263	PRO
2	M	348	PRO
1	N	130	THR
2	O	263	PRO
2	O	348	PRO
1	P	130	THR
2	Q	263	PRO
2	Q	348	PRO
1	R	130	THR
2	S	263	PRO
2	S	348	PRO
1	A	173	PRO
2	B	175	PRO
1	C	173	PRO
2	D	175	PRO
1	E	173	PRO
2	F	175	PRO
1	G	173	PRO
2	H	175	PRO
1	I	173	PRO
2	J	175	PRO
1	L	173	PRO
2	M	175	PRO
1	N	173	PRO
2	O	175	PRO
1	P	173	PRO
2	Q	175	PRO
1	R	173	PRO

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Mol	Chain	Res	Type
2	S	175	PRO
1	A	348	PRO
2	B	72	PRO
3	K	307	SER
1	C	348	PRO
2	D	72	PRO
3	a	224	SER
1	E	348	PRO
2	F	72	PRO
3	b	224	SER
1	G	348	PRO
2	H	72	PRO
3	c	224	SER
1	I	348	PRO
2	J	72	PRO
3	d	224	SER
1	L	348	PRO
2	M	72	PRO
3	e	224	SER
1	N	348	PRO
2	O	72	PRO
3	f	224	SER
1	P	348	PRO
2	Q	72	PRO
3	g	224	SER
1	R	348	PRO
2	S	72	PRO
3	h	224	SER
1	A	298	PRO
2	B	142	GLY
1	C	298	PRO
2	D	142	GLY
1	E	298	PRO
2	F	142	GLY
1	G	298	PRO
2	H	142	GLY
1	I	298	PRO
2	J	142	GLY
1	L	298	PRO
2	M	142	GLY
1	N	298	PRO
2	O	142	GLY

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Mol	Chain	Res	Type
1	P	298	PRO
2	Q	142	GLY
1	R	298	PRO
2	S	142	GLY
1	A	273	ALA
1	C	273	ALA
1	E	273	ALA
1	G	273	ALA
1	I	273	ALA
1	L	273	ALA
1	N	273	ALA
1	P	273	ALA
1	R	273	ALA

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	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	C	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	E	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	G	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	I	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	L	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	N	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	P	359/377 (95%)	354 (99%)	5 (1%)	59	71
1	R	359/377 (95%)	354 (99%)	5 (1%)	59	71
2	B	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	D	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	F	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	H	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	J	367/381 (96%)	364 (99%)	3 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	O	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	Q	367/381 (96%)	364 (99%)	3 (1%)	73	77
2	S	367/381 (96%)	364 (99%)	3 (1%)	73	77
3	K	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	a	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	b	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	c	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	d	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	e	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	f	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	g	310/319 (97%)	309 (100%)	1 (0%)	86	85
3	h	310/319 (97%)	309 (100%)	1 (0%)	86	85
All	All	9324/9693 (96%)	9243 (99%)	81 (1%)	68	75

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	89	PRO
1	A	175	PRO
1	A	263	PRO
1	A	325	PRO
2	B	32	PRO
2	B	89	PRO
2	B	245	PRO
3	K	194	THR
1	C	63	PRO
1	C	89	PRO
1	C	175	PRO
1	C	263	PRO
1	C	325	PRO
2	D	32	PRO
2	D	89	PRO
2	D	245	PRO
3	a	111	THR
1	E	63	PRO

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Mol	Chain	Res	Type
1	E	89	PRO
1	E	175	PRO
1	E	263	PRO
1	E	325	PRO
2	F	32	PRO
2	F	89	PRO
2	F	245	PRO
3	b	111	THR
1	G	63	PRO
1	G	89	PRO
1	G	175	PRO
1	G	263	PRO
1	G	325	PRO
2	H	32	PRO
2	H	89	PRO
2	H	245	PRO
3	c	111	THR
1	I	63	PRO
1	I	89	PRO
1	I	175	PRO
1	I	263	PRO
1	I	325	PRO
2	J	32	PRO
2	J	89	PRO
2	J	245	PRO
3	d	111	THR
1	L	63	PRO
1	L	89	PRO
1	L	175	PRO
1	L	263	PRO
1	L	325	PRO
2	M	32	PRO
2	M	89	PRO
2	M	245	PRO
3	e	111	THR
1	N	63	PRO
1	N	89	PRO
1	N	175	PRO
1	N	263	PRO
1	N	325	PRO
2	O	32	PRO
2	O	89	PRO

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Mol	Chain	Res	Type
2	O	245	PRO
3	f	111	THR
1	P	63	PRO
1	P	89	PRO
1	P	175	PRO
1	P	263	PRO
1	P	325	PRO
2	Q	32	PRO
2	Q	89	PRO
2	Q	245	PRO
3	g	111	THR
1	R	63	PRO
1	R	89	PRO
1	R	175	PRO
1	R	263	PRO
1	R	325	PRO
2	S	32	PRO
2	S	89	PRO
2	S	245	PRO
3	h	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	107	HIS
1	A	133	GLN
1	A	192	HIS
1	A	393	HIS
2	B	8	GLN
2	B	15	GLN
2	B	136	GLN
2	B	281	GLN
3	K	208	GLN
3	K	267	ASN
3	K	315	GLN
1	C	11	GLN
1	C	107	HIS
1	C	133	GLN
1	C	192	HIS
1	C	283	HIS
1	C	393	HIS

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Mol	Chain	Res	Type
2	D	8	GLN
2	D	15	GLN
2	D	136	GLN
2	D	281	GLN
2	D	331	GLN
3	a	125	GLN
3	a	184	ASN
3	a	232	GLN
1	E	11	GLN
1	E	107	HIS
1	E	133	GLN
1	E	192	HIS
1	E	393	HIS
2	F	8	GLN
2	F	15	GLN
2	F	136	GLN
2	F	281	GLN
2	F	331	GLN
3	b	125	GLN
3	b	184	ASN
3	b	228	HIS
3	b	232	GLN
1	G	11	GLN
1	G	107	HIS
1	G	133	GLN
1	G	192	HIS
1	G	393	HIS
2	H	8	GLN
2	H	15	GLN
2	H	101	ASN
2	H	136	GLN
2	H	281	GLN
2	H	331	GLN
3	c	125	GLN
3	c	184	ASN
3	c	232	GLN
1	I	11	GLN
1	I	107	HIS
1	I	133	GLN
1	I	192	HIS
1	I	393	HIS
2	J	8	GLN

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Mol	Chain	Res	Type
2	J	15	GLN
2	J	136	GLN
2	J	281	GLN
2	J	331	GLN
3	d	125	GLN
3	d	184	ASN
3	d	232	GLN
1	L	11	GLN
1	L	107	HIS
1	L	133	GLN
1	L	192	HIS
1	L	393	HIS
2	M	8	GLN
2	M	15	GLN
2	M	101	ASN
2	M	136	GLN
2	M	281	GLN
2	M	331	GLN
3	e	125	GLN
3	e	184	ASN
3	e	228	HIS
3	e	232	GLN
1	N	11	GLN
1	N	107	HIS
1	N	133	GLN
1	N	192	HIS
1	N	393	HIS
2	O	8	GLN
2	O	15	GLN
2	O	136	GLN
2	O	281	GLN
2	O	331	GLN
3	f	125	GLN
3	f	184	ASN
3	f	232	GLN
1	P	11	GLN
1	P	107	HIS
1	P	133	GLN
1	P	192	HIS
1	P	283	HIS
1	P	393	HIS
2	Q	8	GLN

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Mol	Chain	Res	Type
2	Q	15	GLN
2	Q	101	ASN
2	Q	136	GLN
2	Q	281	GLN
2	Q	331	GLN
3	g	125	GLN
3	g	184	ASN
3	g	232	GLN
1	R	11	GLN
1	R	107	HIS
1	R	133	GLN
1	R	192	HIS
1	R	283	HIS
1	R	393	HIS
2	S	8	GLN
2	S	15	GLN
2	S	136	GLN
2	S	281	GLN
2	S	331	GLN
3	h	125	GLN
3	h	184	ASN
3	h	232	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 18 are monoatomic - leaving 36 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	GDP	S	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.69	6 (13%)
7	TA1	F	502	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	13 (12%)
7	TA1	H	502	-	68,68,68	2.21	25 (36%)	105,105,105	1.50	13 (12%)
6	GDP	D	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.70	6 (13%)
7	TA1	S	502	-	68,68,68	2.21	26 (38%)	105,105,105	1.50	13 (12%)
4	GTP	P	501	5	33,34,34	0.97	1 (3%)	50,54,54	1.50	8 (16%)
8	ANP	b	401	5	33,33,33	1.98	10 (30%)	45,52,52	3.17	25 (55%)
8	ANP	h	401	5	33,33,33	1.96	10 (30%)	45,52,52	3.17	24 (53%)
7	TA1	J	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.50	13 (12%)
8	ANP	g	401	5	33,33,33	1.97	10 (30%)	45,52,52	3.17	24 (53%)
6	GDP	M	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.69	6 (13%)
7	TA1	Q	502	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	13 (12%)
4	GTP	L	501	5	33,34,34	0.96	1 (3%)	50,54,54	1.49	8 (16%)
6	GDP	Q	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.70	6 (13%)
4	GTP	I	501	5	33,34,34	0.97	1 (3%)	50,54,54	1.48	8 (16%)
6	GDP	F	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.69	6 (13%)
4	GTP	C	501	5	33,34,34	0.96	1 (3%)	50,54,54	1.50	8 (16%)
7	TA1	D	502	-	68,68,68	2.20	25 (36%)	105,105,105	1.50	13 (12%)
8	ANP	c	401	5	33,33,33	1.99	10 (30%)	45,52,52	3.16	23 (51%)
8	ANP	f	401	5	33,33,33	1.97	9 (27%)	45,52,52	3.16	24 (53%)
8	ANP	d	401	5	33,33,33	1.97	10 (30%)	45,52,52	3.16	23 (51%)
6	GDP	O	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.70	6 (13%)
7	TA1	O	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.50	13 (12%)
6	GDP	J	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.70	6 (13%)
6	GDP	H	501	-	29,30,30	1.23	4 (13%)	45,47,47	1.70	6 (13%)
8	ANP	K	501	5	33,33,33	1.96	9 (27%)	45,52,52	3.17	24 (53%)
4	GTP	N	501	5	33,34,34	0.96	1 (3%)	50,54,54	1.49	8 (16%)
4	GTP	R	501	5	33,34,34	0.96	1 (3%)	50,54,54	1.48	8 (16%)
7	TA1	M	502	-	68,68,68	2.20	27 (39%)	105,105,105	1.50	13 (12%)
4	GTP	E	501	5	33,34,34	0.96	1 (3%)	50,54,54	1.49	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GDP	B	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.70	6 (13%)
8	ANP	e	401	5	33,33,33	1.98	9 (27%)	45,52,52	3.16	24 (53%)
7	TA1	B	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.50	13 (12%)
4	GTP	A	501	5	33,34,34	0.97	1 (3%)	50,54,54	1.49	8 (16%)
8	ANP	a	401	5	33,33,33	1.97	10 (30%)	45,52,52	3.17	24 (53%)
4	GTP	G	501	5	33,34,34	0.96	1 (3%)	50,54,54	1.49	8 (16%)

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	GDP	S	501	-	-	3/16/32/32	0/3/3/3
7	TA1	F	502	-	-	9/41/127/127	0/7/7/7
7	TA1	H	502	-	-	9/41/127/127	0/7/7/7
6	GDP	D	501	-	-	3/16/32/32	0/3/3/3
7	TA1	S	502	-	-	9/41/127/127	0/7/7/7
4	GTP	P	501	5	-	5/22/38/38	0/3/3/3
8	ANP	b	401	5	-	3/18/38/38	0/3/3/3
8	ANP	h	401	5	-	3/18/38/38	0/3/3/3
7	TA1	J	502	-	-	9/41/127/127	0/7/7/7
8	ANP	g	401	5	-	3/18/38/38	0/3/3/3
6	GDP	M	501	-	-	3/16/32/32	0/3/3/3
7	TA1	Q	502	-	-	9/41/127/127	0/7/7/7
4	GTP	L	501	5	-	5/22/38/38	0/3/3/3
6	GDP	Q	501	-	-	3/16/32/32	0/3/3/3
4	GTP	I	501	5	-	5/22/38/38	0/3/3/3
6	GDP	F	501	-	-	3/16/32/32	0/3/3/3
4	GTP	C	501	5	-	5/22/38/38	0/3/3/3
7	TA1	D	502	-	-	9/41/127/127	0/7/7/7
8	ANP	c	401	5	-	3/18/38/38	0/3/3/3
8	ANP	f	401	5	-	3/18/38/38	0/3/3/3
8	ANP	d	401	5	-	3/18/38/38	0/3/3/3
6	GDP	O	501	-	-	3/16/32/32	0/3/3/3
7	TA1	O	502	-	-	9/41/127/127	0/7/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	J	501	-	-	3/16/32/32	0/3/3/3
6	GDP	H	501	-	-	3/16/32/32	0/3/3/3
8	ANP	K	501	5	-	3/18/38/38	0/3/3/3
4	GTP	N	501	5	-	5/22/38/38	0/3/3/3
4	GTP	R	501	5	-	5/22/38/38	0/3/3/3
7	TA1	M	502	-	-	9/41/127/127	0/7/7/7
4	GTP	E	501	5	-	5/22/38/38	0/3/3/3
6	GDP	B	501	-	-	3/16/32/32	0/3/3/3
8	ANP	e	401	5	-	3/18/38/38	0/3/3/3
7	TA1	B	502	-	-	9/41/127/127	0/7/7/7
4	GTP	A	501	5	-	5/22/38/38	0/3/3/3
8	ANP	a	401	5	-	3/18/38/38	0/3/3/3
4	GTP	G	501	5	-	5/22/38/38	0/3/3/3

All (363) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	502	TA1	C08-C09	6.54	1.50	1.38
7	H	502	TA1	C08-C09	6.53	1.50	1.38
7	B	502	TA1	C08-C09	6.52	1.50	1.38
7	F	502	TA1	C08-C09	6.52	1.50	1.38
7	S	502	TA1	C08-C09	6.49	1.50	1.38
7	D	502	TA1	C08-C09	6.49	1.50	1.38
7	Q	502	TA1	C08-C09	6.49	1.50	1.38
7	M	502	TA1	C08-C09	6.48	1.50	1.38
7	J	502	TA1	C08-C09	6.44	1.49	1.38
8	c	401	ANP	PA-O3A	-5.79	1.53	1.59
8	e	401	ANP	PA-O3A	-5.72	1.53	1.59
7	B	502	TA1	C07-C06	-5.72	1.25	1.38
7	S	502	TA1	C07-C06	-5.71	1.25	1.38
7	J	502	TA1	C07-C06	-5.70	1.25	1.38
7	D	502	TA1	C07-C06	-5.70	1.25	1.38
7	O	502	TA1	C07-C06	-5.69	1.25	1.38
7	F	502	TA1	C07-C06	-5.69	1.25	1.38
7	Q	502	TA1	C07-C06	-5.69	1.25	1.38
7	H	502	TA1	C07-C06	-5.68	1.25	1.38
7	M	502	TA1	C07-C06	-5.68	1.25	1.38
8	d	401	ANP	PA-O3A	-5.65	1.53	1.59
8	b	401	ANP	PA-O3A	-5.65	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	401	ANP	PA-O3A	-5.62	1.53	1.59
8	g	401	ANP	PA-O3A	-5.62	1.53	1.59
8	h	401	ANP	PA-O3A	-5.61	1.53	1.59
8	a	401	ANP	PA-O3A	-5.61	1.53	1.59
8	K	501	ANP	PA-O3A	-5.57	1.53	1.59
7	H	502	TA1	C18-C10	5.44	1.69	1.57
7	J	502	TA1	C18-C10	5.41	1.69	1.57
7	S	502	TA1	C18-C10	5.40	1.69	1.57
7	Q	502	TA1	C18-C10	5.40	1.69	1.57
7	B	502	TA1	C18-C10	5.39	1.69	1.57
7	M	502	TA1	C18-C10	5.37	1.69	1.57
7	O	502	TA1	C18-C10	5.36	1.69	1.57
7	D	502	TA1	C18-C10	5.35	1.69	1.57
7	F	502	TA1	C18-C10	5.32	1.68	1.57
7	H	502	TA1	C09-C04	4.90	1.46	1.39
7	S	502	TA1	C09-C04	4.87	1.46	1.39
8	d	401	ANP	PG-O1G	4.85	1.53	1.46
7	F	502	TA1	C09-C04	4.85	1.46	1.39
7	M	502	TA1	C09-C04	4.85	1.46	1.39
7	D	502	TA1	C09-C04	4.85	1.46	1.39
8	b	401	ANP	PG-O1G	4.82	1.53	1.46
7	Q	502	TA1	C09-C04	4.82	1.46	1.39
8	e	401	ANP	PG-O1G	4.81	1.53	1.46
7	J	502	TA1	C09-C04	4.81	1.46	1.39
7	B	502	TA1	C09-C04	4.81	1.46	1.39
8	a	401	ANP	PG-O1G	4.80	1.53	1.46
7	O	502	TA1	C09-C04	4.77	1.46	1.39
8	c	401	ANP	PG-O1G	4.77	1.53	1.46
8	g	401	ANP	PG-O1G	4.77	1.53	1.46
8	f	401	ANP	PG-O1G	4.76	1.53	1.46
8	K	501	ANP	PG-O1G	4.74	1.53	1.46
8	h	401	ANP	PG-O1G	4.71	1.53	1.46
7	J	502	TA1	C45-C24	4.27	1.61	1.54
7	S	502	TA1	C45-C24	4.25	1.61	1.54
7	H	502	TA1	C45-C24	4.23	1.61	1.54
7	Q	502	TA1	C45-C24	4.22	1.61	1.54
7	D	502	TA1	C45-C24	4.21	1.61	1.54
7	B	502	TA1	C45-C24	4.20	1.61	1.54
7	O	502	TA1	C45-C24	4.20	1.61	1.54
7	F	502	TA1	C45-C24	4.19	1.61	1.54
7	M	502	TA1	C45-C24	4.18	1.61	1.54
8	h	401	ANP	PA-O5'	4.00	1.75	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	501	ANP	PA-O5'	3.99	1.75	1.59
8	e	401	ANP	PA-O5'	3.98	1.75	1.59
8	b	401	ANP	PA-O5'	3.98	1.75	1.59
8	c	401	ANP	PA-O5'	3.98	1.75	1.59
8	d	401	ANP	PA-O5'	3.97	1.74	1.59
8	f	401	ANP	PA-O5'	3.97	1.74	1.59
8	g	401	ANP	PA-O5'	3.96	1.74	1.59
8	a	401	ANP	PA-O5'	3.95	1.74	1.59
7	S	502	TA1	C36-C31	3.80	1.45	1.39
7	H	502	TA1	C36-C31	3.78	1.45	1.39
7	J	502	TA1	C36-C31	3.77	1.45	1.39
7	M	502	TA1	C36-C31	3.77	1.45	1.39
7	F	502	TA1	C36-C31	3.76	1.45	1.39
7	Q	502	TA1	C36-C31	3.76	1.45	1.39
7	O	502	TA1	C36-C31	3.76	1.45	1.39
7	B	502	TA1	C36-C31	3.74	1.45	1.39
7	D	502	TA1	C36-C31	3.74	1.45	1.39
7	D	502	TA1	O02-C03	3.55	1.41	1.34
7	O	502	TA1	O02-C03	3.54	1.41	1.34
7	S	502	TA1	O02-C03	3.54	1.41	1.34
7	B	502	TA1	O02-C03	3.52	1.41	1.34
7	J	502	TA1	O02-C03	3.51	1.41	1.34
7	M	502	TA1	O02-C03	3.51	1.41	1.34
7	Q	502	TA1	O02-C03	3.51	1.41	1.34
7	H	502	TA1	O02-C03	3.51	1.41	1.34
7	F	502	TA1	O02-C03	3.50	1.41	1.34
7	D	502	TA1	C25-C24	3.47	1.39	1.34
7	O	502	TA1	C25-C24	3.45	1.39	1.34
7	F	502	TA1	C25-C24	3.40	1.39	1.34
7	S	502	TA1	C25-C24	3.39	1.39	1.34
7	H	502	TA1	C25-C24	3.38	1.39	1.34
7	M	502	TA1	C25-C24	3.37	1.39	1.34
7	Q	502	TA1	C25-C24	3.34	1.39	1.34
7	B	502	TA1	C25-C24	3.33	1.39	1.34
7	F	502	TA1	C46-C45	3.32	1.60	1.53
7	O	502	TA1	C46-C45	3.31	1.60	1.53
7	J	502	TA1	C25-C24	3.31	1.39	1.34
7	J	502	TA1	C46-C45	3.29	1.60	1.53
7	D	502	TA1	C46-C45	3.27	1.60	1.53
7	H	502	TA1	C46-C45	3.26	1.60	1.53
7	Q	502	TA1	C46-C45	3.26	1.60	1.53
7	B	502	TA1	C46-C45	3.25	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	502	TA1	C46-C45	3.25	1.60	1.53
7	S	502	TA1	C46-C45	3.22	1.60	1.53
7	B	502	TA1	C11-C10	3.18	1.61	1.54
7	B	502	TA1	C43-C01	3.18	1.60	1.54
8	d	401	ANP	O5'-C5'	-3.18	1.32	1.44
8	b	401	ANP	O5'-C5'	-3.18	1.32	1.44
8	g	401	ANP	O5'-C5'	-3.18	1.32	1.44
8	a	401	ANP	O5'-C5'	-3.18	1.32	1.44
8	e	401	ANP	O5'-C5'	-3.17	1.32	1.44
7	S	502	TA1	C11-C10	3.17	1.61	1.54
8	h	401	ANP	O5'-C5'	-3.17	1.32	1.44
7	S	502	TA1	C43-C01	3.16	1.60	1.54
8	K	501	ANP	O5'-C5'	-3.16	1.32	1.44
8	c	401	ANP	O5'-C5'	-3.16	1.32	1.44
8	f	401	ANP	O5'-C5'	-3.16	1.32	1.44
7	O	502	TA1	C43-C01	3.16	1.60	1.54
7	O	502	TA1	C11-C10	3.15	1.61	1.54
7	Q	502	TA1	C11-C10	3.15	1.61	1.54
7	H	502	TA1	C43-C01	3.15	1.60	1.54
7	J	502	TA1	C43-C01	3.15	1.60	1.54
7	F	502	TA1	C11-C10	3.14	1.61	1.54
7	Q	502	TA1	C43-C01	3.13	1.60	1.54
7	F	502	TA1	C43-C01	3.13	1.60	1.54
7	M	502	TA1	C43-C01	3.13	1.60	1.54
7	D	502	TA1	C43-C01	3.13	1.60	1.54
7	D	502	TA1	C11-C10	3.12	1.61	1.54
7	M	502	TA1	C11-C10	3.12	1.61	1.54
7	H	502	TA1	C11-C10	3.11	1.61	1.54
7	J	502	TA1	C11-C10	3.11	1.61	1.54
6	J	501	GDP	C6-N1	-3.05	1.33	1.38
6	S	501	GDP	C6-N1	-3.05	1.33	1.38
6	Q	501	GDP	C6-N1	-3.04	1.33	1.38
6	F	501	GDP	C6-N1	-3.04	1.33	1.38
6	H	501	GDP	C6-N1	-3.03	1.33	1.38
6	O	501	GDP	C6-N1	-3.03	1.33	1.38
6	M	501	GDP	C6-N1	-3.01	1.33	1.38
6	B	501	GDP	C6-N1	-2.98	1.33	1.38
6	D	501	GDP	C6-N1	-2.98	1.33	1.38
7	O	502	TA1	C43-C26	2.97	1.58	1.52
7	F	502	TA1	C43-C26	2.95	1.58	1.52
7	Q	502	TA1	C43-C26	2.94	1.58	1.52
7	B	502	TA1	C43-C26	2.93	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	502	TA1	C43-C26	2.92	1.58	1.52
7	J	502	TA1	C43-C26	2.92	1.58	1.52
7	M	502	TA1	C43-C26	2.92	1.58	1.52
7	S	502	TA1	C43-C26	2.91	1.58	1.52
7	D	502	TA1	C43-C26	2.90	1.58	1.52
7	Q	502	TA1	C26-C25	2.70	1.56	1.51
7	J	502	TA1	C26-C25	2.68	1.56	1.51
7	H	502	TA1	C26-C25	2.68	1.56	1.51
7	M	502	TA1	C26-C25	2.67	1.56	1.51
6	O	501	GDP	C5-C4	2.66	1.46	1.38
6	D	501	GDP	C5-C4	2.66	1.46	1.38
7	F	502	TA1	C26-C25	2.65	1.56	1.51
6	J	501	GDP	C5-C4	2.65	1.46	1.38
6	B	501	GDP	C5-C4	2.65	1.46	1.38
7	O	502	TA1	C26-C25	2.64	1.56	1.51
7	S	502	TA1	C26-C25	2.64	1.56	1.51
6	H	501	GDP	C4-N9	-2.64	1.31	1.38
6	H	501	GDP	C5-C4	2.63	1.45	1.38
7	B	502	TA1	C26-C25	2.63	1.56	1.51
6	M	501	GDP	C5-C4	2.63	1.45	1.38
6	S	501	GDP	C5-C4	2.62	1.45	1.38
7	D	502	TA1	C26-C25	2.62	1.56	1.51
6	J	501	GDP	C4-N9	-2.62	1.31	1.38
6	Q	501	GDP	C5-C4	2.62	1.45	1.38
7	M	502	TA1	C01-C45	2.62	1.66	1.56
6	F	501	GDP	C5-C4	2.61	1.45	1.38
6	B	501	GDP	C4-N9	-2.60	1.31	1.38
6	D	501	GDP	C4-N9	-2.59	1.31	1.38
6	M	501	GDP	C4-N9	-2.59	1.31	1.38
7	Q	502	TA1	C01-C45	2.58	1.66	1.56
7	S	502	TA1	C01-C45	2.58	1.66	1.56
6	O	501	GDP	C4-N9	-2.58	1.31	1.38
6	Q	501	GDP	C4-N9	-2.58	1.31	1.38
7	O	502	TA1	C01-C45	2.57	1.66	1.56
6	S	501	GDP	C4-N9	-2.57	1.31	1.38
6	F	501	GDP	C4-N9	-2.57	1.31	1.38
7	D	502	TA1	C01-C45	2.57	1.66	1.56
7	H	502	TA1	C01-C45	2.57	1.66	1.56
7	B	502	TA1	C01-C45	2.56	1.66	1.56
7	F	502	TA1	C18-C20	2.56	1.62	1.55
7	J	502	TA1	C01-C45	2.56	1.66	1.56
7	M	502	TA1	C18-C20	2.56	1.62	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	502	TA1	C18-C20	2.56	1.62	1.55
7	F	502	TA1	C01-C45	2.55	1.66	1.56
7	D	502	TA1	C18-C20	2.55	1.62	1.55
7	Q	502	TA1	C18-C20	2.53	1.62	1.55
7	B	502	TA1	C18-C20	2.53	1.62	1.55
7	J	502	TA1	C18-C20	2.53	1.62	1.55
7	S	502	TA1	C18-C20	2.53	1.62	1.55
7	H	502	TA1	C18-C20	2.52	1.62	1.55
8	g	401	ANP	PB-N3B	2.51	1.69	1.63
8	b	401	ANP	PB-N3B	2.50	1.69	1.63
8	d	401	ANP	PB-N3B	2.49	1.69	1.63
7	B	502	TA1	C04-C03	-2.49	1.44	1.50
8	K	501	ANP	PB-N3B	2.49	1.69	1.63
7	H	502	TA1	C04-C03	-2.48	1.44	1.50
8	c	401	ANP	PB-N3B	2.48	1.69	1.63
8	e	401	ANP	PB-N3B	2.47	1.69	1.63
8	f	401	ANP	PB-N3B	2.47	1.69	1.63
7	Q	502	TA1	C04-C03	-2.46	1.44	1.50
8	h	401	ANP	PB-N3B	2.46	1.69	1.63
8	a	401	ANP	PB-N3B	2.45	1.69	1.63
7	J	502	TA1	C04-C03	-2.45	1.44	1.50
7	M	502	TA1	C04-C03	-2.45	1.44	1.50
7	O	502	TA1	C41-C42	2.45	1.43	1.38
7	S	502	TA1	C04-C03	-2.44	1.44	1.50
7	D	502	TA1	C04-C03	-2.43	1.44	1.50
6	D	501	GDP	C5-N7	-2.43	1.34	1.39
7	F	502	TA1	C04-C03	-2.42	1.44	1.50
6	H	501	GDP	C5-N7	-2.42	1.34	1.39
6	B	501	GDP	C5-N7	-2.42	1.34	1.39
6	S	501	GDP	C5-N7	-2.42	1.34	1.39
7	O	502	TA1	C04-C03	-2.40	1.44	1.50
6	M	501	GDP	C5-N7	-2.40	1.34	1.39
6	F	501	GDP	C5-N7	-2.40	1.34	1.39
7	B	502	TA1	C41-C42	2.39	1.43	1.38
6	Q	501	GDP	C5-N7	-2.38	1.34	1.39
6	O	501	GDP	C5-N7	-2.38	1.34	1.39
7	J	502	TA1	C41-C42	2.37	1.43	1.38
8	c	401	ANP	PG-O3G	-2.37	1.50	1.56
6	J	501	GDP	C5-N7	-2.37	1.34	1.39
8	a	401	ANP	PG-O3G	-2.37	1.50	1.56
8	g	401	ANP	PG-O3G	-2.36	1.50	1.56
7	F	502	TA1	C16-C15	2.36	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	502	TA1	C16-C15	2.35	1.57	1.52
7	D	502	TA1	C41-C42	2.35	1.42	1.38
7	M	502	TA1	C41-C42	2.35	1.42	1.38
8	f	401	ANP	PG-O3G	-2.35	1.50	1.56
8	e	401	ANP	PG-O3G	-2.35	1.50	1.56
7	S	502	TA1	C41-C42	2.34	1.42	1.38
7	J	502	TA1	C16-C15	2.34	1.57	1.52
7	H	502	TA1	C41-C42	2.34	1.42	1.38
7	F	502	TA1	C41-C42	2.34	1.42	1.38
8	d	401	ANP	PG-O3G	-2.33	1.50	1.56
7	S	502	TA1	C16-C15	2.33	1.57	1.52
8	d	401	ANP	C5-N7	-2.33	1.34	1.39
8	K	501	ANP	PG-O3G	-2.32	1.50	1.56
8	b	401	ANP	PG-O3G	-2.32	1.50	1.56
8	h	401	ANP	PG-O3G	-2.32	1.50	1.56
7	Q	502	TA1	C41-C42	2.32	1.42	1.38
8	g	401	ANP	C5-N7	-2.31	1.34	1.39
8	f	401	ANP	C5-N7	-2.31	1.34	1.39
7	M	502	TA1	C16-C15	2.30	1.56	1.52
8	b	401	ANP	C5-N7	-2.29	1.34	1.39
7	O	502	TA1	C16-C15	2.29	1.56	1.52
7	Q	502	TA1	C16-C15	2.29	1.56	1.52
8	c	401	ANP	C5-N7	-2.28	1.34	1.39
7	B	502	TA1	C16-C15	2.28	1.56	1.52
8	h	401	ANP	C5-N7	-2.27	1.34	1.39
8	K	501	ANP	C5-N7	-2.26	1.34	1.39
8	e	401	ANP	C5-N7	-2.26	1.35	1.39
8	a	401	ANP	C5-N7	-2.25	1.35	1.39
7	F	502	TA1	C37-C29	2.24	1.54	1.52
7	D	502	TA1	C16-C15	2.24	1.56	1.52
7	M	502	TA1	C37-C29	2.24	1.54	1.52
7	Q	502	TA1	C37-C29	2.22	1.54	1.52
7	J	502	TA1	C37-C29	2.21	1.54	1.52
4	I	501	GTP	C5-N7	-2.20	1.34	1.39
7	H	502	TA1	C37-C29	2.19	1.54	1.52
7	D	502	TA1	C37-C29	2.18	1.54	1.52
7	O	502	TA1	C37-C29	2.18	1.54	1.52
8	c	401	ANP	C1'-N9	-2.17	1.40	1.46
7	D	502	TA1	C06-C05	2.17	1.42	1.38
7	S	502	TA1	C06-C05	2.16	1.42	1.38
8	f	401	ANP	C1'-N9	-2.16	1.40	1.46
8	g	401	ANP	C1'-N9	-2.16	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	502	TA1	C06-C05	2.15	1.42	1.38
7	B	502	TA1	C37-C29	2.15	1.54	1.52
8	K	501	ANP	C1'-N9	-2.15	1.40	1.46
8	b	401	ANP	C1'-N9	-2.15	1.40	1.46
7	Q	502	TA1	C10-C02	2.15	1.62	1.57
7	F	502	TA1	C10-C02	2.14	1.62	1.57
7	J	502	TA1	O09-C21	2.14	1.49	1.44
7	D	502	TA1	C10-C02	2.14	1.62	1.57
8	d	401	ANP	C1'-N9	-2.14	1.40	1.46
4	C	501	GTP	C5-N7	-2.14	1.34	1.39
7	S	502	TA1	C37-C29	2.14	1.54	1.52
7	H	502	TA1	C10-C02	2.14	1.62	1.57
7	H	502	TA1	O09-C21	2.14	1.49	1.44
7	S	502	TA1	C08-C07	2.14	1.42	1.38
4	P	501	GTP	C5-N7	-2.13	1.34	1.39
7	D	502	TA1	O09-C21	2.13	1.49	1.44
8	a	401	ANP	C1'-N9	-2.13	1.40	1.46
7	D	502	TA1	C08-C07	2.13	1.42	1.38
8	h	401	ANP	C1'-N9	-2.13	1.40	1.46
7	M	502	TA1	O09-C21	2.13	1.49	1.44
7	B	502	TA1	C10-C02	2.13	1.62	1.57
8	e	401	ANP	C1'-N9	-2.13	1.40	1.46
7	B	502	TA1	O09-C21	2.13	1.49	1.44
7	M	502	TA1	C10-C02	2.13	1.62	1.57
7	H	502	TA1	C06-C05	2.13	1.42	1.38
7	Q	502	TA1	C08-C07	2.12	1.42	1.38
4	A	501	GTP	C5-N7	-2.12	1.34	1.39
7	D	502	TA1	C33-C32	2.12	1.42	1.38
7	M	502	TA1	C06-C05	2.12	1.42	1.38
7	O	502	TA1	O09-C21	2.11	1.49	1.44
7	M	502	TA1	C33-C32	2.11	1.42	1.38
4	L	501	GTP	C5-N7	-2.11	1.34	1.39
7	O	502	TA1	C10-C02	2.11	1.62	1.57
7	F	502	TA1	C08-C07	2.11	1.42	1.38
7	O	502	TA1	C06-C05	2.11	1.42	1.38
4	N	501	GTP	C5-N7	-2.11	1.34	1.39
7	J	502	TA1	C06-C05	2.11	1.42	1.38
7	J	502	TA1	C08-C07	2.10	1.42	1.38
7	J	502	TA1	C10-C02	2.10	1.62	1.57
7	B	502	TA1	C06-C05	2.10	1.42	1.38
7	O	502	TA1	C33-C32	2.10	1.42	1.38
7	F	502	TA1	O09-C21	2.10	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	502	TA1	C08-C07	2.10	1.42	1.38
7	S	502	TA1	C10-C02	2.10	1.62	1.57
7	B	502	TA1	C08-C07	2.10	1.42	1.38
7	F	502	TA1	C39-C38	2.10	1.42	1.38
7	S	502	TA1	C39-C38	2.10	1.42	1.38
4	G	501	GTP	C5-N7	-2.10	1.34	1.39
4	R	501	GTP	C5-N7	-2.09	1.34	1.39
7	S	502	TA1	O09-C21	2.09	1.49	1.44
7	O	502	TA1	C08-C07	2.09	1.42	1.38
7	H	502	TA1	C08-C07	2.08	1.42	1.38
7	O	502	TA1	C39-C38	2.08	1.42	1.38
7	F	502	TA1	C33-C32	2.07	1.42	1.38
7	Q	502	TA1	C39-C38	2.07	1.42	1.38
8	b	401	ANP	O4'-C1'	2.07	1.46	1.42
4	E	501	GTP	C5-N7	-2.07	1.34	1.39
7	Q	502	TA1	C06-C05	2.07	1.42	1.38
7	J	502	TA1	C33-C32	2.06	1.42	1.38
7	J	502	TA1	C39-C38	2.06	1.42	1.38
7	Q	502	TA1	O09-C21	2.06	1.49	1.44
8	f	401	ANP	O4'-C1'	2.06	1.46	1.42
8	g	401	ANP	O4'-C1'	2.06	1.46	1.42
8	a	401	ANP	PG-O2G	-2.05	1.51	1.56
7	H	502	TA1	C33-C32	2.05	1.42	1.38
7	B	502	TA1	C33-C32	2.05	1.42	1.38
7	H	502	TA1	C39-C38	2.05	1.42	1.38
8	a	401	ANP	O4'-C1'	2.05	1.46	1.42
8	e	401	ANP	O4'-C1'	2.04	1.46	1.42
7	M	502	TA1	C39-C38	2.04	1.42	1.38
7	D	502	TA1	C39-C38	2.04	1.42	1.38
7	B	502	TA1	C39-C38	2.04	1.42	1.38
8	b	401	ANP	PG-O2G	-2.03	1.51	1.56
8	h	401	ANP	PG-O2G	-2.03	1.51	1.56
7	J	502	TA1	C34-C33	2.03	1.42	1.38
8	c	401	ANP	PG-O2G	-2.02	1.51	1.56
8	d	401	ANP	O4'-C1'	2.02	1.46	1.42
7	S	502	TA1	C34-C33	2.02	1.42	1.38
8	c	401	ANP	O4'-C1'	2.02	1.46	1.42
7	S	502	TA1	C33-C32	2.02	1.42	1.38
7	O	502	TA1	O02-C02	2.02	1.48	1.45
8	K	501	ANP	O4'-C1'	2.02	1.46	1.42
8	d	401	ANP	PG-O2G	-2.01	1.51	1.56
8	g	401	ANP	PG-O2G	-2.01	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	401	ANP	O4'-C1'	2.01	1.46	1.42
7	Q	502	TA1	C33-C32	2.01	1.42	1.38
7	B	502	TA1	C34-C33	2.01	1.42	1.38
7	M	502	TA1	C18-C17	2.00	1.61	1.55
7	M	502	TA1	O02-C02	2.00	1.48	1.45

All (458) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	401	ANP	C5'-C4'-C3'	-7.56	88.00	115.21
8	e	401	ANP	C5'-C4'-C3'	-7.56	88.01	115.21
8	a	401	ANP	C5'-C4'-C3'	-7.55	88.02	115.21
8	d	401	ANP	C5'-C4'-C3'	-7.55	88.03	115.21
8	K	501	ANP	C5'-C4'-C3'	-7.55	88.03	115.21
8	c	401	ANP	C5'-C4'-C3'	-7.55	88.05	115.21
8	h	401	ANP	C5'-C4'-C3'	-7.55	88.05	115.21
8	b	401	ANP	C5'-C4'-C3'	-7.54	88.08	115.21
8	g	401	ANP	C5'-C4'-C3'	-7.53	88.10	115.21
8	g	401	ANP	O5'-C5'-C4'	6.02	129.50	108.99
8	b	401	ANP	O5'-C5'-C4'	6.02	129.48	108.99
8	h	401	ANP	O5'-C5'-C4'	6.01	129.46	108.99
8	a	401	ANP	O5'-C5'-C4'	6.00	129.42	108.99
8	K	501	ANP	O5'-C5'-C4'	5.99	129.40	108.99
8	d	401	ANP	O5'-C5'-C4'	5.99	129.38	108.99
8	f	401	ANP	O5'-C5'-C4'	5.99	129.38	108.99
8	e	401	ANP	O5'-C5'-C4'	5.99	129.38	108.99
8	c	401	ANP	O5'-C5'-C4'	5.98	129.37	108.99
8	d	401	ANP	O4'-C1'-N9	5.95	119.51	108.09
8	K	501	ANP	O4'-C1'-N9	5.94	119.50	108.09
8	e	401	ANP	O4'-C1'-N9	5.93	119.49	108.09
8	h	401	ANP	O4'-C1'-N9	5.93	119.47	108.09
8	b	401	ANP	O4'-C1'-N9	5.92	119.45	108.09
8	g	401	ANP	O4'-C1'-N9	5.92	119.45	108.09
7	B	502	TA1	C07-C06-C05	5.91	127.53	120.24
8	c	401	ANP	O4'-C1'-N9	5.91	119.44	108.09
7	F	502	TA1	C08-C09-C04	-5.91	114.56	120.36
8	a	401	ANP	O4'-C1'-N9	5.90	119.42	108.09
8	f	401	ANP	O4'-C1'-N9	5.90	119.42	108.09
7	O	502	TA1	C08-C09-C04	-5.88	114.59	120.36
7	D	502	TA1	C07-C06-C05	5.87	127.49	120.24
7	H	502	TA1	C08-C09-C04	-5.87	114.60	120.36
7	O	502	TA1	C07-C06-C05	5.87	127.48	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	502	TA1	C08-C09-C04	-5.87	114.60	120.36
7	B	502	TA1	C08-C09-C04	-5.85	114.61	120.36
7	F	502	TA1	C07-C06-C05	5.85	127.46	120.24
7	J	502	TA1	C07-C06-C05	5.85	127.46	120.24
7	D	502	TA1	C08-C09-C04	-5.85	114.62	120.36
7	S	502	TA1	C07-C06-C05	5.85	127.45	120.24
7	H	502	TA1	C07-C06-C05	5.84	127.45	120.24
7	M	502	TA1	C07-C06-C05	5.84	127.45	120.24
7	Q	502	TA1	C08-C09-C04	-5.84	114.62	120.36
7	Q	502	TA1	C07-C06-C05	5.83	127.44	120.24
7	J	502	TA1	C08-C09-C04	-5.82	114.64	120.36
7	M	502	TA1	C08-C09-C04	-5.80	114.67	120.36
6	Q	501	GDP	C5-C4-N3	-5.36	119.86	128.39
8	b	401	ANP	C5-C4-N3	-5.35	119.34	126.72
6	D	501	GDP	C5-C4-N3	-5.35	119.87	128.39
6	J	501	GDP	C5-C4-N3	-5.35	119.88	128.39
8	a	401	ANP	C5-C4-N3	-5.35	119.36	126.72
6	H	501	GDP	C5-C4-N3	-5.35	119.88	128.39
6	O	501	GDP	C5-C4-N3	-5.34	119.89	128.39
6	B	501	GDP	C5-C4-N3	-5.33	119.90	128.39
8	K	501	ANP	C5-C4-N3	-5.33	119.38	126.72
6	M	501	GDP	C5-C4-N3	-5.32	119.92	128.39
8	g	401	ANP	C5-C4-N3	-5.32	119.39	126.72
8	h	401	ANP	C5-C4-N3	-5.31	119.41	126.72
6	F	501	GDP	C5-C4-N3	-5.31	119.94	128.39
8	c	401	ANP	C5-C4-N3	-5.31	119.41	126.72
8	f	401	ANP	C5-C4-N3	-5.29	119.43	126.72
6	S	501	GDP	C5-C4-N3	-5.29	119.98	128.39
8	e	401	ANP	C5-C4-N3	-5.28	119.45	126.72
8	d	401	ANP	C5-C4-N3	-5.27	119.47	126.72
8	K	501	ANP	O3A-PB-N3B	-5.26	92.01	106.59
8	e	401	ANP	O3A-PB-N3B	-5.25	92.03	106.59
8	d	401	ANP	O3A-PB-N3B	-5.25	92.04	106.59
8	b	401	ANP	O3A-PB-N3B	-5.24	92.04	106.59
8	g	401	ANP	O3A-PB-N3B	-5.24	92.04	106.59
8	h	401	ANP	O3A-PB-N3B	-5.24	92.05	106.59
8	f	401	ANP	O3A-PB-N3B	-5.24	92.06	106.59
8	a	401	ANP	O3A-PB-N3B	-5.24	92.06	106.59
8	c	401	ANP	O3A-PB-N3B	-5.23	92.08	106.59
8	b	401	ANP	N3-C2-N1	-5.11	120.84	128.58
8	g	401	ANP	N3-C2-N1	-5.11	120.84	128.58
8	K	501	ANP	N3-C2-N1	-5.09	120.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	c	401	ANP	N3-C2-N1	-5.09	120.88	128.58
8	a	401	ANP	N3-C2-N1	-5.09	120.88	128.58
8	f	401	ANP	N3-C2-N1	-5.08	120.89	128.58
8	d	401	ANP	N3-C2-N1	-5.07	120.90	128.58
8	e	401	ANP	N3-C2-N1	-5.07	120.91	128.58
8	h	401	ANP	N3-C2-N1	-5.07	120.91	128.58
8	f	401	ANP	O2A-PA-O3A	5.07	120.97	107.27
8	h	401	ANP	O2A-PA-O3A	5.07	120.97	107.27
8	K	501	ANP	O2A-PA-O3A	5.06	120.94	107.27
8	b	401	ANP	O2A-PA-O3A	5.06	120.94	107.27
8	a	401	ANP	O2A-PA-O3A	5.05	120.93	107.27
8	c	401	ANP	O2A-PA-O3A	5.05	120.93	107.27
8	e	401	ANP	O2A-PA-O3A	5.05	120.93	107.27
8	g	401	ANP	O2A-PA-O3A	5.05	120.93	107.27
8	d	401	ANP	O2A-PA-O3A	5.04	120.89	107.27
8	b	401	ANP	N3-C4-N9	4.90	135.50	127.17
8	a	401	ANP	N3-C4-N9	4.89	135.48	127.17
8	g	401	ANP	N3-C4-N9	4.88	135.47	127.17
8	K	501	ANP	N3-C4-N9	4.86	135.44	127.17
8	c	401	ANP	N3-C4-N9	4.85	135.41	127.17
8	f	401	ANP	N3-C4-N9	4.84	135.41	127.17
8	h	401	ANP	N3-C4-N9	4.84	135.40	127.17
8	e	401	ANP	N3-C4-N9	4.84	135.40	127.17
8	g	401	ANP	O2A-PA-O5'	-4.84	85.63	107.57
8	c	401	ANP	O2A-PA-O5'	-4.84	85.64	107.57
8	d	401	ANP	O2A-PA-O5'	-4.84	85.64	107.57
8	e	401	ANP	O2A-PA-O5'	-4.84	85.65	107.57
8	b	401	ANP	O2A-PA-O5'	-4.83	85.65	107.57
8	h	401	ANP	O2A-PA-O5'	-4.83	85.67	107.57
8	d	401	ANP	N3-C4-N9	4.83	135.38	127.17
8	a	401	ANP	O2A-PA-O5'	-4.83	85.67	107.57
8	K	501	ANP	O2A-PA-O5'	-4.83	85.68	107.57
8	f	401	ANP	O2A-PA-O5'	-4.82	85.70	107.57
8	K	501	ANP	O5'-PA-O1A	-4.70	90.32	108.94
8	h	401	ANP	O5'-PA-O1A	-4.69	90.33	108.94
8	g	401	ANP	O5'-PA-O1A	-4.69	90.34	108.94
8	e	401	ANP	O5'-PA-O1A	-4.68	90.37	108.94
8	d	401	ANP	O5'-PA-O1A	-4.68	90.37	108.94
8	c	401	ANP	O5'-PA-O1A	-4.68	90.38	108.94
8	b	401	ANP	O5'-PA-O1A	-4.68	90.38	108.94
8	f	401	ANP	O5'-PA-O1A	-4.68	90.38	108.94
8	a	401	ANP	O5'-PA-O1A	-4.68	90.40	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	C2-N3-C4	4.39	119.86	112.30
6	D	501	GDP	C2-N3-C4	4.38	119.85	112.30
6	O	501	GDP	C2-N3-C4	4.38	119.85	112.30
6	M	501	GDP	C2-N3-C4	4.37	119.83	112.30
6	J	501	GDP	C2-N3-C4	4.37	119.83	112.30
4	P	501	GTP	C5-C4-N3	-4.37	121.44	128.39
6	H	501	GDP	C2-N3-C4	4.37	119.82	112.30
4	C	501	GTP	C5-C4-N3	-4.36	121.45	128.39
4	N	501	GTP	C5-C4-N3	-4.36	121.45	128.39
6	Q	501	GDP	C2-N3-C4	4.35	119.80	112.30
6	S	501	GDP	C2-N3-C4	4.35	119.79	112.30
4	G	501	GTP	C5-C4-N3	-4.35	121.47	128.39
4	E	501	GTP	C5-C4-N3	-4.34	121.47	128.39
4	A	501	GTP	C5-C4-N3	-4.33	121.50	128.39
4	L	501	GTP	C5-C4-N3	-4.33	121.50	128.39
6	F	501	GDP	C2-N3-C4	4.33	119.75	112.30
4	R	501	GTP	C5-C4-N3	-4.30	121.55	128.39
4	I	501	GTP	C5-C4-N3	-4.26	121.61	128.39
7	F	502	TA1	C09-C04-C03	-4.12	111.32	120.40
7	O	502	TA1	C09-C04-C03	-4.11	111.34	120.40
7	D	502	TA1	C09-C04-C03	-4.10	111.37	120.40
7	S	502	TA1	C09-C04-C03	-4.09	111.37	120.40
7	Q	502	TA1	C09-C04-C03	-4.09	111.37	120.40
4	C	501	GTP	C2-N3-C4	4.09	119.35	112.30
4	E	501	GTP	C2-N3-C4	4.09	119.34	112.30
4	P	501	GTP	C2-N3-C4	4.08	119.33	112.30
7	M	502	TA1	C09-C04-C03	-4.08	111.40	120.40
7	H	502	TA1	C09-C04-C03	-4.08	111.41	120.40
7	B	502	TA1	C09-C04-C03	-4.08	111.41	120.40
4	N	501	GTP	C2-N3-C4	4.07	119.30	112.30
4	G	501	GTP	C2-N3-C4	4.06	119.30	112.30
7	J	502	TA1	C09-C04-C03	-4.06	111.44	120.40
4	A	501	GTP	C2-N3-C4	4.06	119.29	112.30
4	L	501	GTP	C2-N3-C4	4.04	119.26	112.30
4	I	501	GTP	C2-N3-C4	4.01	119.20	112.30
4	R	501	GTP	C2-N3-C4	4.00	119.19	112.30
8	b	401	ANP	C2-N3-C4	4.00	121.61	111.83
8	g	401	ANP	C2-N3-C4	4.00	121.59	111.83
8	a	401	ANP	C2-N3-C4	3.99	121.57	111.83
8	K	501	ANP	C2-N3-C4	3.97	121.54	111.83
8	d	401	ANP	C2-N3-C4	3.97	121.52	111.83
8	f	401	ANP	C2-N3-C4	3.96	121.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	c	401	ANP	C2-N3-C4	3.96	121.50	111.83
6	J	501	GDP	N9-C4-N3	3.96	133.87	125.95
8	h	401	ANP	C2-N3-C4	3.96	121.49	111.83
6	O	501	GDP	N9-C4-N3	3.95	133.85	125.95
8	e	401	ANP	C2-N3-C4	3.95	121.48	111.83
6	D	501	GDP	N9-C4-N3	3.93	133.81	125.95
6	H	501	GDP	N9-C4-N3	3.93	133.81	125.95
6	M	501	GDP	N9-C4-N3	3.93	133.81	125.95
6	B	501	GDP	N9-C4-N3	3.92	133.79	125.95
6	Q	501	GDP	N9-C4-N3	3.92	133.79	125.95
6	S	501	GDP	N9-C4-N3	3.91	133.77	125.95
6	F	501	GDP	N9-C4-N3	3.89	133.73	125.95
8	d	401	ANP	C5-N7-C8	3.69	109.26	103.45
8	c	401	ANP	C5-N7-C8	3.68	109.24	103.45
8	h	401	ANP	C5-N7-C8	3.68	109.23	103.45
8	e	401	ANP	C5-N7-C8	3.67	109.22	103.45
8	f	401	ANP	C5-N7-C8	3.67	109.22	103.45
8	K	501	ANP	C5-N7-C8	3.67	109.22	103.45
8	a	401	ANP	C5-N7-C8	3.66	109.21	103.45
8	g	401	ANP	C5-N7-C8	3.66	109.21	103.45
8	b	401	ANP	C5-N7-C8	3.65	109.18	103.45
7	M	502	TA1	C05-C04-C03	3.65	128.43	120.40
7	Q	502	TA1	C05-C04-C03	3.65	128.43	120.40
7	H	502	TA1	C05-C04-C03	3.64	128.42	120.40
7	S	502	TA1	C05-C04-C03	3.63	128.39	120.40
7	D	502	TA1	C05-C04-C03	3.62	128.38	120.40
7	O	502	TA1	C05-C04-C03	3.62	128.38	120.40
7	F	502	TA1	C05-C04-C03	3.62	128.38	120.40
7	J	502	TA1	C05-C04-C03	3.62	128.38	120.40
7	B	502	TA1	C05-C04-C03	3.62	128.37	120.40
6	O	501	GDP	C6-C5-N7	3.59	136.83	130.29
6	D	501	GDP	C6-C5-N7	3.59	136.82	130.29
6	S	501	GDP	C6-C5-N7	3.59	136.82	130.29
6	B	501	GDP	C6-C5-N7	3.59	136.82	130.29
6	F	501	GDP	C6-C5-N7	3.58	136.81	130.29
6	J	501	GDP	C6-C5-N7	3.57	136.79	130.29
6	H	501	GDP	C6-C5-N7	3.57	136.78	130.29
6	M	501	GDP	C6-C5-N7	3.56	136.76	130.29
6	Q	501	GDP	C6-C5-N7	3.56	136.76	130.29
8	h	401	ANP	N9-C8-N7	-3.46	109.03	113.94
8	g	401	ANP	O2B-PB-O3A	3.45	116.14	104.64
8	g	401	ANP	N9-C8-N7	-3.44	109.05	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	501	ANP	N9-C8-N7	-3.44	109.05	113.94
8	K	501	ANP	O2B-PB-O3A	3.44	116.12	104.64
8	b	401	ANP	O2B-PB-O3A	3.44	116.11	104.64
8	d	401	ANP	O2B-PB-O3A	3.44	116.11	104.64
8	d	401	ANP	N9-C8-N7	-3.43	109.06	113.94
8	a	401	ANP	O2B-PB-O3A	3.43	116.09	104.64
8	f	401	ANP	N9-C8-N7	-3.43	109.08	113.94
8	e	401	ANP	O2B-PB-O3A	3.43	116.08	104.64
8	e	401	ANP	N9-C8-N7	-3.43	109.08	113.94
8	a	401	ANP	N9-C8-N7	-3.42	109.09	113.94
8	h	401	ANP	O2B-PB-O3A	3.42	116.05	104.64
8	c	401	ANP	O2B-PB-O3A	3.41	116.04	104.64
8	f	401	ANP	O2B-PB-O3A	3.41	116.03	104.64
8	c	401	ANP	N9-C8-N7	-3.40	109.12	113.94
8	b	401	ANP	N9-C8-N7	-3.39	109.12	113.94
7	H	502	TA1	C17-C18-C20	3.25	109.87	102.58
7	J	502	TA1	C17-C18-C20	3.24	109.85	102.58
7	Q	502	TA1	C17-C18-C20	3.24	109.85	102.58
7	S	502	TA1	C17-C18-C20	3.23	109.83	102.58
7	B	502	TA1	C17-C18-C20	3.23	109.83	102.58
7	O	502	TA1	C17-C18-C20	3.22	109.81	102.58
7	F	502	TA1	C17-C18-C20	3.22	109.80	102.58
7	M	502	TA1	C17-C18-C20	3.21	109.80	102.58
7	D	502	TA1	C17-C18-C20	3.19	109.74	102.58
8	f	401	ANP	PA-O5'-C5'	-3.13	103.39	121.35
8	d	401	ANP	PA-O5'-C5'	-3.13	103.41	121.35
8	a	401	ANP	PA-O5'-C5'	-3.12	103.44	121.35
8	K	501	ANP	PA-O5'-C5'	-3.12	103.45	121.35
8	c	401	ANP	PA-O5'-C5'	-3.12	103.45	121.35
8	h	401	ANP	PA-O5'-C5'	-3.12	103.45	121.35
8	e	401	ANP	PA-O5'-C5'	-3.12	103.46	121.35
8	g	401	ANP	PA-O5'-C5'	-3.12	103.48	121.35
8	b	401	ANP	PA-O5'-C5'	-3.12	103.49	121.35
4	A	501	GTP	N9-C8-N7	-3.11	107.64	113.40
4	C	501	GTP	N9-C8-N7	-3.10	107.65	113.40
4	P	501	GTP	N9-C8-N7	-3.09	107.67	113.40
4	N	501	GTP	N9-C8-N7	-3.08	107.68	113.40
4	G	501	GTP	N9-C8-N7	-3.08	107.69	113.40
4	L	501	GTP	N9-C8-N7	-3.08	107.70	113.40
4	I	501	GTP	N9-C8-N7	-3.07	107.70	113.40
4	R	501	GTP	N9-C8-N7	-3.06	107.73	113.40
4	E	501	GTP	N9-C8-N7	-3.05	107.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GTP	C2-N1-C6	-2.97	119.73	125.11
4	P	501	GTP	C2-N1-C6	-2.96	119.74	125.11
7	J	502	TA1	O04-C11-C14	-2.96	101.86	108.13
7	H	502	TA1	C45-C01-C02	2.95	115.18	111.93
4	N	501	GTP	C2-N1-C6	-2.95	119.75	125.11
4	R	501	GTP	C2-N1-C6	-2.95	119.75	125.11
7	H	502	TA1	O04-C11-C14	-2.95	101.87	108.13
7	B	502	TA1	O04-C11-C14	-2.95	101.87	108.13
7	S	502	TA1	O04-C11-C14	-2.95	101.87	108.13
7	Q	502	TA1	O04-C11-C14	-2.95	101.88	108.13
7	F	502	TA1	O04-C11-C14	-2.94	101.90	108.13
7	M	502	TA1	O04-C11-C14	-2.94	101.90	108.13
7	O	502	TA1	O04-C11-C14	-2.94	101.90	108.13
7	S	502	TA1	C45-C01-C02	2.94	115.16	111.93
4	L	501	GTP	C2-N1-C6	-2.93	119.79	125.11
7	D	502	TA1	O04-C11-C14	-2.93	101.92	108.13
7	F	502	TA1	C45-C01-C02	2.93	115.15	111.93
4	I	501	GTP	C2-N1-C6	-2.92	119.81	125.11
4	A	501	GTP	C2-N1-C6	-2.91	119.83	125.11
7	J	502	TA1	C45-C01-C02	2.91	115.13	111.93
7	D	502	TA1	C45-C01-C02	2.91	115.13	111.93
4	E	501	GTP	C2-N1-C6	-2.90	119.84	125.11
4	G	501	GTP	C2-N1-C6	-2.90	119.84	125.11
7	B	502	TA1	C45-C01-C02	2.90	115.11	111.93
7	Q	502	TA1	C45-C01-C02	2.89	115.11	111.93
7	M	502	TA1	C45-C01-C02	2.86	115.07	111.93
7	O	502	TA1	C45-C01-C02	2.85	115.06	111.93
4	G	501	GTP	N9-C4-N3	2.81	131.57	125.95
4	C	501	GTP	N9-C4-N3	2.81	131.57	125.95
4	E	501	GTP	N9-C4-N3	2.80	131.56	125.95
4	N	501	GTP	N9-C4-N3	2.80	131.55	125.95
4	A	501	GTP	N9-C4-N3	2.79	131.53	125.95
4	P	501	GTP	N9-C4-N3	2.78	131.52	125.95
8	g	401	ANP	C2'-C1'-N9	-2.77	106.42	113.30
8	d	401	ANP	C2'-C1'-N9	-2.76	106.44	113.30
8	e	401	ANP	C2'-C1'-N9	-2.76	106.44	113.30
8	b	401	ANP	C2'-C1'-N9	-2.76	106.45	113.30
4	R	501	GTP	N9-C4-N3	2.76	131.47	125.95
8	a	401	ANP	C2'-C1'-N9	-2.76	106.45	113.30
4	L	501	GTP	N9-C4-N3	2.76	131.47	125.95
8	h	401	ANP	C2'-C1'-N9	-2.75	106.46	113.30
4	I	501	GTP	N9-C4-N3	2.75	131.45	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	501	ANP	C2'-C1'-N9	-2.74	106.48	113.30
8	c	401	ANP	C2'-C1'-N9	-2.74	106.49	113.30
8	f	401	ANP	C2'-C1'-N9	-2.73	106.51	113.30
8	d	401	ANP	O2A-PA-O1A	2.73	125.16	112.44
8	f	401	ANP	O2A-PA-O1A	2.73	125.13	112.44
8	a	401	ANP	O2A-PA-O1A	2.72	125.11	112.44
8	K	501	ANP	O2A-PA-O1A	2.72	125.10	112.44
8	h	401	ANP	O2A-PA-O1A	2.72	125.09	112.44
8	g	401	ANP	O2A-PA-O1A	2.71	125.04	112.44
8	b	401	ANP	O1G-PG-N3B	2.71	115.76	111.77
8	c	401	ANP	O2A-PA-O1A	2.71	125.04	112.44
8	b	401	ANP	O2A-PA-O1A	2.70	125.03	112.44
8	e	401	ANP	O2A-PA-O1A	2.70	125.02	112.44
8	K	501	ANP	O1G-PG-N3B	2.70	115.75	111.77
8	h	401	ANP	O1G-PG-N3B	2.70	115.74	111.77
8	d	401	ANP	O1G-PG-N3B	2.69	115.74	111.77
8	f	401	ANP	O1G-PG-N3B	2.69	115.73	111.77
8	e	401	ANP	O1G-PG-N3B	2.69	115.73	111.77
8	g	401	ANP	O1G-PG-N3B	2.69	115.73	111.77
8	a	401	ANP	O4'-C4'-C5'	-2.68	100.74	109.33
8	e	401	ANP	O4'-C4'-C5'	-2.68	100.74	109.33
8	h	401	ANP	O4'-C4'-C5'	-2.68	100.77	109.33
8	b	401	ANP	O4'-C4'-C5'	-2.67	100.78	109.33
8	c	401	ANP	O4'-C4'-C5'	-2.67	100.78	109.33
8	c	401	ANP	O1G-PG-N3B	2.66	115.69	111.77
8	f	401	ANP	O4'-C4'-C5'	-2.66	100.80	109.33
8	d	401	ANP	O4'-C4'-C5'	-2.66	100.82	109.33
8	g	401	ANP	O4'-C4'-C5'	-2.66	100.83	109.33
8	a	401	ANP	O1G-PG-N3B	2.65	115.68	111.77
8	K	501	ANP	O4'-C4'-C5'	-2.65	100.84	109.33
6	O	501	GDP	C4-C5-N7	-2.64	106.49	110.67
6	D	501	GDP	C4-C5-N7	-2.64	106.49	110.67
8	d	401	ANP	C2'-C3'-C4'	2.64	107.70	102.61
6	H	501	GDP	C4-C5-N7	-2.63	106.50	110.67
6	Q	501	GDP	C4-C5-N7	-2.63	106.50	110.67
8	c	401	ANP	C2'-C3'-C4'	2.63	107.68	102.61
8	a	401	ANP	C2'-C3'-C4'	2.63	107.68	102.61
6	F	501	GDP	C4-C5-N7	-2.62	106.51	110.67
6	J	501	GDP	C4-C5-N7	-2.62	106.52	110.67
8	K	501	ANP	C2'-C3'-C4'	2.62	107.67	102.61
6	B	501	GDP	C4-C5-N7	-2.61	106.53	110.67
8	f	401	ANP	C2'-C3'-C4'	2.60	107.63	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	401	ANP	C2'-C3'-C4'	2.60	107.63	102.61
8	h	401	ANP	C2'-C3'-C4'	2.60	107.62	102.61
8	e	401	ANP	C2'-C3'-C4'	2.59	107.62	102.61
8	g	401	ANP	C2'-C3'-C4'	2.59	107.62	102.61
6	S	501	GDP	C4-C5-N7	-2.59	106.56	110.67
6	M	501	GDP	C4-C5-N7	-2.59	106.57	110.67
7	M	502	TA1	O01-C01-C43	2.51	113.44	107.04
7	S	502	TA1	O01-C01-C43	2.49	113.41	107.04
7	J	502	TA1	O01-C01-C43	2.49	113.39	107.04
7	B	502	TA1	O01-C01-C43	2.48	113.39	107.04
7	H	502	TA1	O01-C01-C43	2.48	113.39	107.04
4	I	501	GTP	O6-C6-C5	-2.48	119.98	126.53
7	B	502	TA1	C06-C05-C04	-2.48	117.93	120.36
7	Q	502	TA1	O01-C01-C43	2.48	113.37	107.04
7	D	502	TA1	O01-C01-C43	2.48	113.37	107.04
8	K	501	ANP	C4-N9-C8	2.48	108.34	105.74
7	D	502	TA1	C06-C05-C04	-2.47	117.93	120.36
7	O	502	TA1	O01-C01-C43	2.47	113.36	107.04
4	R	501	GTP	O6-C6-C5	-2.47	120.01	126.53
7	F	502	TA1	C06-C05-C04	-2.47	117.94	120.36
8	a	401	ANP	C4-N9-C8	2.47	108.33	105.74
4	E	501	GTP	O6-C6-C5	-2.47	120.01	126.53
7	O	502	TA1	C06-C05-C04	-2.47	117.94	120.36
7	F	502	TA1	O01-C01-C43	2.46	113.34	107.04
8	e	401	ANP	C4-N9-C8	2.46	108.32	105.74
8	h	401	ANP	C4-N9-C8	2.46	108.32	105.74
4	P	501	GTP	O6-C6-C5	-2.46	120.04	126.53
4	C	501	GTP	O6-C6-C5	-2.46	120.04	126.53
4	L	501	GTP	O6-C6-C5	-2.45	120.05	126.53
4	N	501	GTP	O6-C6-C5	-2.45	120.06	126.53
4	A	501	GTP	O6-C6-C5	-2.45	120.06	126.53
8	g	401	ANP	C4-N9-C8	2.45	108.31	105.74
4	G	501	GTP	O6-C6-C5	-2.45	120.07	126.53
7	S	502	TA1	C06-C05-C04	-2.44	117.96	120.36
8	b	401	ANP	C4-N9-C8	2.44	108.30	105.74
8	f	401	ANP	C4-N9-C8	2.43	108.29	105.74
7	J	502	TA1	C06-C05-C04	-2.42	117.98	120.36
8	d	401	ANP	C4-N9-C8	2.41	108.27	105.74
4	P	501	GTP	C5-C6-N1	2.41	119.39	113.25
4	C	501	GTP	C5-C6-N1	2.41	119.38	113.25
7	M	502	TA1	C06-C05-C04	-2.41	118.00	120.36
7	H	502	TA1	C06-C05-C04	-2.40	118.01	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	502	TA1	C06-C05-C04	-2.39	118.01	120.36
4	R	501	GTP	C5-C6-N1	2.39	119.34	113.25
8	g	401	ANP	O2G-PG-O1G	-2.39	107.46	113.45
8	c	401	ANP	C4-N9-C8	2.39	108.25	105.74
8	e	401	ANP	O2G-PG-O1G	-2.38	107.47	113.45
4	E	501	GTP	C5-C6-N1	2.38	119.32	113.25
4	I	501	GTP	C5-C6-N1	2.38	119.32	113.25
8	d	401	ANP	O2G-PG-O1G	-2.38	107.48	113.45
8	K	501	ANP	O2G-PG-O1G	-2.38	107.48	113.45
4	A	501	GTP	C5-C6-N1	2.38	119.31	113.25
4	N	501	GTP	C5-C6-N1	2.38	119.30	113.25
8	b	401	ANP	O2G-PG-O1G	-2.37	107.50	113.45
4	L	501	GTP	C5-C6-N1	2.37	119.28	113.25
4	G	501	GTP	C5-C6-N1	2.36	119.26	113.25
8	f	401	ANP	O2G-PG-O1G	-2.36	107.54	113.45
8	c	401	ANP	O2G-PG-O1G	-2.35	107.55	113.45
8	h	401	ANP	O2G-PG-O1G	-2.35	107.55	113.45
8	a	401	ANP	O2G-PG-O1G	-2.35	107.55	113.45
4	C	501	GTP	C8-N7-C5	2.29	108.35	104.26
4	A	501	GTP	C8-N7-C5	2.28	108.33	104.26
4	I	501	GTP	C8-N7-C5	2.26	108.29	104.26
4	P	501	GTP	C8-N7-C5	2.25	108.27	104.26
4	L	501	GTP	C8-N7-C5	2.24	108.26	104.26
4	E	501	GTP	C8-N7-C5	2.24	108.25	104.26
4	N	501	GTP	C8-N7-C5	2.24	108.25	104.26
4	R	501	GTP	C8-N7-C5	2.24	108.25	104.26
4	G	501	GTP	C8-N7-C5	2.23	108.22	104.26
7	J	502	TA1	C14-C11-C15	-2.22	83.09	85.38
7	J	502	TA1	C10-C18-C17	-2.21	102.36	106.55
7	B	502	TA1	C10-C18-C17	-2.20	102.36	106.55
7	S	502	TA1	C10-C18-C17	-2.20	102.37	106.55
7	M	502	TA1	C14-C11-C15	-2.20	83.11	85.38
7	F	502	TA1	C14-C11-C15	-2.20	83.11	85.38
7	B	502	TA1	C14-C11-C15	-2.20	83.11	85.38
7	H	502	TA1	C10-C18-C17	-2.20	102.38	106.55
7	D	502	TA1	C10-C18-C17	-2.19	102.39	106.55
7	M	502	TA1	C10-C18-C17	-2.19	102.39	106.55
7	J	502	TA1	O06-C15-C11	2.19	92.97	90.58
6	F	501	GDP	C2'-C3'-C4'	2.19	106.83	102.61
6	S	501	GDP	C2'-C3'-C4'	2.19	106.83	102.61
7	Q	502	TA1	C14-C11-C15	-2.19	83.12	85.38
7	F	502	TA1	C10-C18-C17	-2.18	102.40	106.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	502	TA1	C14-C11-C15	-2.18	83.13	85.38
7	Q	502	TA1	C10-C18-C17	-2.18	102.41	106.55
7	O	502	TA1	C14-C11-C15	-2.18	83.13	85.38
6	J	501	GDP	C2'-C3'-C4'	2.17	106.81	102.61
6	M	501	GDP	C2'-C3'-C4'	2.17	106.81	102.61
6	D	501	GDP	C2'-C3'-C4'	2.17	106.80	102.61
7	S	502	TA1	O06-C15-C11	2.17	92.95	90.58
6	H	501	GDP	C2'-C3'-C4'	2.17	106.80	102.61
7	S	502	TA1	C14-C11-C15	-2.16	83.15	85.38
7	O	502	TA1	C10-C18-C17	-2.16	102.44	106.55
6	B	501	GDP	C2'-C3'-C4'	2.16	106.78	102.61
7	F	502	TA1	O06-C15-C11	2.16	92.94	90.58
6	O	501	GDP	C2'-C3'-C4'	2.16	106.78	102.61
7	H	502	TA1	C14-C11-C15	-2.16	83.15	85.38
7	D	502	TA1	O06-C15-C11	2.15	92.93	90.58
7	M	502	TA1	O06-C15-C11	2.15	92.93	90.58
7	Q	502	TA1	O06-C15-C11	2.14	92.92	90.58
6	Q	501	GDP	C2'-C3'-C4'	2.14	106.74	102.61
7	O	502	TA1	O06-C15-C11	2.14	92.92	90.58
7	B	502	TA1	O06-C15-C11	2.14	92.91	90.58
7	H	502	TA1	O06-C15-C11	2.13	92.91	90.58
7	F	502	TA1	C21-O09-C22	2.08	120.23	115.95
7	O	502	TA1	C21-O09-C22	2.07	120.22	115.95
7	B	502	TA1	C21-O09-C22	2.07	120.22	115.95
7	Q	502	TA1	C21-O09-C22	2.06	120.21	115.95
7	S	502	TA1	C21-O09-C22	2.06	120.20	115.95
7	H	502	TA1	C21-O09-C22	2.06	120.20	115.95
7	J	502	TA1	C21-O09-C22	2.05	120.18	115.95
8	b	401	ANP	O4'-C4'-C3'	2.05	109.22	105.15
7	M	502	TA1	C21-O09-C22	2.04	120.15	115.95
7	D	502	TA1	C21-O09-C22	2.04	120.15	115.95
8	K	501	ANP	C4-C5-N7	-2.03	108.26	110.58
8	h	401	ANP	O4'-C4'-C3'	2.03	109.19	105.15
8	a	401	ANP	C4-C5-N7	-2.03	108.26	110.58
8	c	401	ANP	C4-C5-N7	-2.03	108.26	110.58
8	g	401	ANP	O4'-C4'-C3'	2.03	109.17	105.15
8	f	401	ANP	O4'-C4'-C3'	2.03	109.17	105.15
8	e	401	ANP	O4'-C4'-C3'	2.02	109.17	105.15
8	K	501	ANP	O4'-C4'-C3'	2.02	109.16	105.15
8	d	401	ANP	O4'-C4'-C3'	2.02	109.16	105.15
8	b	401	ANP	C2-N1-C6	2.01	122.04	118.73
8	e	401	ANP	C4-C5-N7	-2.01	108.28	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	401	ANP	C4-C5-N7	-2.01	108.28	110.58
8	b	401	ANP	C4-C5-N7	-2.01	108.29	110.58
8	a	401	ANP	O4'-C4'-C3'	2.01	109.13	105.15
8	f	401	ANP	C2-N1-C6	2.00	122.02	118.73
8	g	401	ANP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
4	E	501	GTP	C5'-O5'-PA-O3A
4	E	501	GTP	C5'-O5'-PA-O1A
4	E	501	GTP	C5'-O5'-PA-O2A
4	G	501	GTP	C5'-O5'-PA-O3A
4	G	501	GTP	C5'-O5'-PA-O1A
4	G	501	GTP	C5'-O5'-PA-O2A
4	I	501	GTP	C5'-O5'-PA-O3A
4	I	501	GTP	C5'-O5'-PA-O1A
4	I	501	GTP	C5'-O5'-PA-O2A
4	L	501	GTP	C5'-O5'-PA-O3A
4	L	501	GTP	C5'-O5'-PA-O1A
4	L	501	GTP	C5'-O5'-PA-O2A
4	N	501	GTP	C5'-O5'-PA-O3A
4	N	501	GTP	C5'-O5'-PA-O1A
4	N	501	GTP	C5'-O5'-PA-O2A
4	P	501	GTP	C5'-O5'-PA-O3A
4	P	501	GTP	C5'-O5'-PA-O1A
4	P	501	GTP	C5'-O5'-PA-O2A
4	R	501	GTP	C5'-O5'-PA-O3A
4	R	501	GTP	C5'-O5'-PA-O1A
4	R	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O1A
6	F	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
6	F	501	GDP	C5'-O5'-PA-O1A
6	H	501	GDP	C5'-O5'-PA-O3A
6	H	501	GDP	C5'-O5'-PA-O1A
6	J	501	GDP	C5'-O5'-PA-O3A
6	J	501	GDP	C5'-O5'-PA-O1A
6	M	501	GDP	C5'-O5'-PA-O3A
6	M	501	GDP	C5'-O5'-PA-O1A
6	O	501	GDP	C5'-O5'-PA-O3A
6	O	501	GDP	C5'-O5'-PA-O1A
6	Q	501	GDP	C5'-O5'-PA-O3A
6	Q	501	GDP	C5'-O5'-PA-O1A
6	S	501	GDP	C5'-O5'-PA-O3A
6	S	501	GDP	C5'-O5'-PA-O1A
8	K	501	ANP	PB-N3B-PG-O1G
8	K	501	ANP	PG-N3B-PB-O1B
8	a	401	ANP	PB-N3B-PG-O1G
8	a	401	ANP	PG-N3B-PB-O1B
8	b	401	ANP	PB-N3B-PG-O1G
8	b	401	ANP	PG-N3B-PB-O1B
8	c	401	ANP	PB-N3B-PG-O1G
8	c	401	ANP	PG-N3B-PB-O1B
8	d	401	ANP	PB-N3B-PG-O1G
8	d	401	ANP	PG-N3B-PB-O1B
8	e	401	ANP	PB-N3B-PG-O1G
8	e	401	ANP	PG-N3B-PB-O1B
8	f	401	ANP	PB-N3B-PG-O1G
8	f	401	ANP	PG-N3B-PB-O1B
8	g	401	ANP	PB-N3B-PG-O1G
8	g	401	ANP	PG-N3B-PB-O1B
8	h	401	ANP	PB-N3B-PG-O1G
8	h	401	ANP	PG-N3B-PB-O1B
7	B	502	TA1	O02-C03-C04-C09
7	D	502	TA1	O02-C03-C04-C09
7	F	502	TA1	O02-C03-C04-C09
7	H	502	TA1	O02-C03-C04-C09
7	J	502	TA1	O02-C03-C04-C09
7	M	502	TA1	O02-C03-C04-C09
7	O	502	TA1	O02-C03-C04-C09
7	Q	502	TA1	O02-C03-C04-C09
7	S	502	TA1	O02-C03-C04-C09
7	B	502	TA1	O02-C03-C04-C05
7	D	502	TA1	O02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
7	F	502	TA1	O02-C03-C04-C05
7	H	502	TA1	O02-C03-C04-C05
7	J	502	TA1	O02-C03-C04-C05
7	M	502	TA1	O02-C03-C04-C05
7	O	502	TA1	O02-C03-C04-C05
7	Q	502	TA1	O02-C03-C04-C05
7	S	502	TA1	O02-C03-C04-C05
4	A	501	GTP	O4'-C4'-C5'-O5'
4	A	501	GTP	C3'-C4'-C5'-O5'
4	C	501	GTP	O4'-C4'-C5'-O5'
4	C	501	GTP	C3'-C4'-C5'-O5'
4	E	501	GTP	O4'-C4'-C5'-O5'
4	E	501	GTP	C3'-C4'-C5'-O5'
4	G	501	GTP	O4'-C4'-C5'-O5'
4	G	501	GTP	C3'-C4'-C5'-O5'
4	I	501	GTP	O4'-C4'-C5'-O5'
4	I	501	GTP	C3'-C4'-C5'-O5'
4	L	501	GTP	O4'-C4'-C5'-O5'
4	L	501	GTP	C3'-C4'-C5'-O5'
4	N	501	GTP	O4'-C4'-C5'-O5'
4	N	501	GTP	C3'-C4'-C5'-O5'
4	P	501	GTP	O4'-C4'-C5'-O5'
4	P	501	GTP	C3'-C4'-C5'-O5'
4	R	501	GTP	O4'-C4'-C5'-O5'
4	R	501	GTP	C3'-C4'-C5'-O5'
7	D	502	TA1	O03-C03-C04-C05
7	F	502	TA1	O03-C03-C04-C05
7	H	502	TA1	O03-C03-C04-C05
7	J	502	TA1	O03-C03-C04-C05
7	M	502	TA1	O03-C03-C04-C05
7	O	502	TA1	O03-C03-C04-C05
7	Q	502	TA1	O03-C03-C04-C05
7	S	502	TA1	O03-C03-C04-C05
7	B	502	TA1	O03-C03-C04-C05
7	Q	502	TA1	O03-C03-C04-C09
7	B	502	TA1	O03-C03-C04-C09
7	D	502	TA1	O03-C03-C04-C09
7	F	502	TA1	O03-C03-C04-C09
7	H	502	TA1	O03-C03-C04-C09
7	J	502	TA1	O03-C03-C04-C09
7	M	502	TA1	O03-C03-C04-C09
7	O	502	TA1	O03-C03-C04-C09

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Mol	Chain	Res	Type	Atoms
7	S	502	TA1	O03-C03-C04-C09
7	B	502	TA1	N01-C30-C31-C36
7	D	502	TA1	N01-C30-C31-C36
7	F	502	TA1	N01-C30-C31-C36
7	H	502	TA1	N01-C30-C31-C36
7	J	502	TA1	N01-C30-C31-C36
7	M	502	TA1	N01-C30-C31-C36
7	O	502	TA1	N01-C30-C31-C36
7	Q	502	TA1	N01-C30-C31-C36
7	S	502	TA1	N01-C30-C31-C36
7	B	502	TA1	O14-C30-C31-C36
7	H	502	TA1	O14-C30-C31-C36
7	J	502	TA1	O14-C30-C31-C36
7	D	502	TA1	O14-C30-C31-C36
7	O	502	TA1	O14-C30-C31-C36
7	Q	502	TA1	O14-C30-C31-C36
7	F	502	TA1	O14-C30-C31-C36
7	M	502	TA1	O14-C30-C31-C36
7	S	502	TA1	O14-C30-C31-C36
7	D	502	TA1	N01-C30-C31-C32
7	F	502	TA1	N01-C30-C31-C32
7	M	502	TA1	N01-C30-C31-C32
7	O	502	TA1	N01-C30-C31-C32
7	Q	502	TA1	N01-C30-C31-C32
7	S	502	TA1	N01-C30-C31-C32
7	B	502	TA1	N01-C30-C31-C32
7	H	502	TA1	N01-C30-C31-C32
7	J	502	TA1	N01-C30-C31-C32
7	D	502	TA1	O14-C30-C31-C32
7	B	502	TA1	O14-C30-C31-C32
7	H	502	TA1	O14-C30-C31-C32
7	J	502	TA1	O14-C30-C31-C32
7	O	502	TA1	O14-C30-C31-C32
7	Q	502	TA1	O14-C30-C31-C32
7	F	502	TA1	O14-C30-C31-C32
7	S	502	TA1	O14-C30-C31-C32
7	M	502	TA1	O14-C30-C31-C32
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O2A
6	F	501	GDP	C5'-O5'-PA-O2A
6	H	501	GDP	C5'-O5'-PA-O2A
6	J	501	GDP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	M	501	GDP	C5'-O5'-PA-O2A
6	O	501	GDP	C5'-O5'-PA-O2A
6	Q	501	GDP	C5'-O5'-PA-O2A
6	S	501	GDP	C5'-O5'-PA-O2A
7	B	502	TA1	C15-C11-O04-C12
7	D	502	TA1	C15-C11-O04-C12
7	F	502	TA1	C15-C11-O04-C12
7	H	502	TA1	C15-C11-O04-C12
7	J	502	TA1	C15-C11-O04-C12
7	M	502	TA1	C15-C11-O04-C12
7	O	502	TA1	C15-C11-O04-C12
7	Q	502	TA1	C15-C11-O04-C12
7	S	502	TA1	C15-C11-O04-C12
8	K	501	ANP	PG-N3B-PB-O3A
8	a	401	ANP	PG-N3B-PB-O3A
8	b	401	ANP	PG-N3B-PB-O3A
8	c	401	ANP	PG-N3B-PB-O3A
8	d	401	ANP	PG-N3B-PB-O3A
8	e	401	ANP	PG-N3B-PB-O3A
8	f	401	ANP	PG-N3B-PB-O3A
8	g	401	ANP	PG-N3B-PB-O3A
8	h	401	ANP	PG-N3B-PB-O3A

There are no ring outliers.

27 monomers are involved in 69 short contacts:

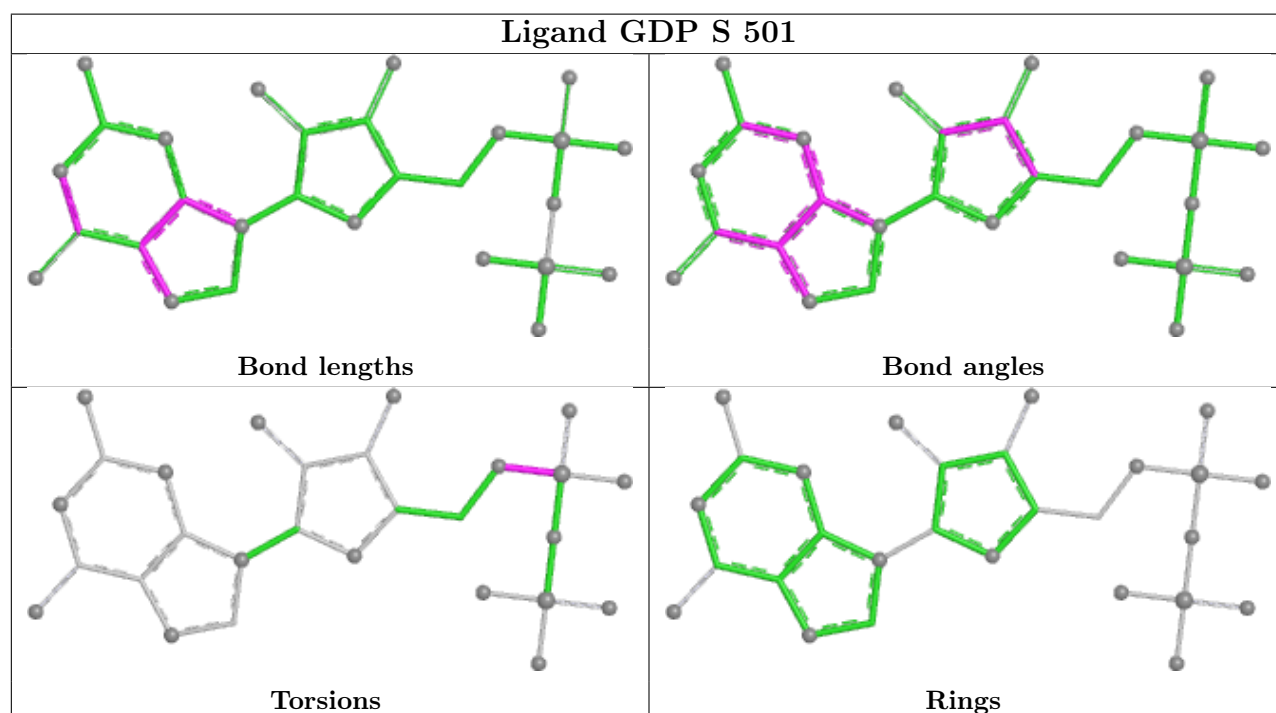
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	502	TA1	3	0
7	H	502	TA1	3	0
7	S	502	TA1	3	0
4	P	501	GTP	2	0
8	b	401	ANP	3	0
8	h	401	ANP	4	0
7	J	502	TA1	3	0
8	g	401	ANP	4	0
7	Q	502	TA1	3	0
4	L	501	GTP	1	0
4	I	501	GTP	1	0
4	C	501	GTP	2	0
7	D	502	TA1	3	0
8	c	401	ANP	3	0
8	f	401	ANP	3	0

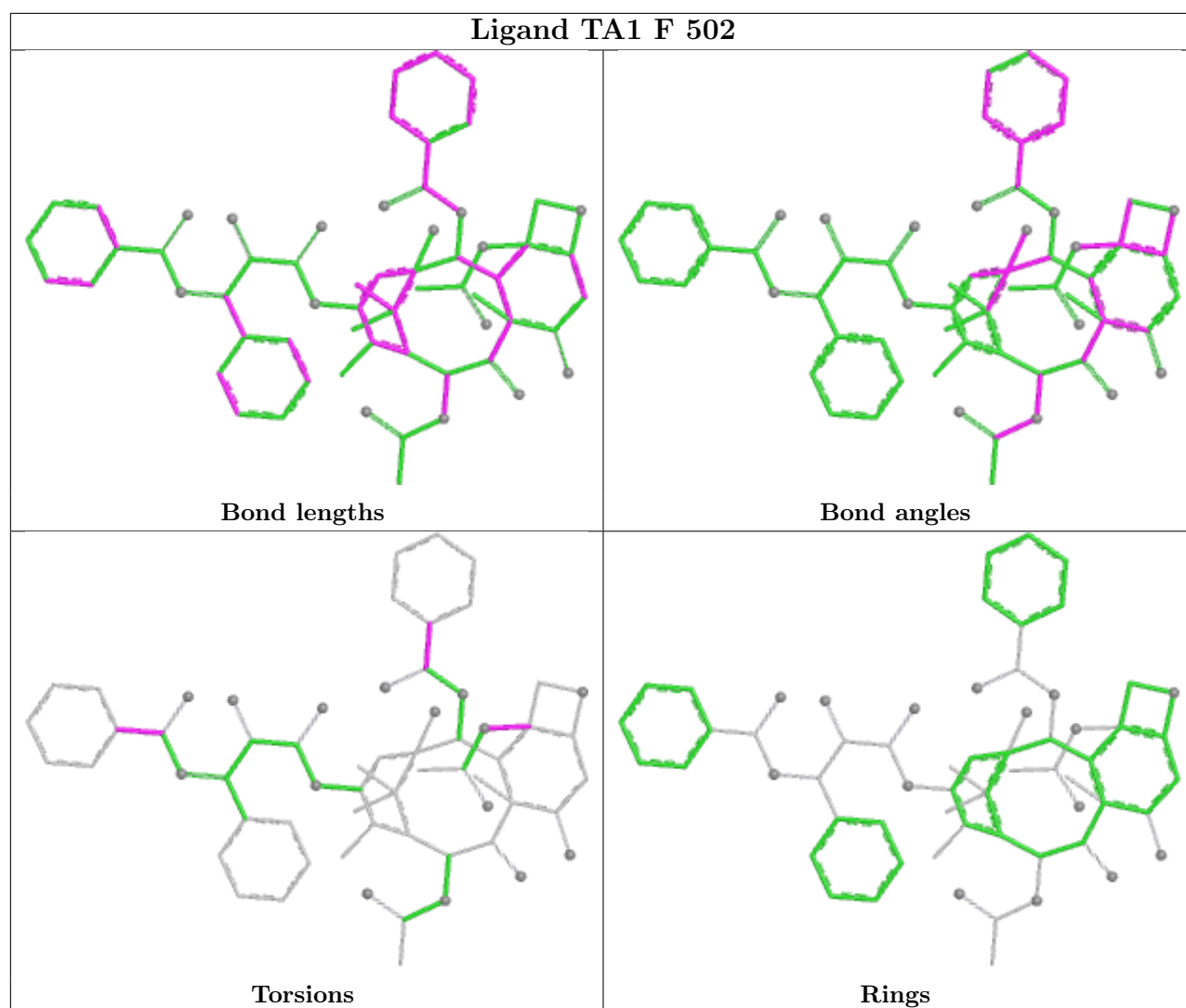
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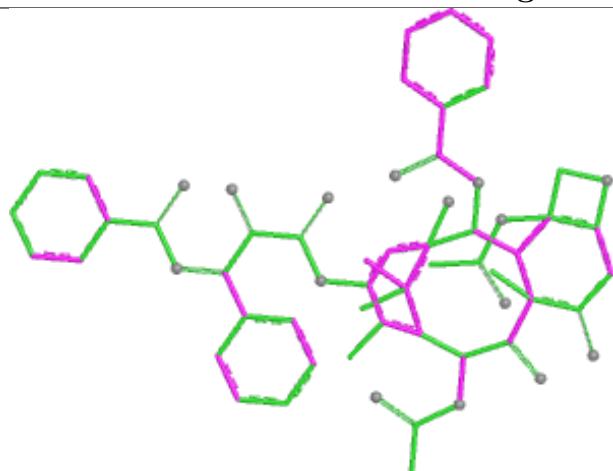
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	d	401	ANP	3	0
7	O	502	TA1	3	0
8	K	501	ANP	3	0
4	N	501	GTP	1	0
4	R	501	GTP	2	0
7	M	502	TA1	3	0
4	E	501	GTP	1	0
8	e	401	ANP	3	0
7	B	502	TA1	3	0
4	A	501	GTP	1	0
8	a	401	ANP	4	0
4	G	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

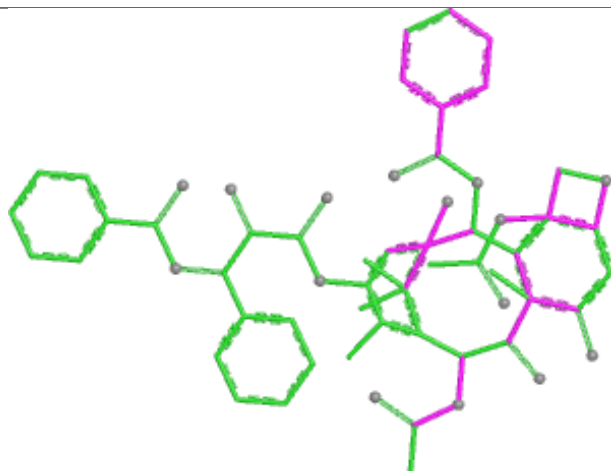




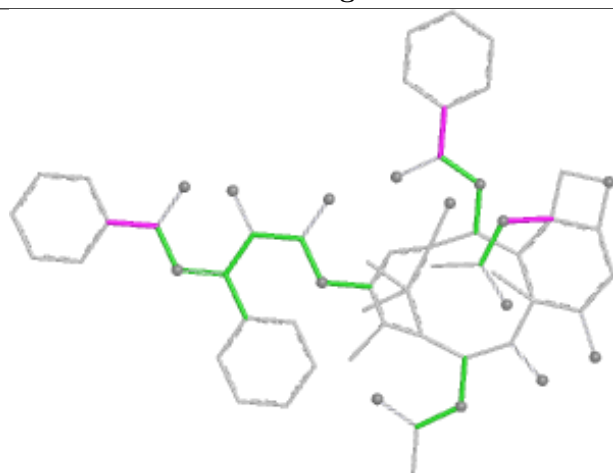
Ligand TA1 H 502



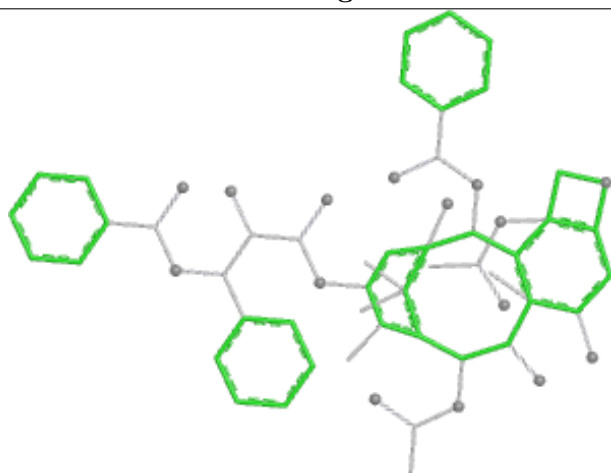
Bond lengths



Bond angles

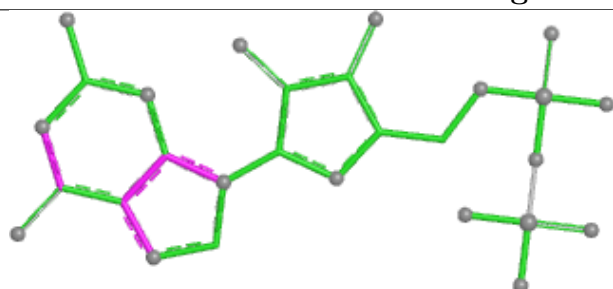


Torsions

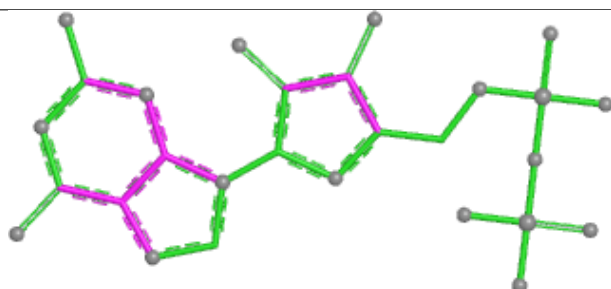


Rings

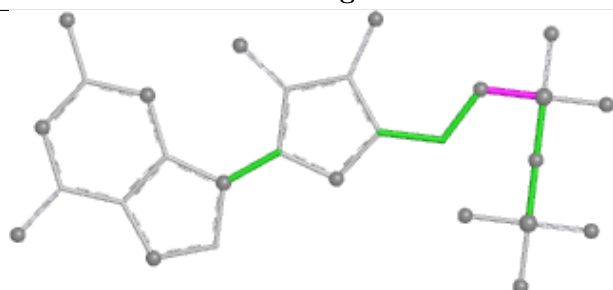
Ligand GDP D 501



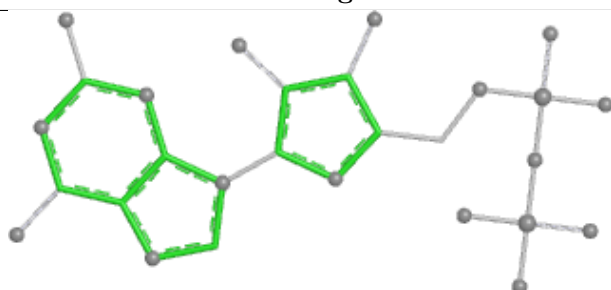
Bond lengths



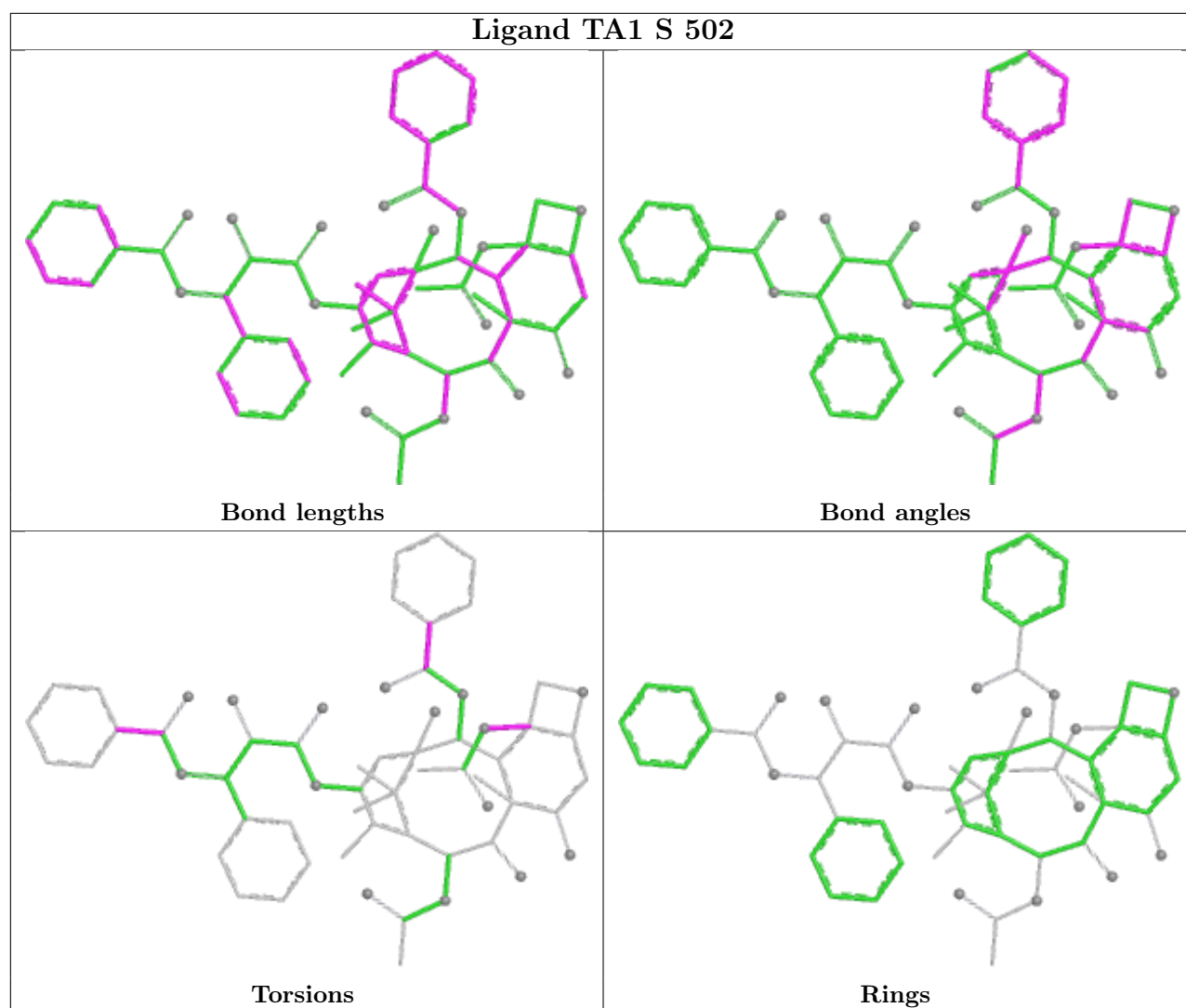
Bond angles

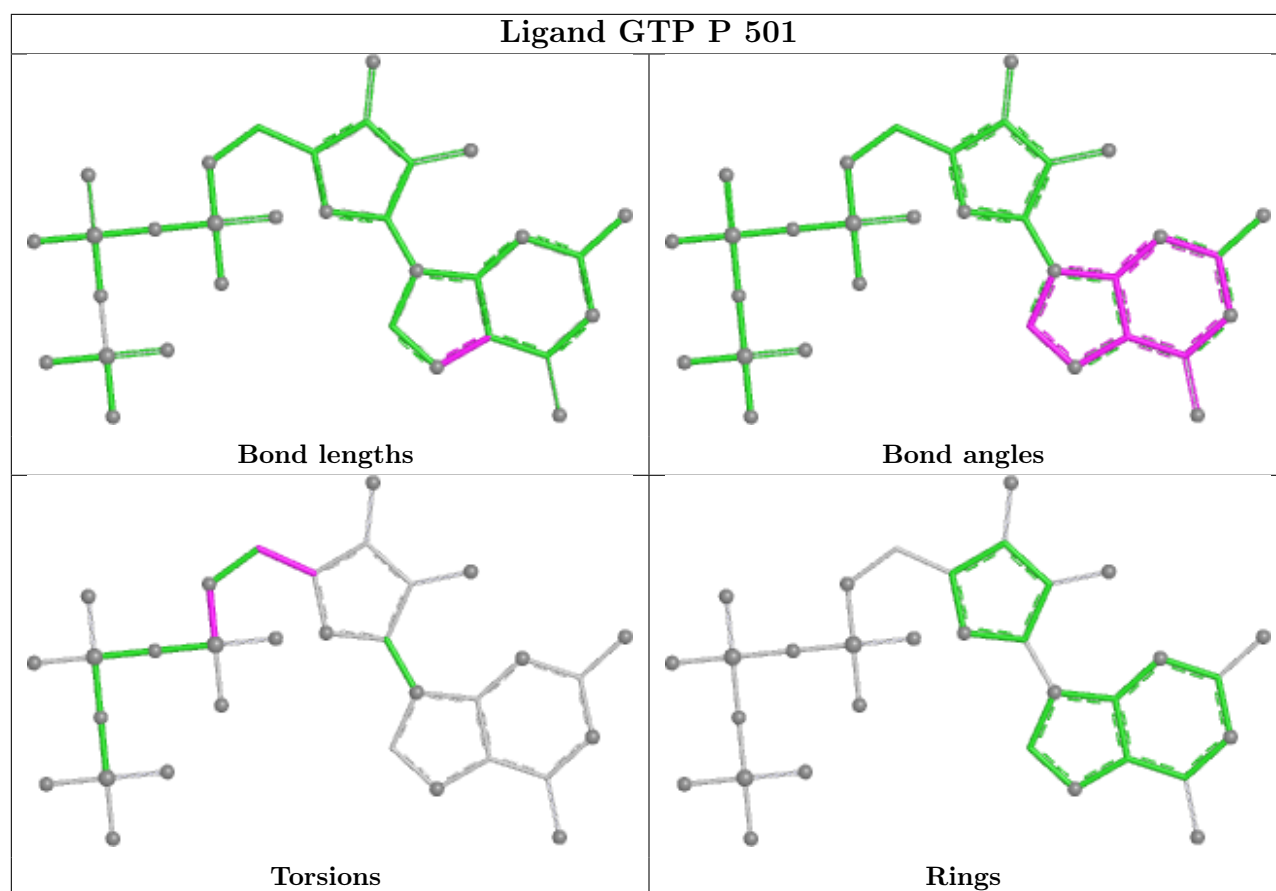


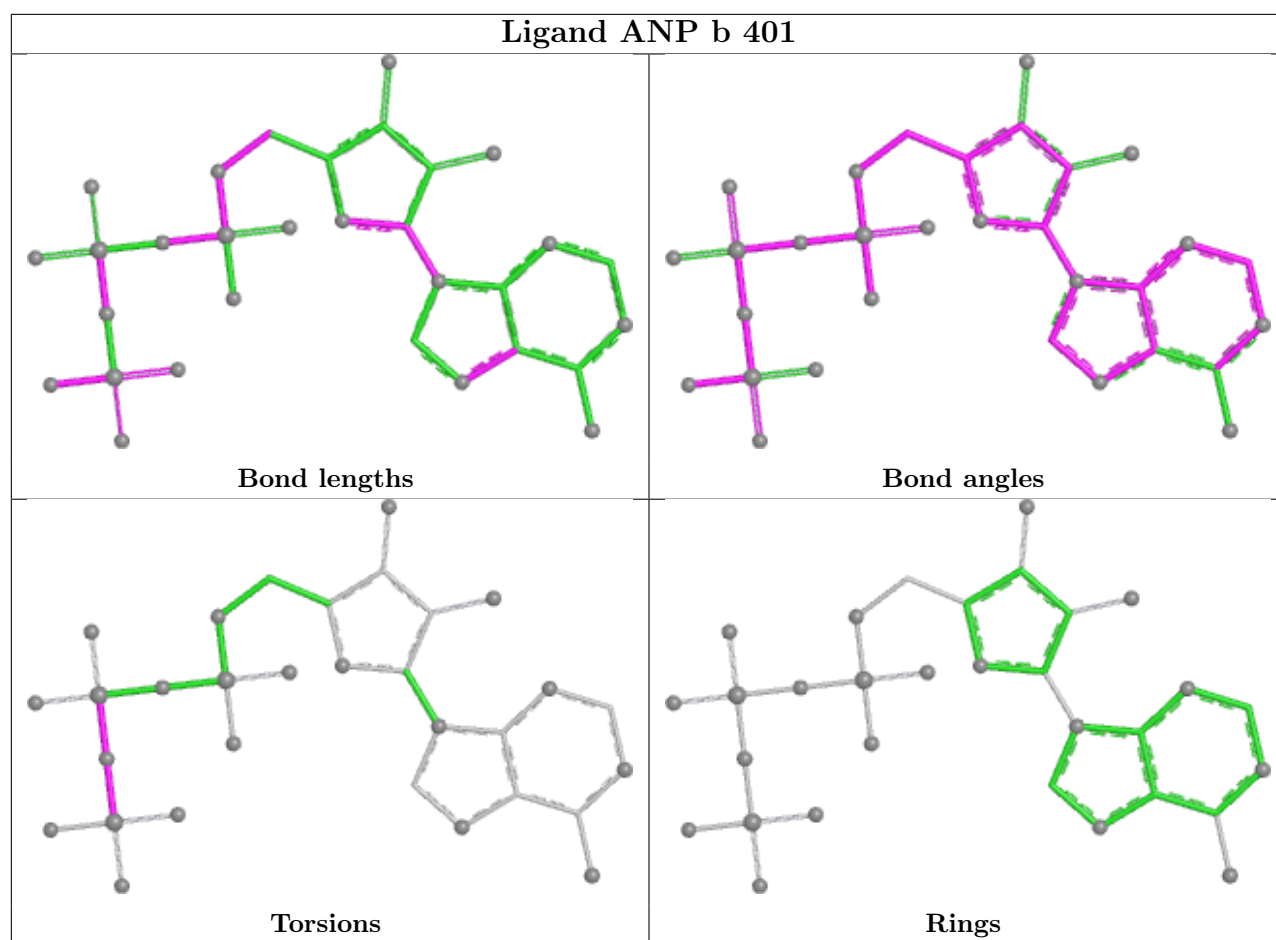
Torsions

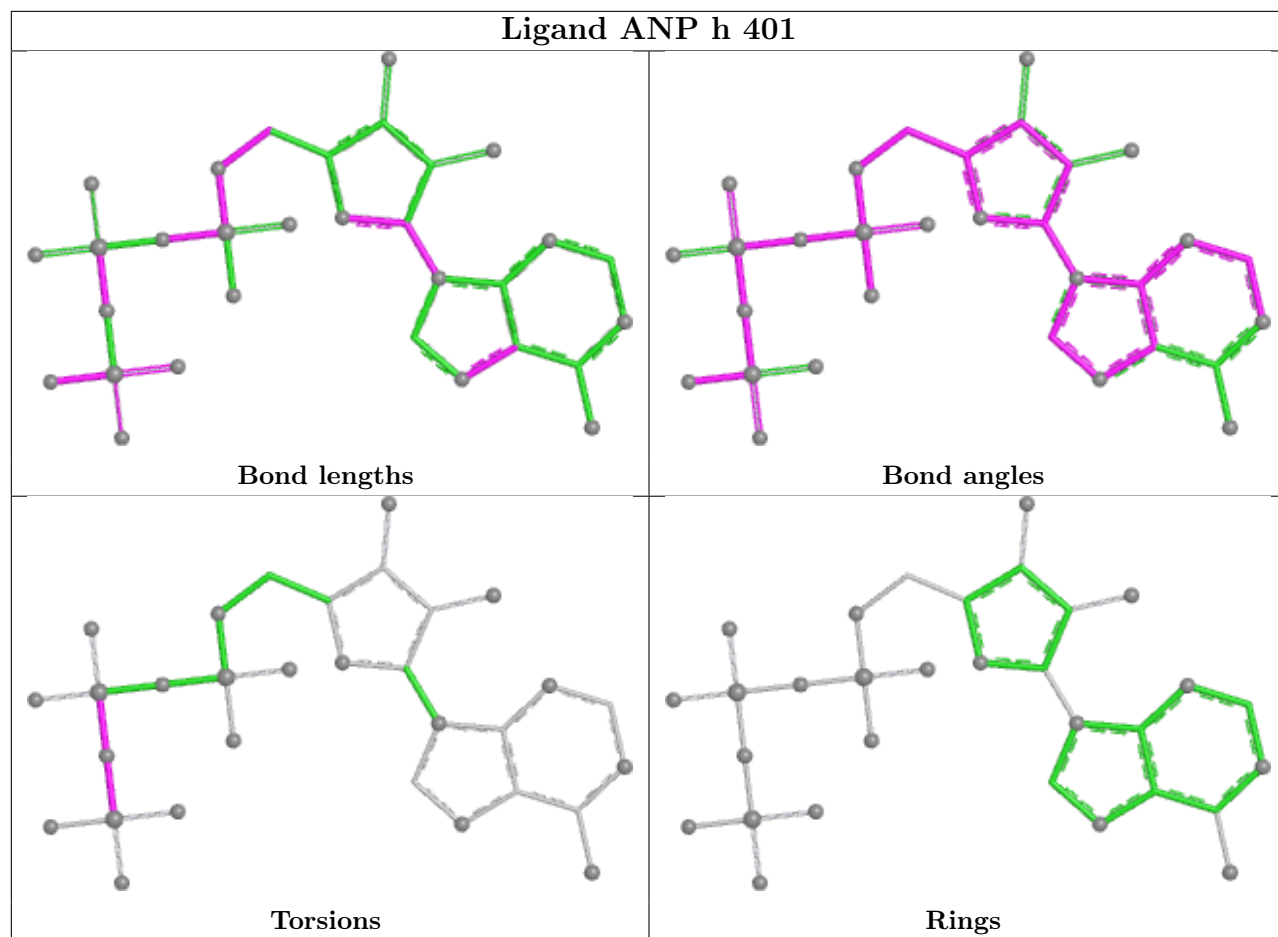


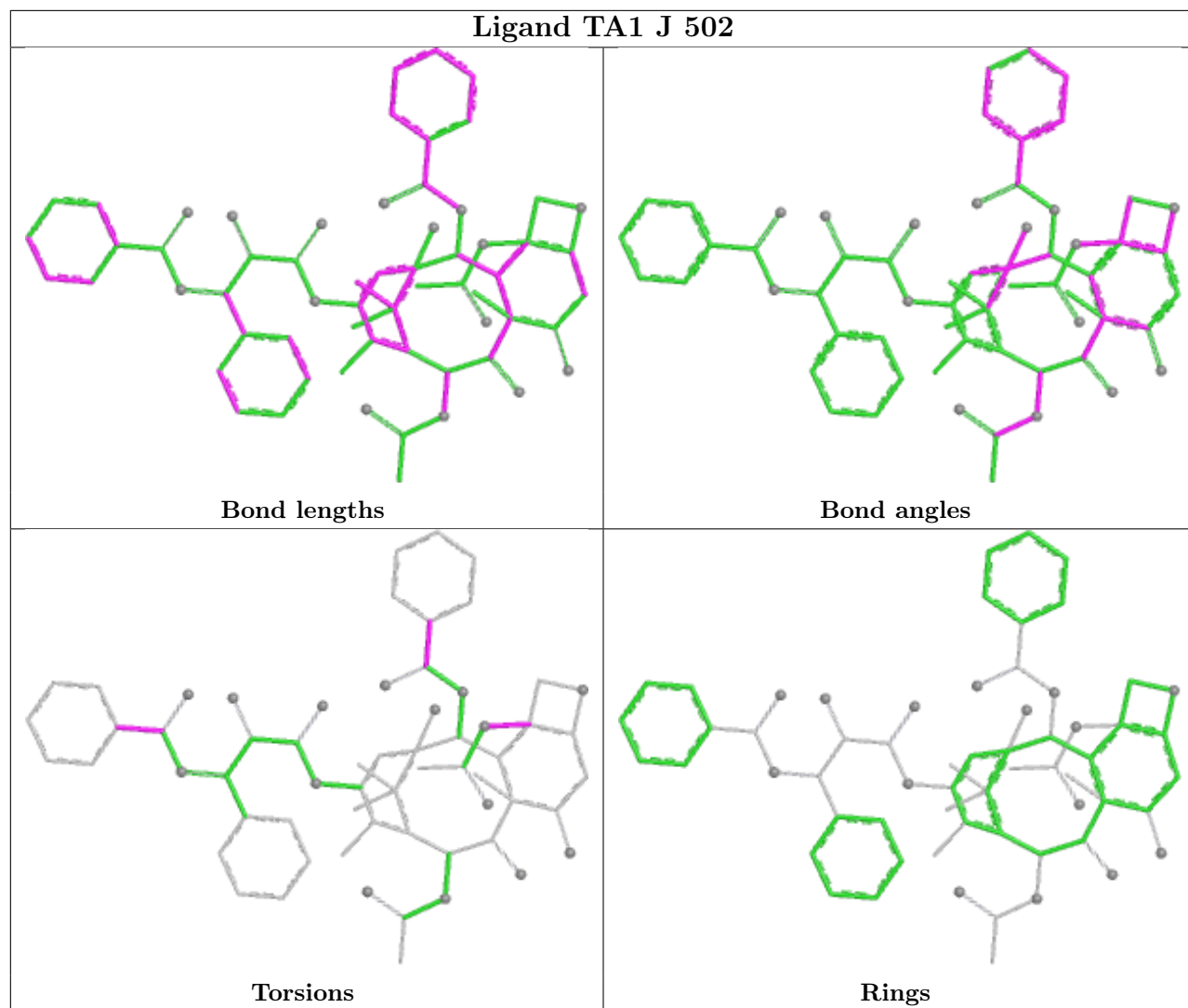
Rings



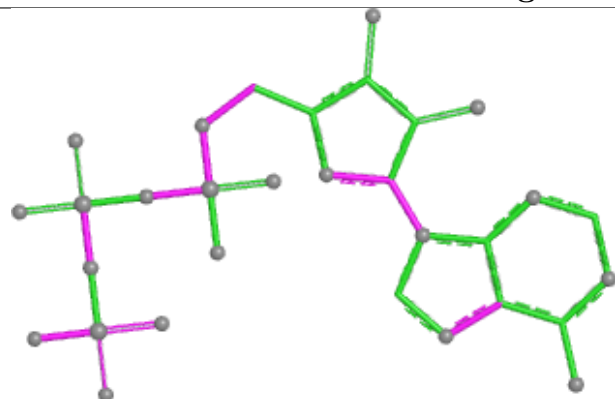




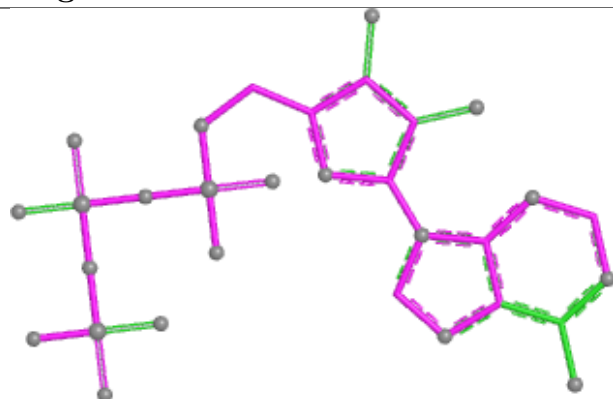




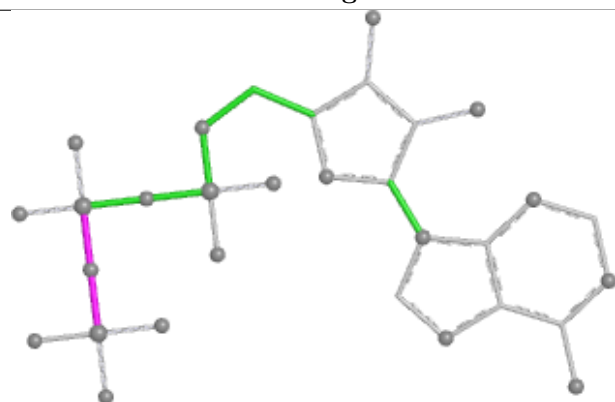
Ligand ANP g 401



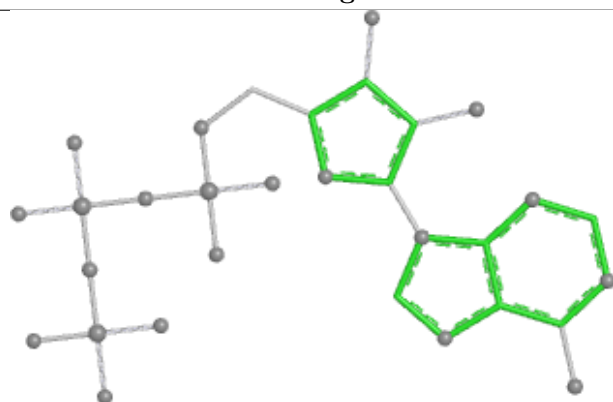
Bond lengths



Bond angles

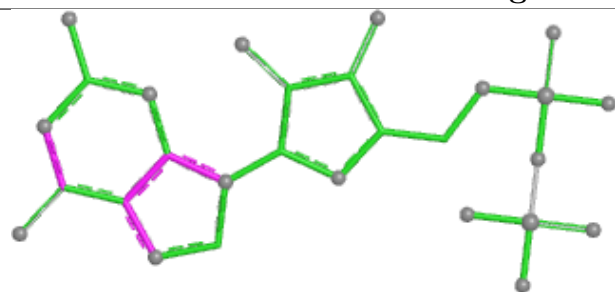


Torsions

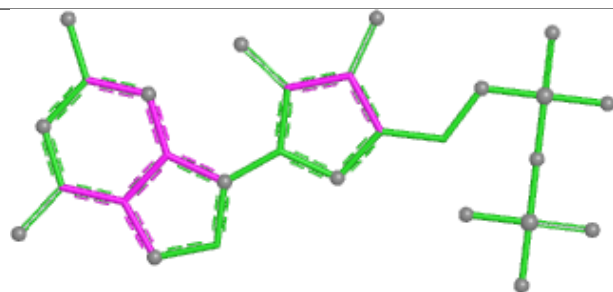


Rings

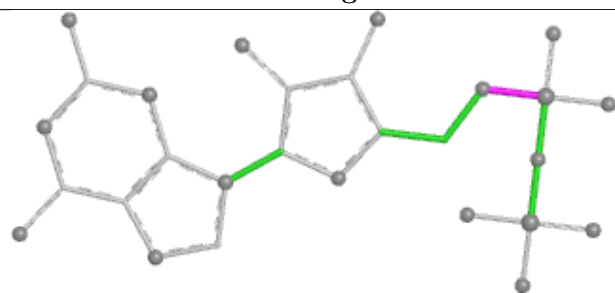
Ligand GDP M 501



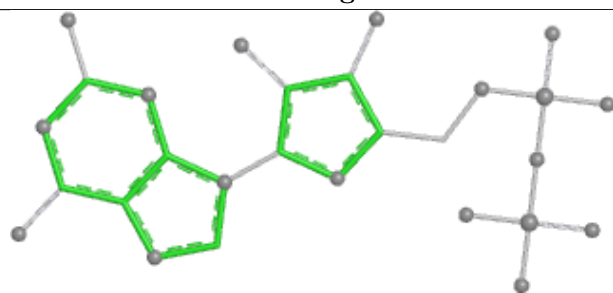
Bond lengths



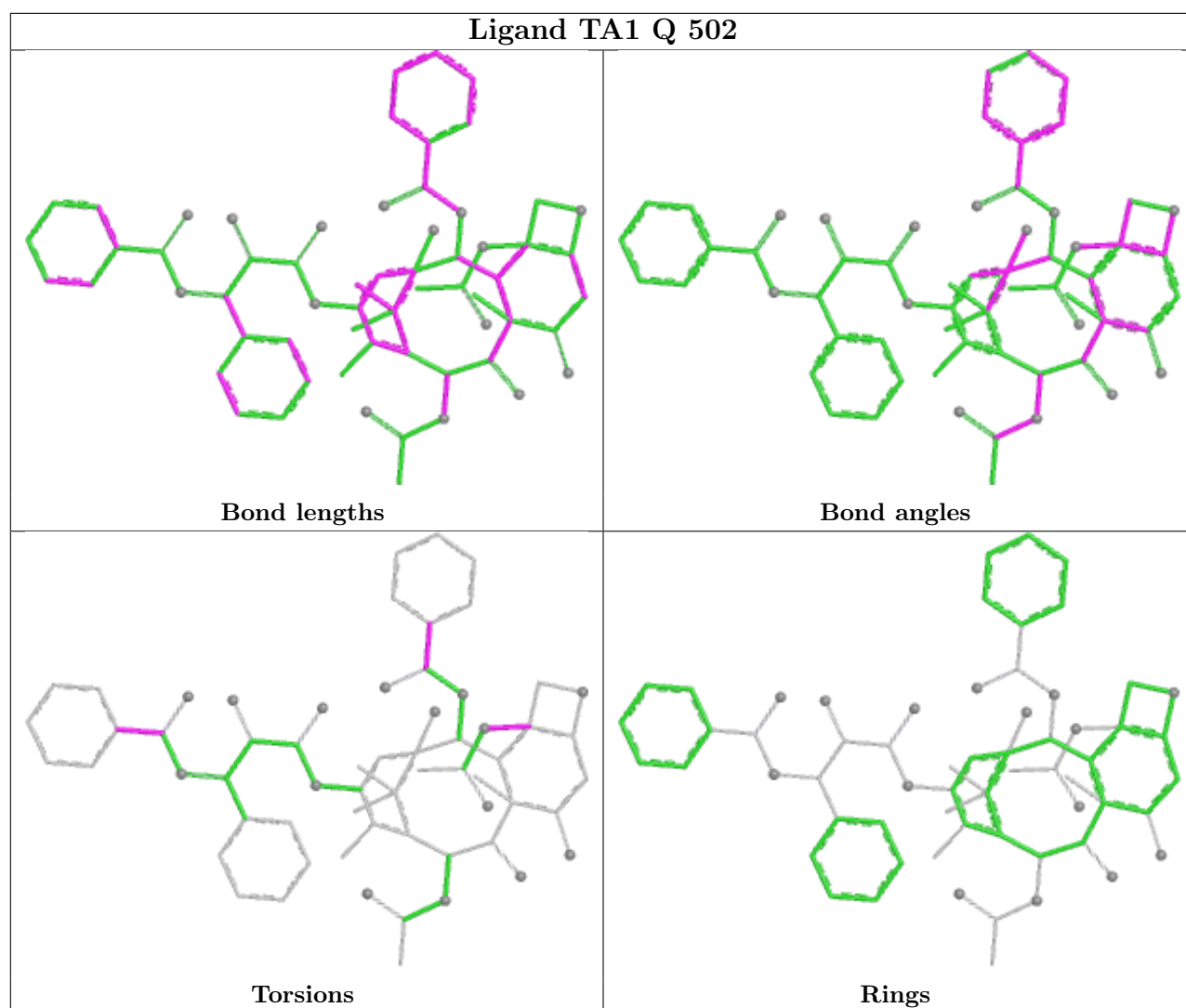
Bond angles



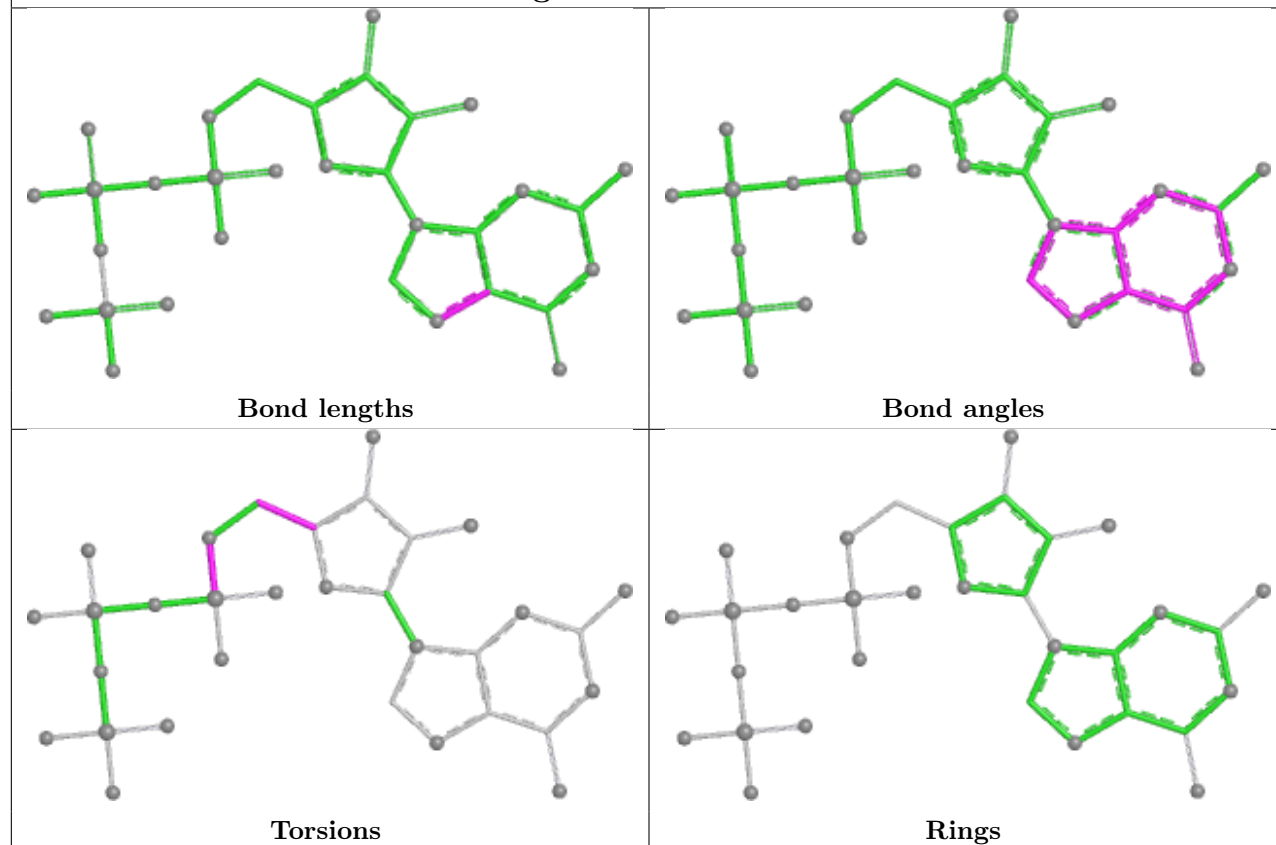
Torsions



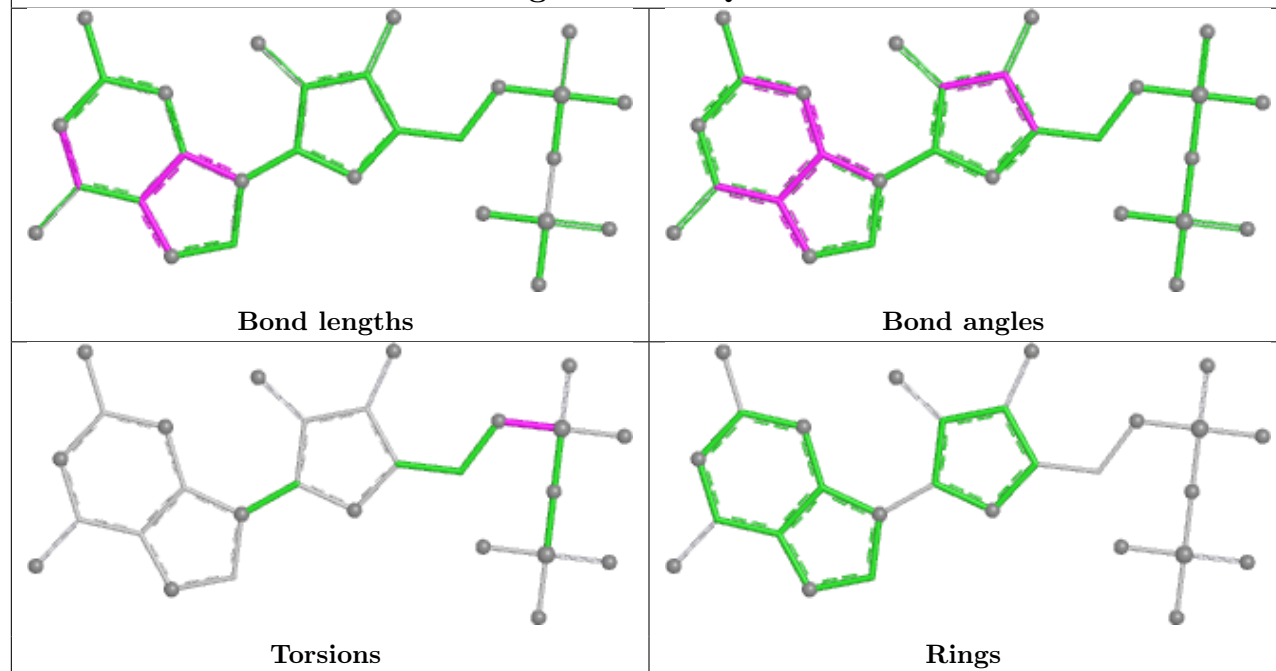
Rings



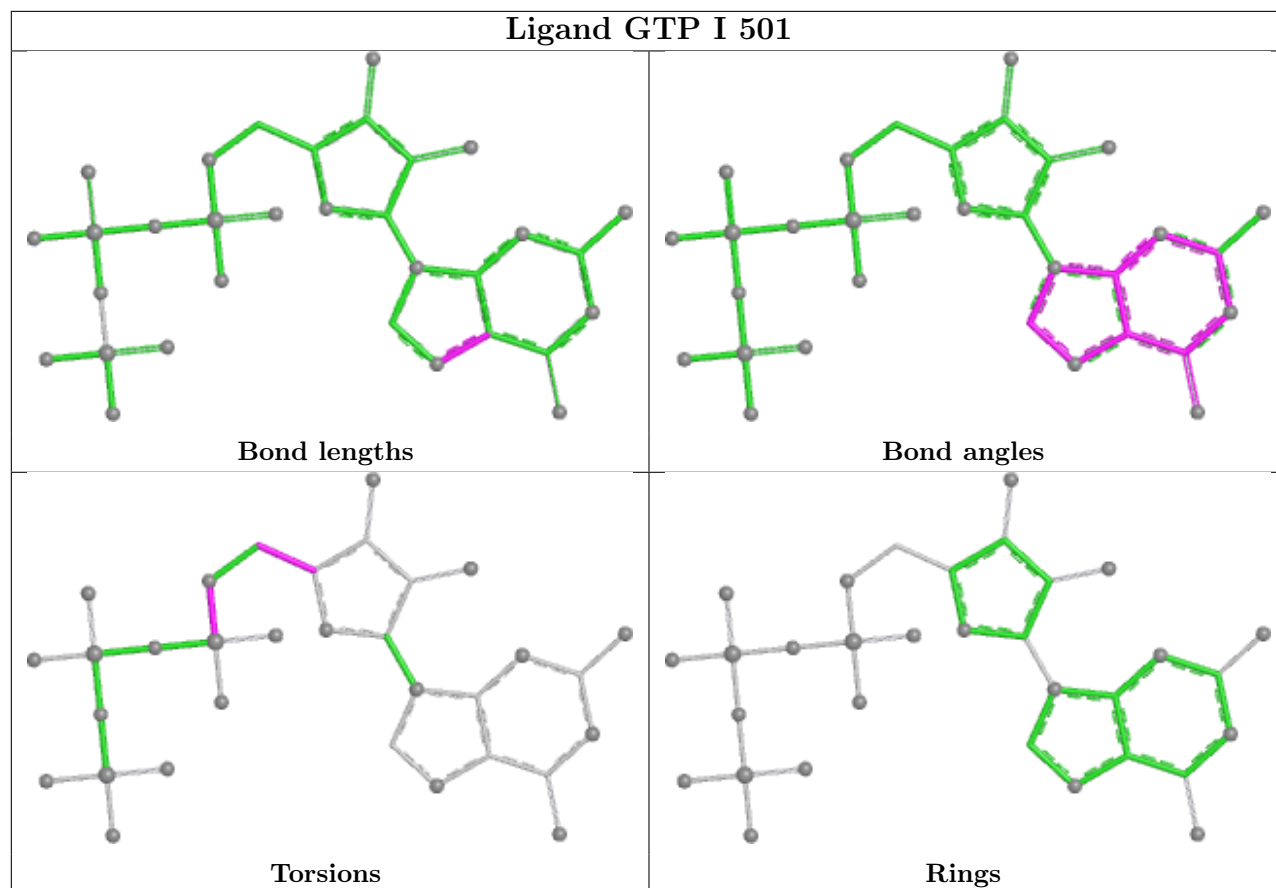
Ligand GTP L 501



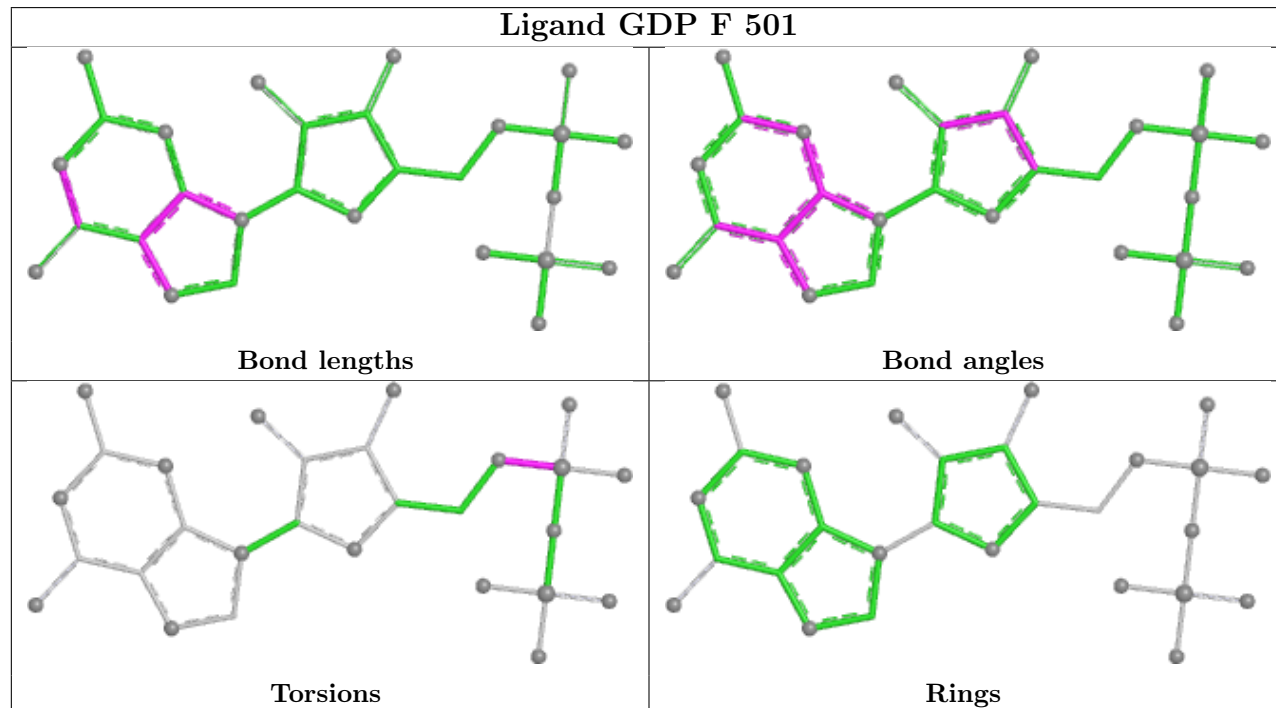
Ligand GDP Q 501

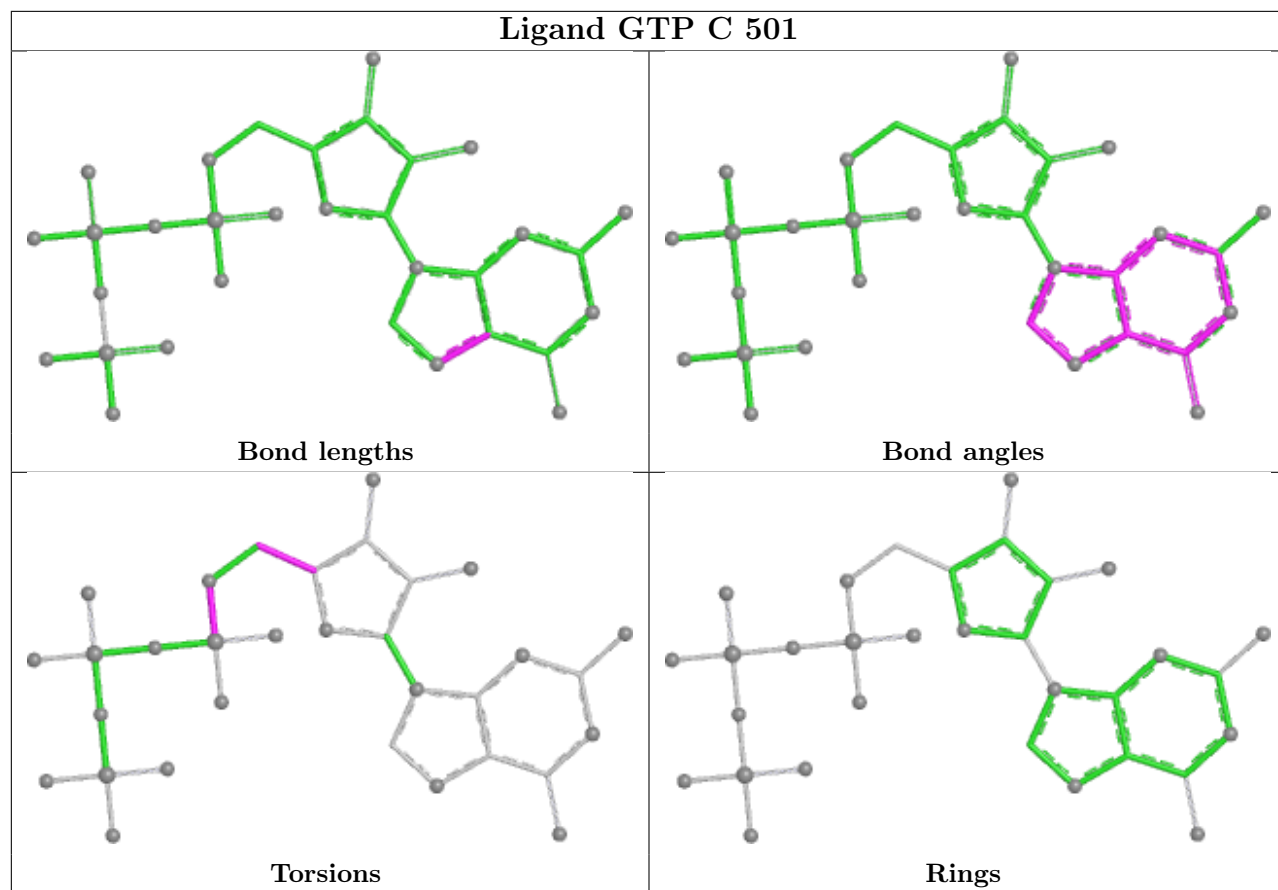


Ligand GTP I 501

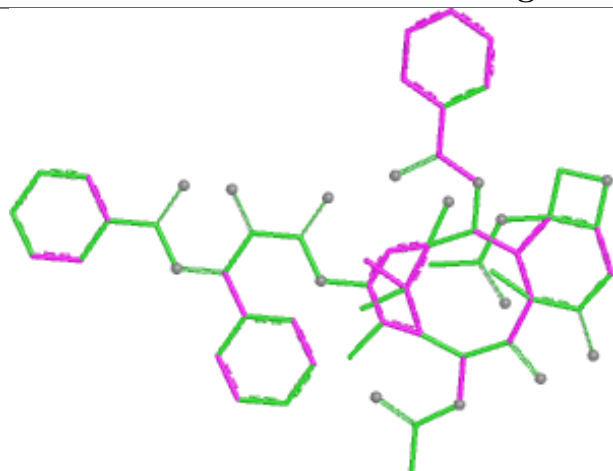


Ligand GDP F 501

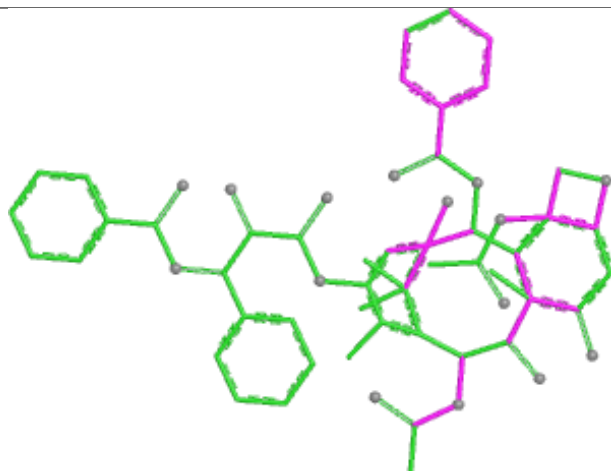




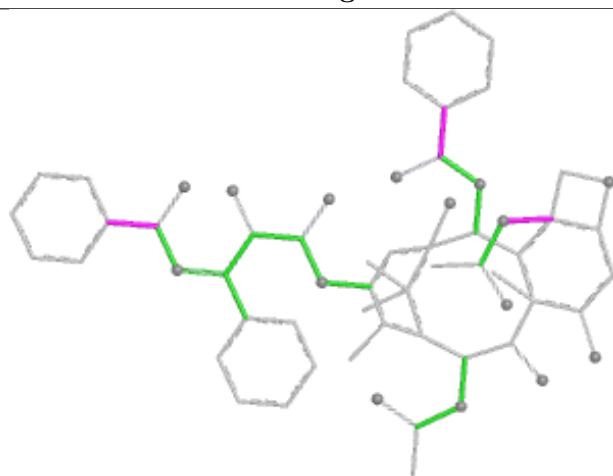
Ligand TA1 D 502



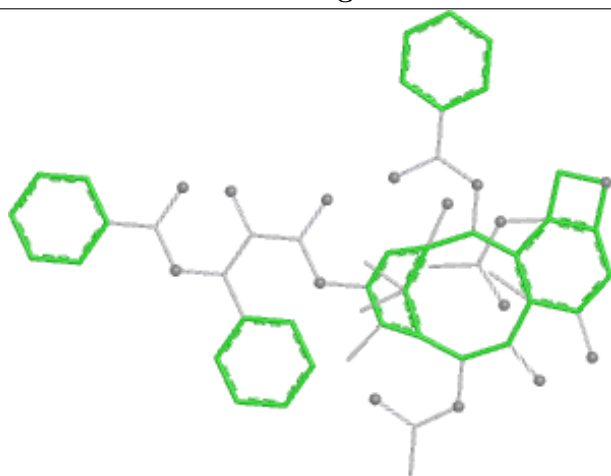
Bond lengths



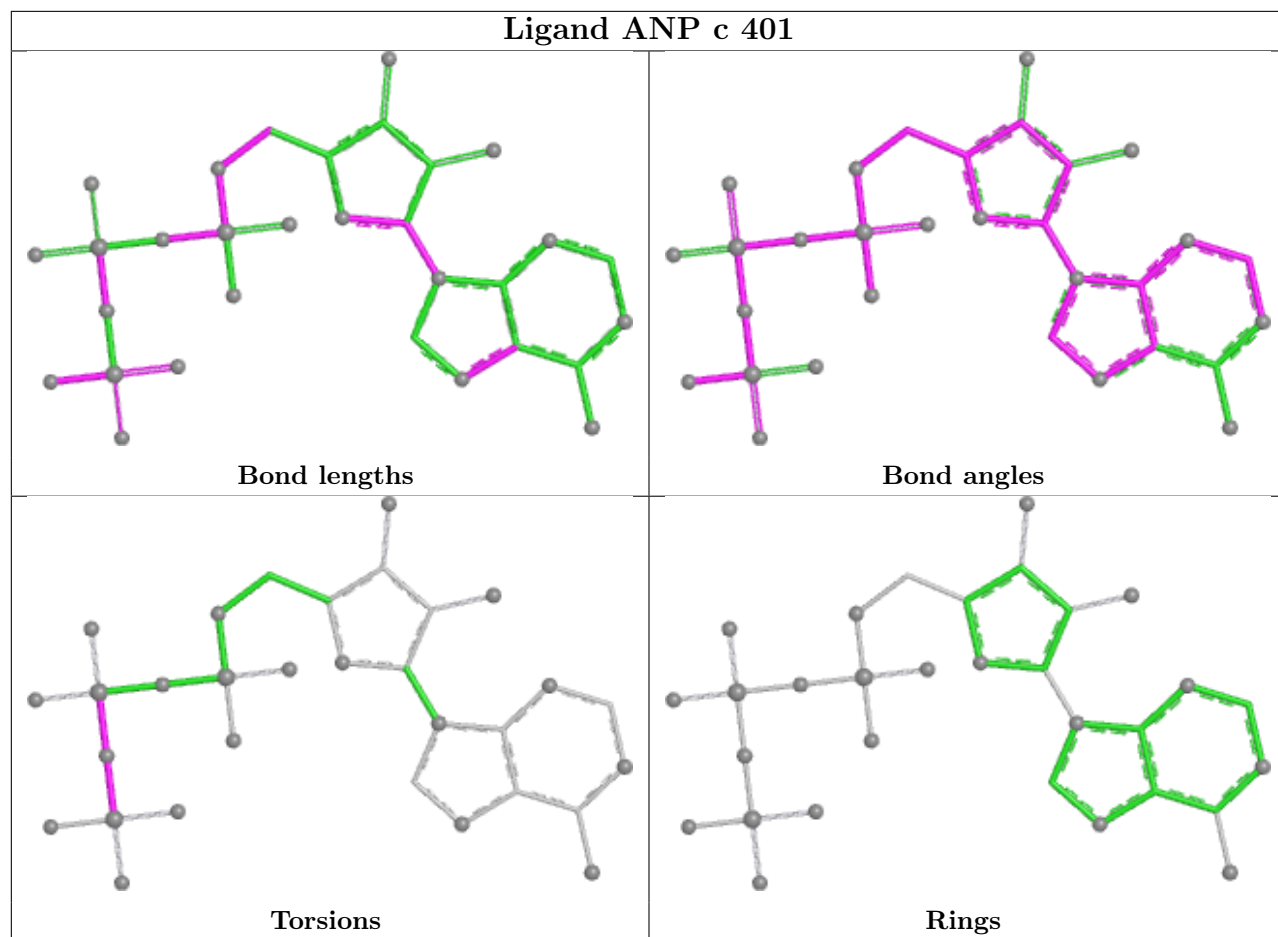
Bond angles

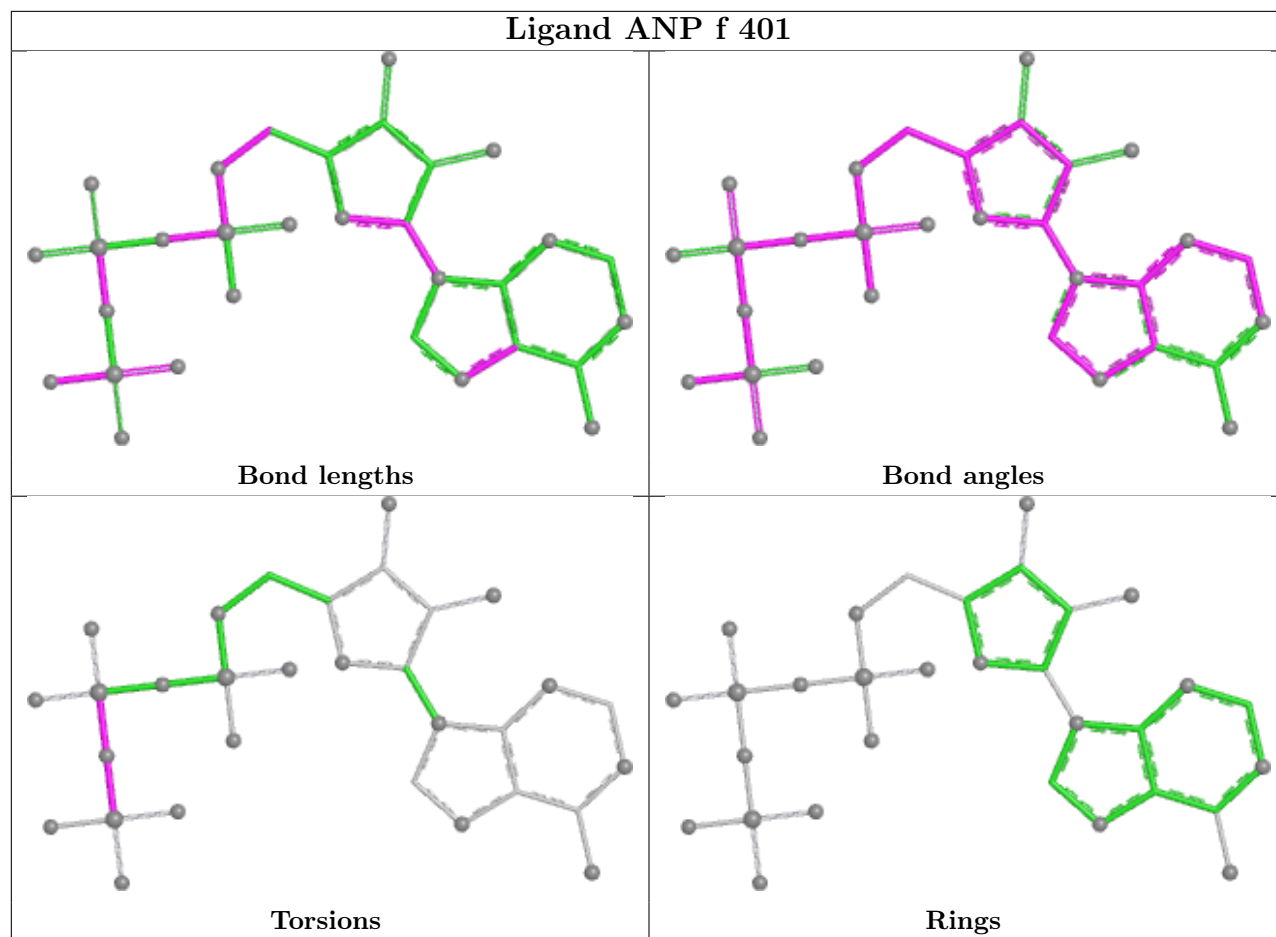


Torsions

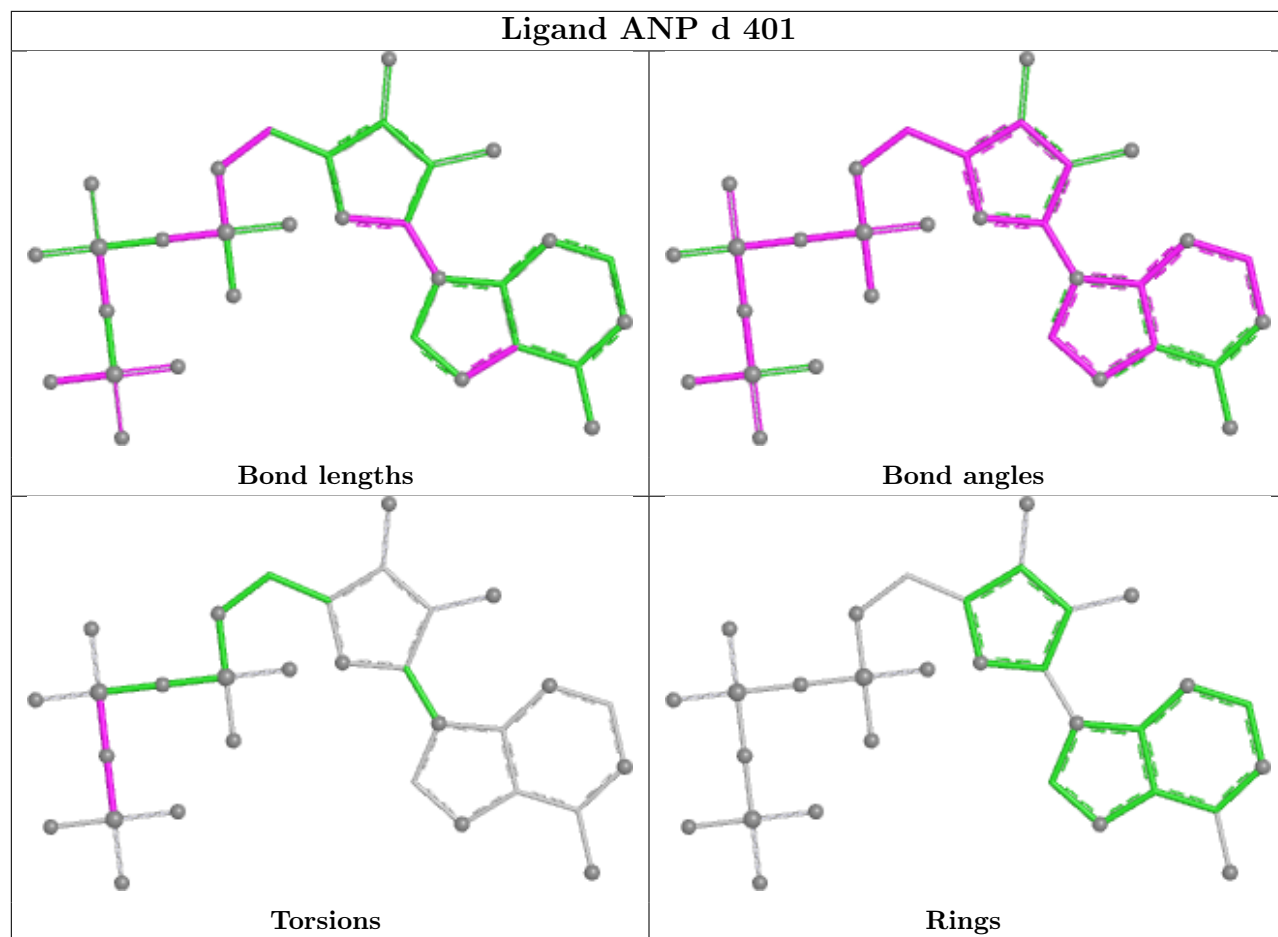


Rings

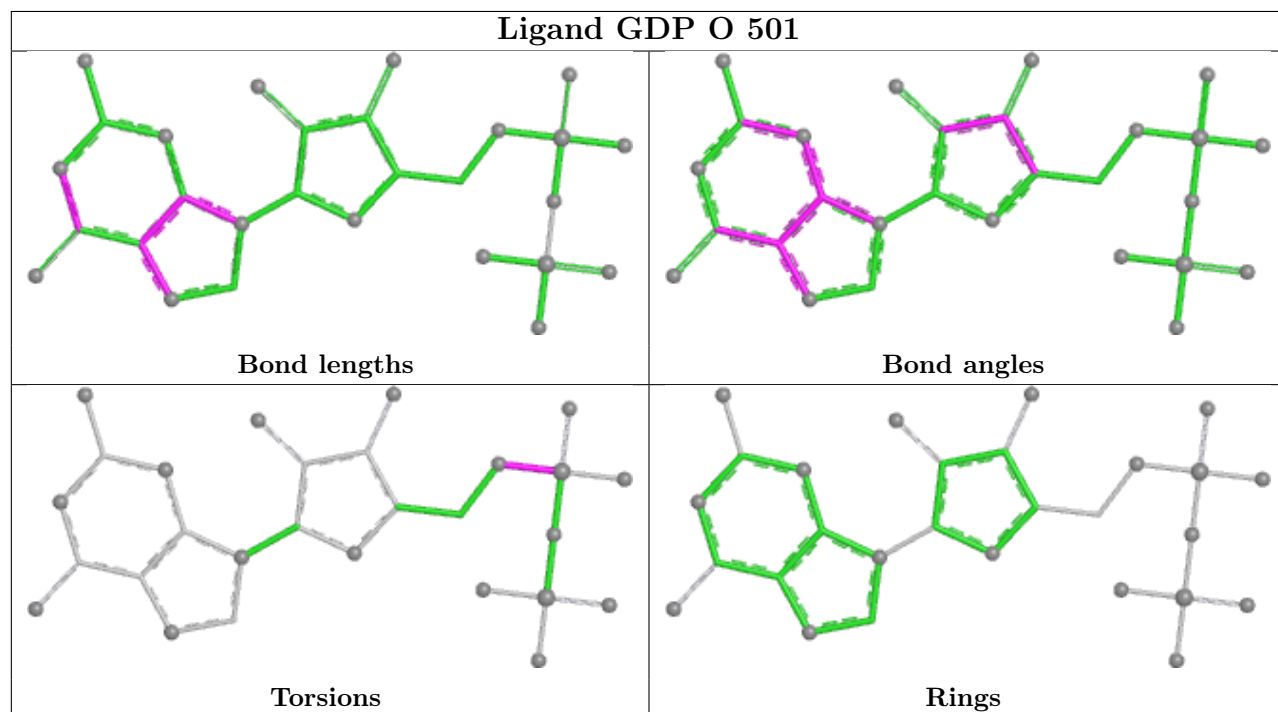


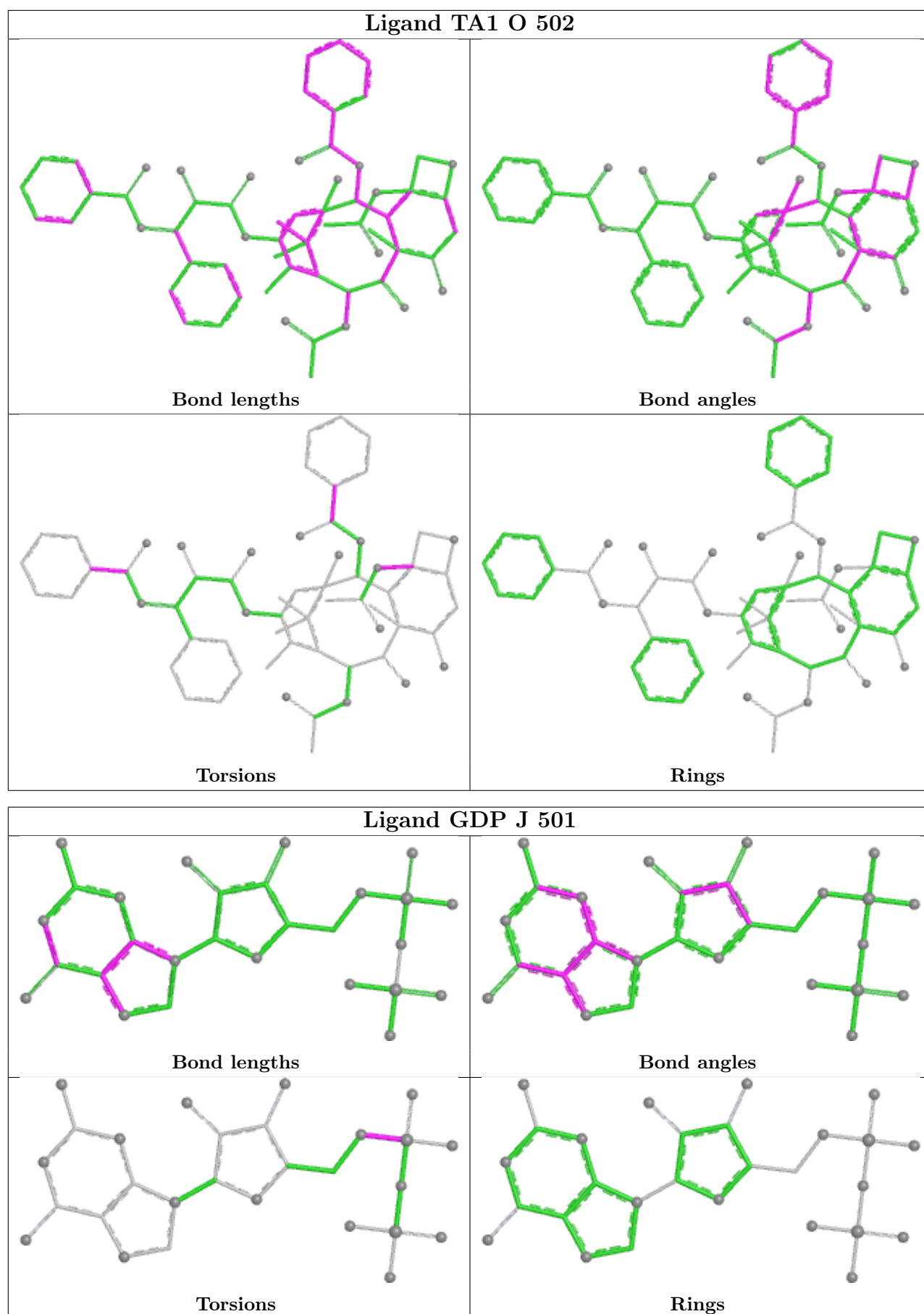


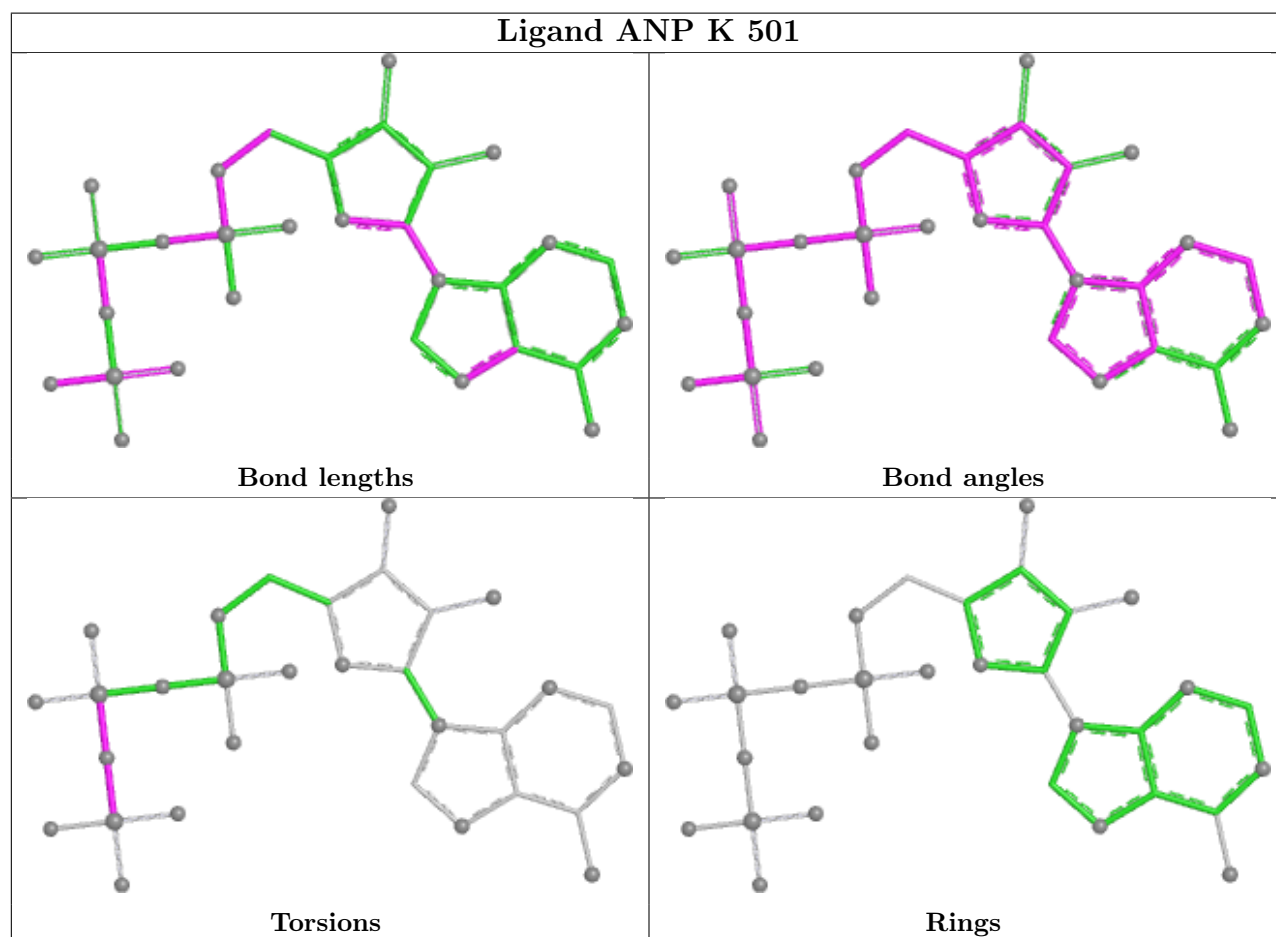
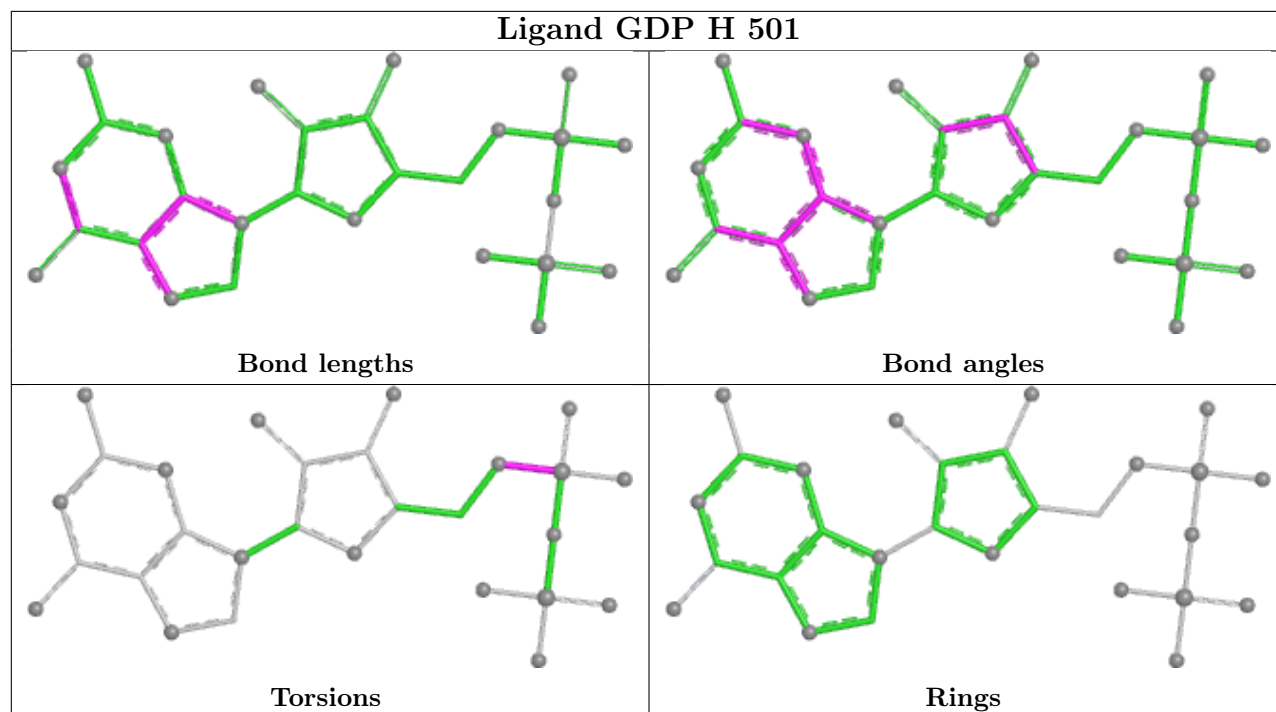
Ligand ANP d 401

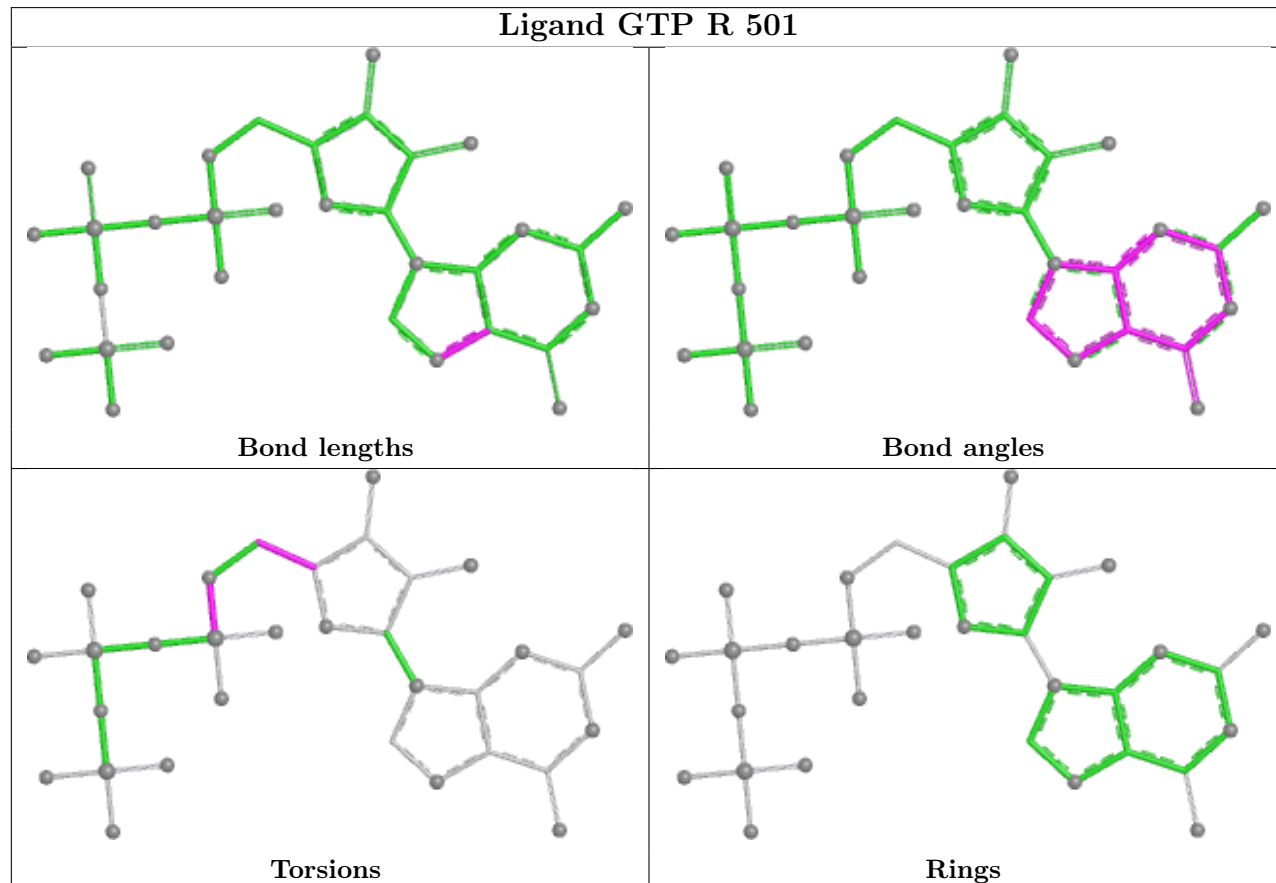
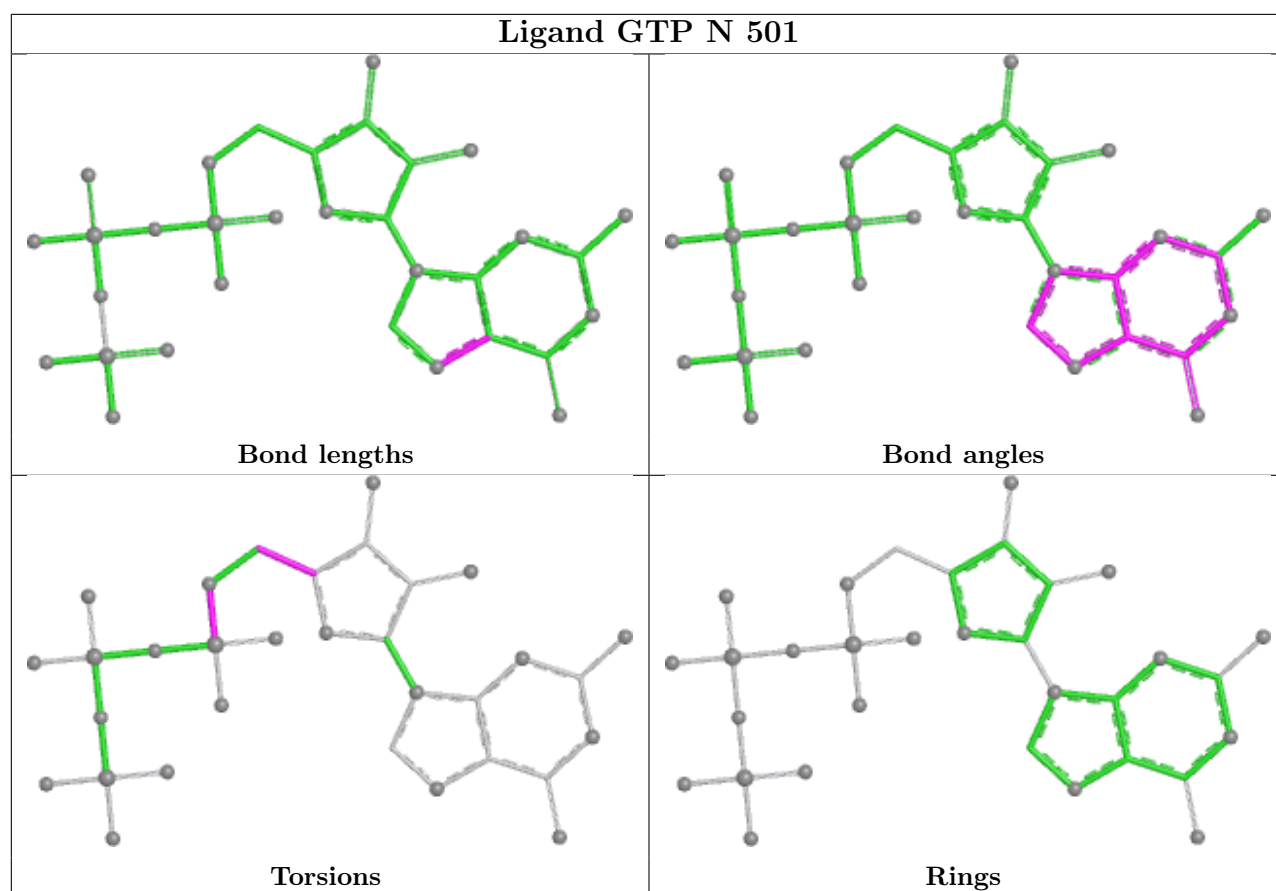


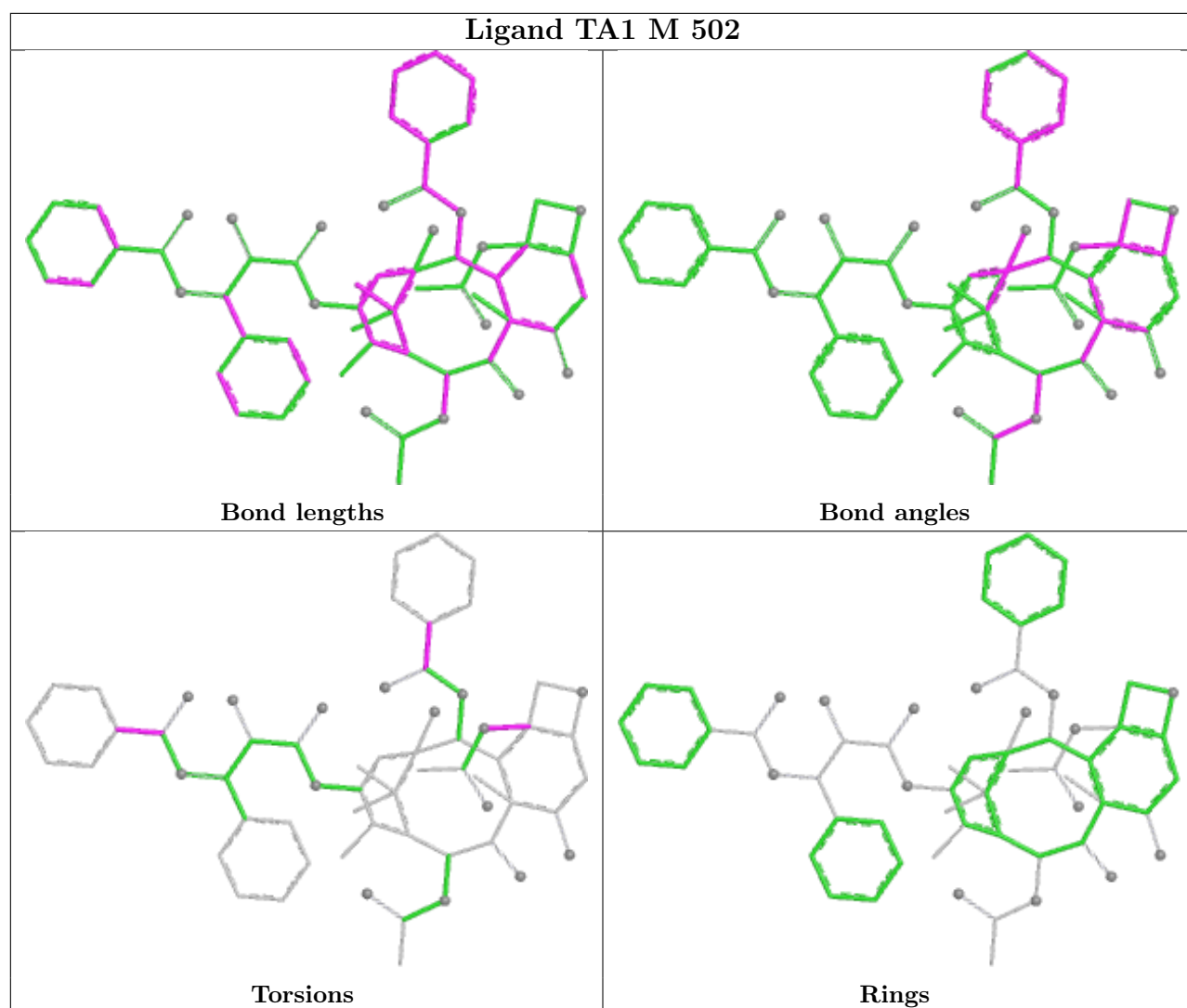
Ligand GDP O 501

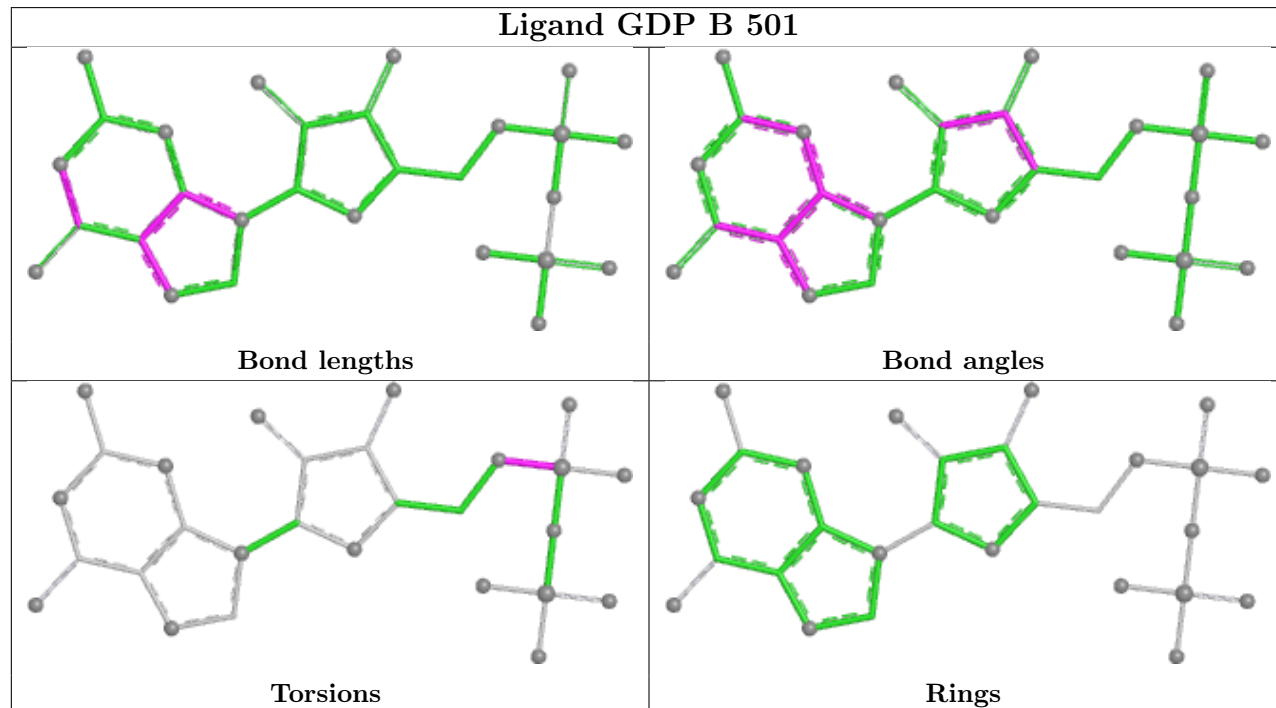
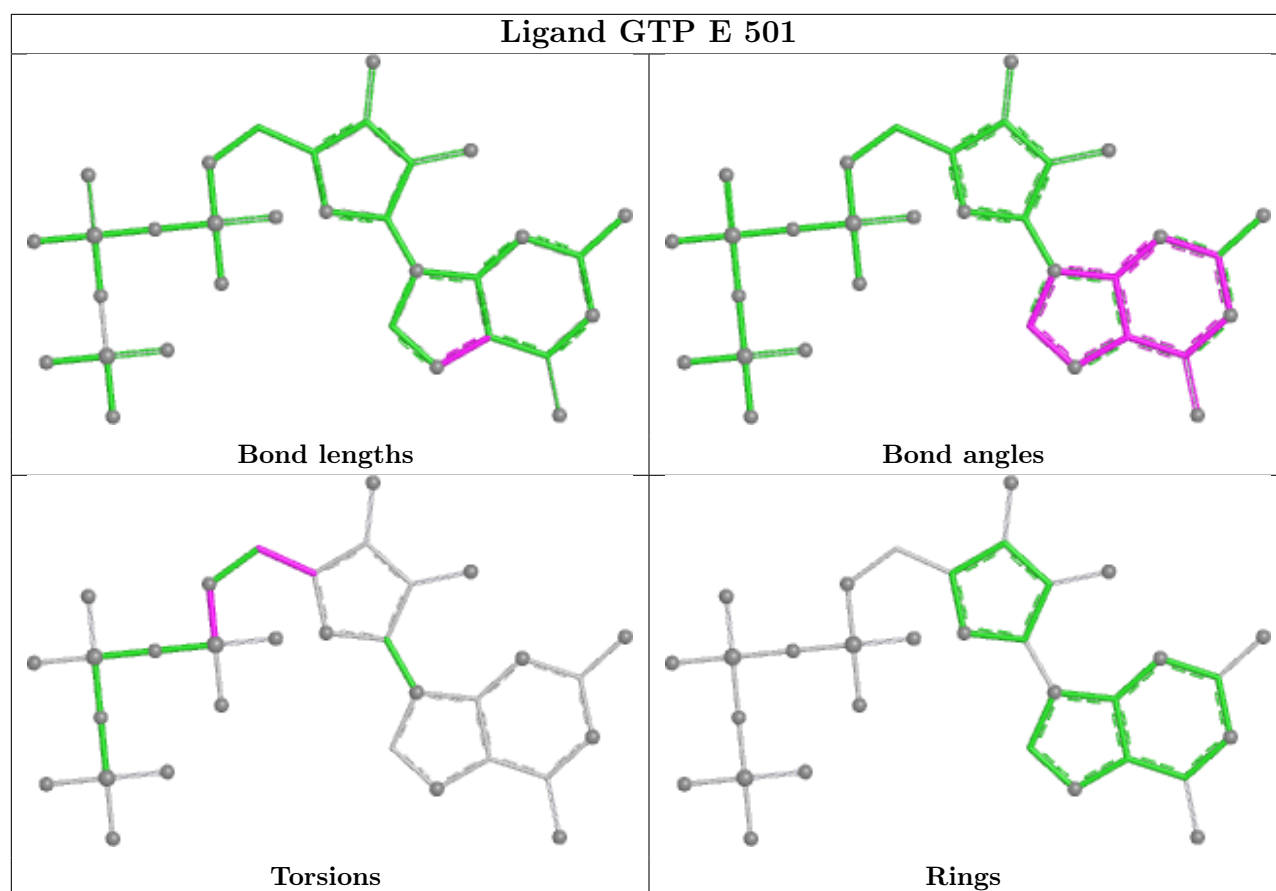




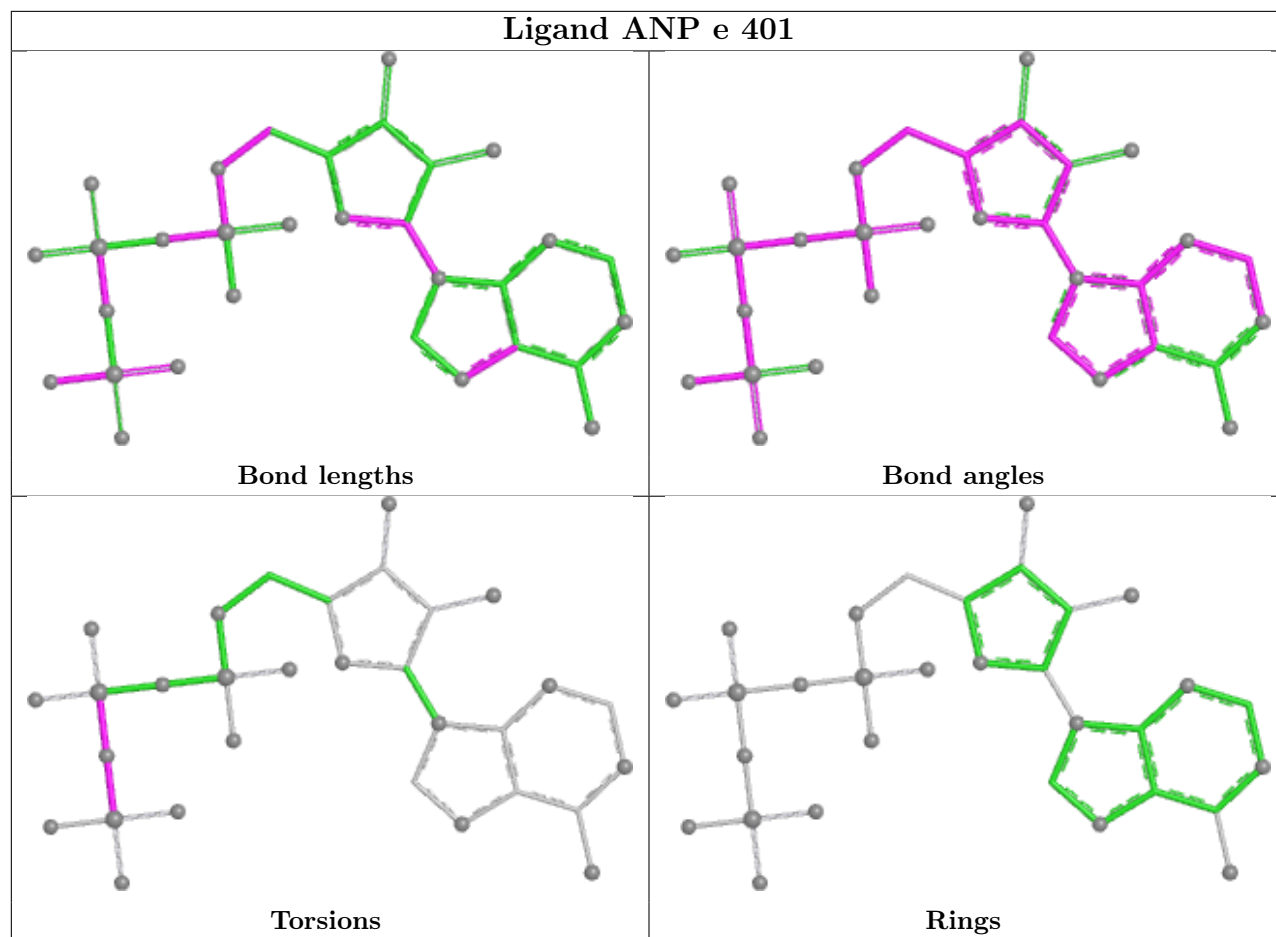


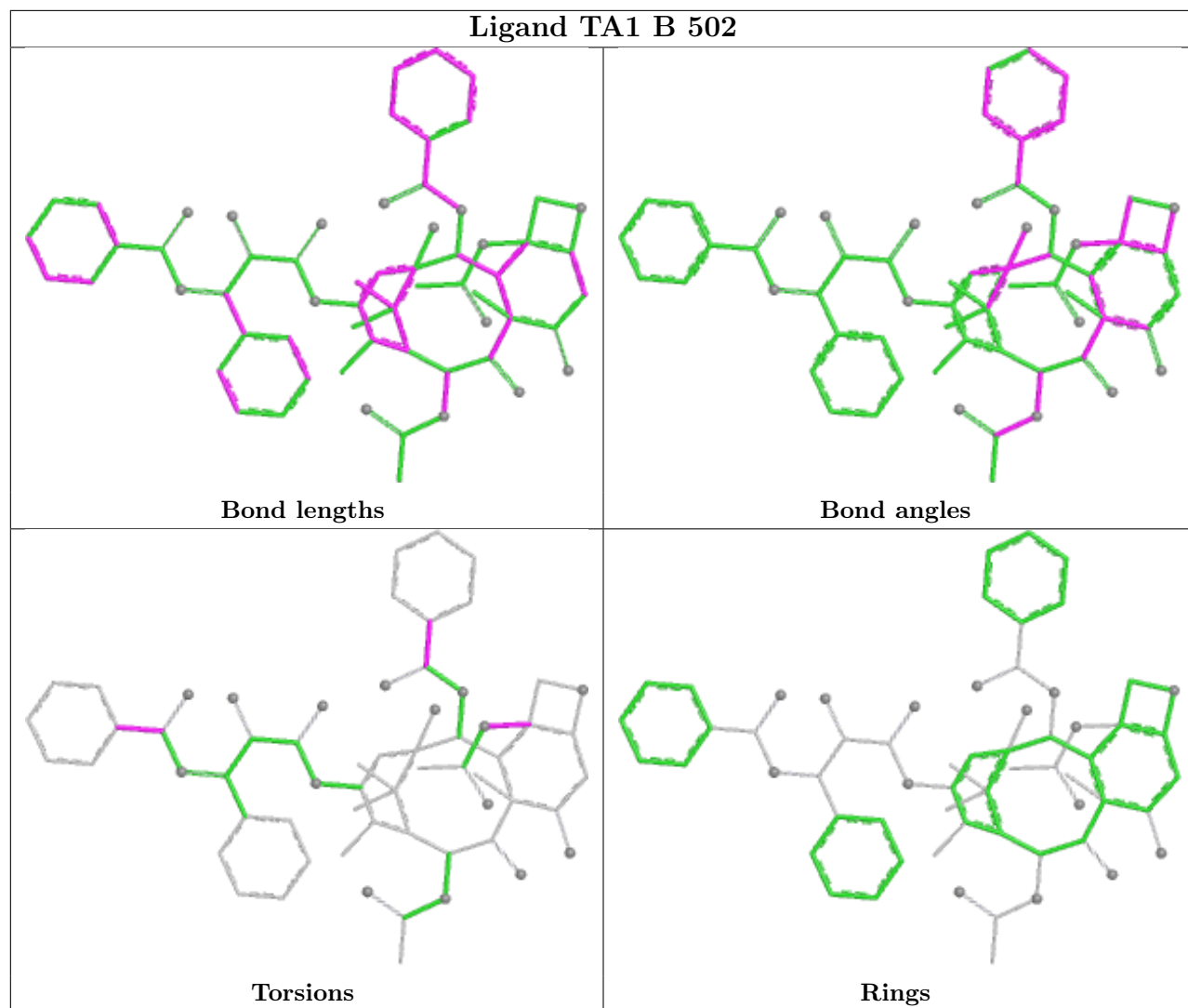


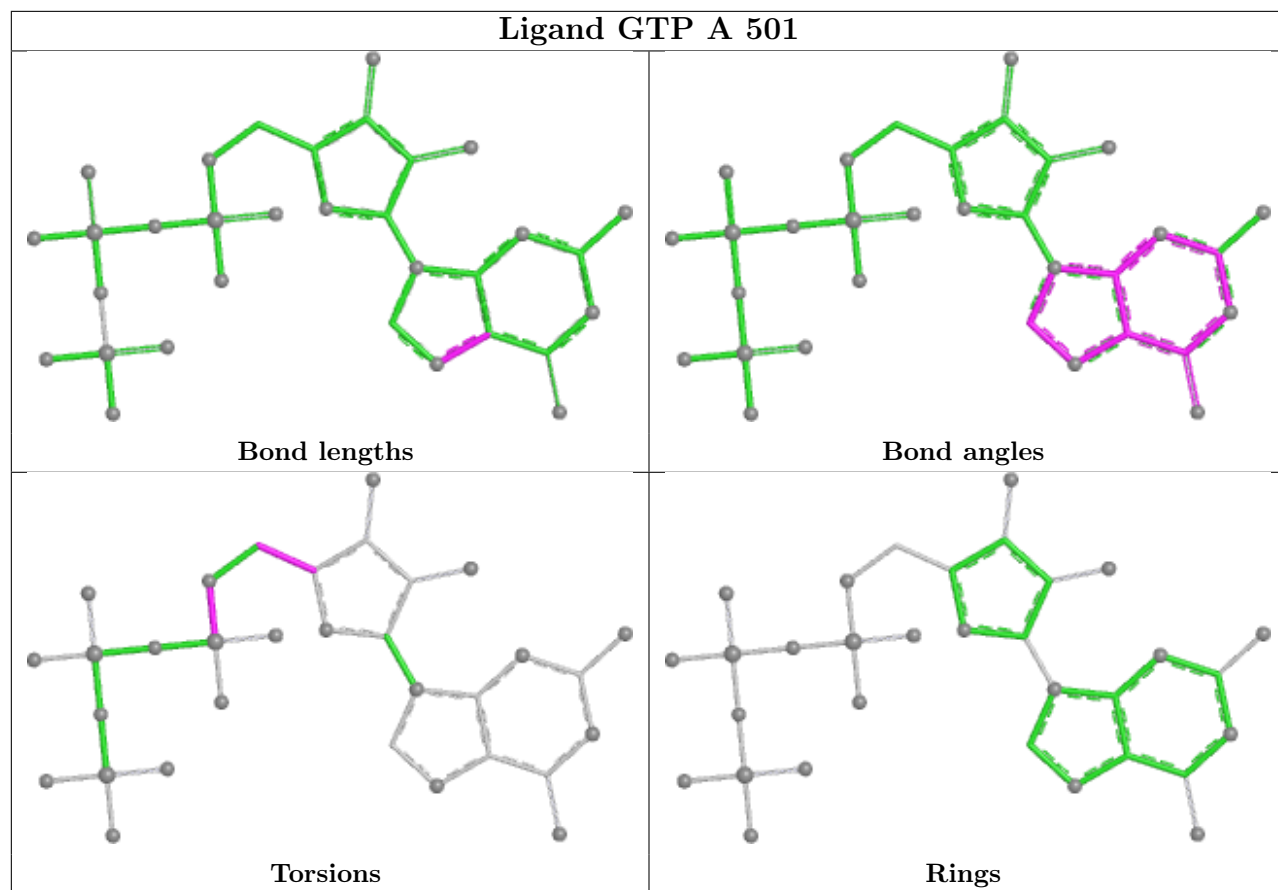




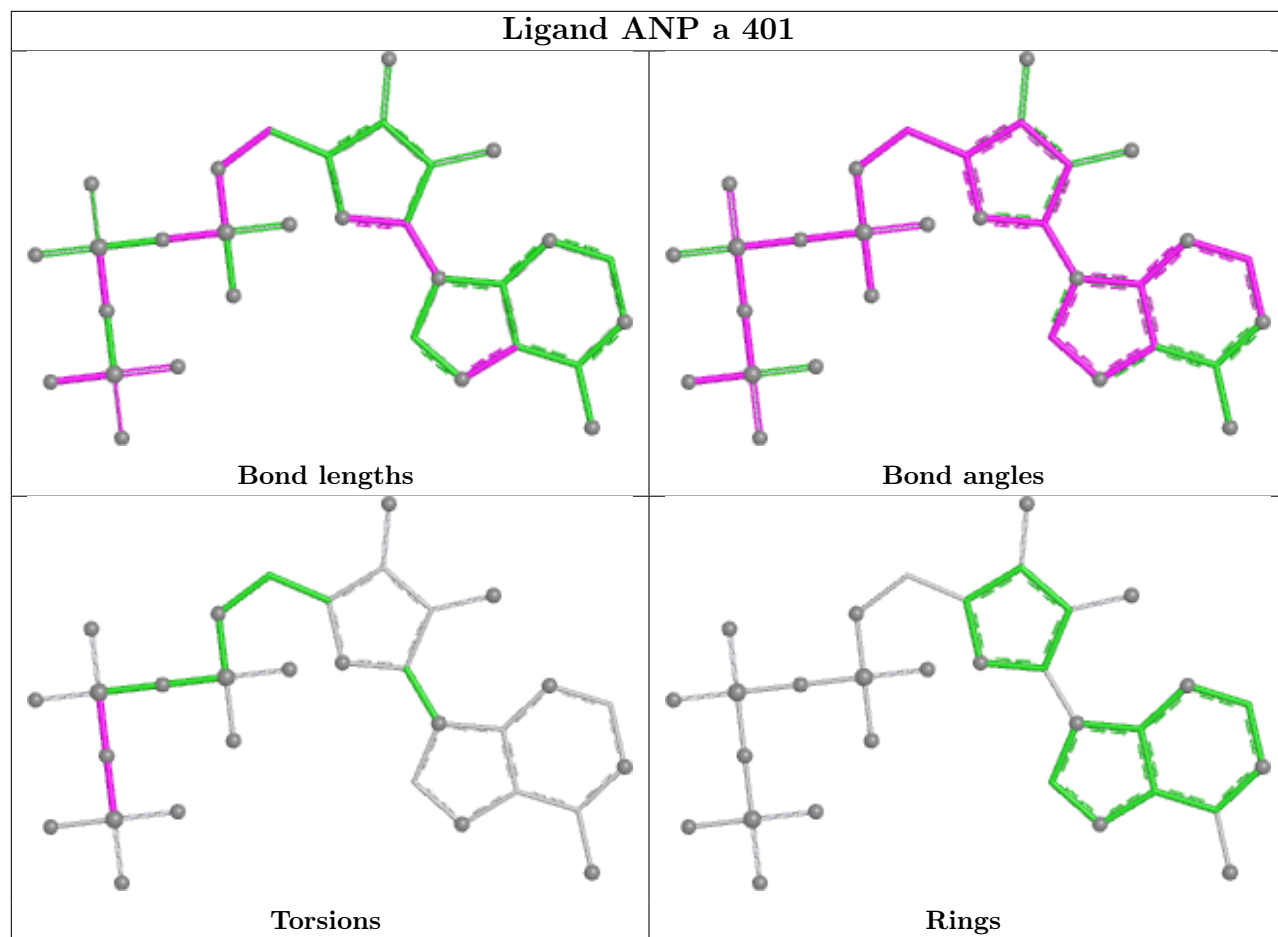
Ligand ANP e 401

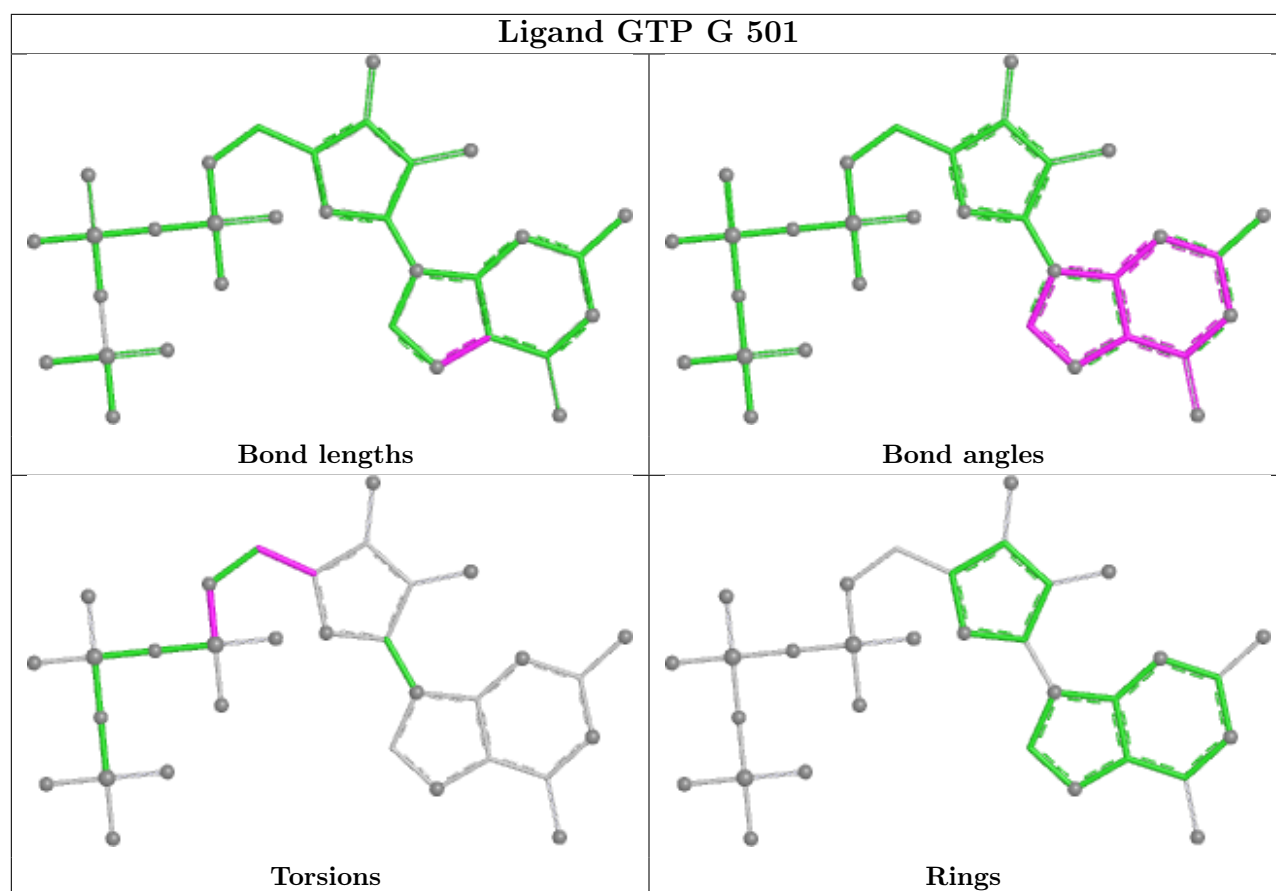






Ligand ANP a 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

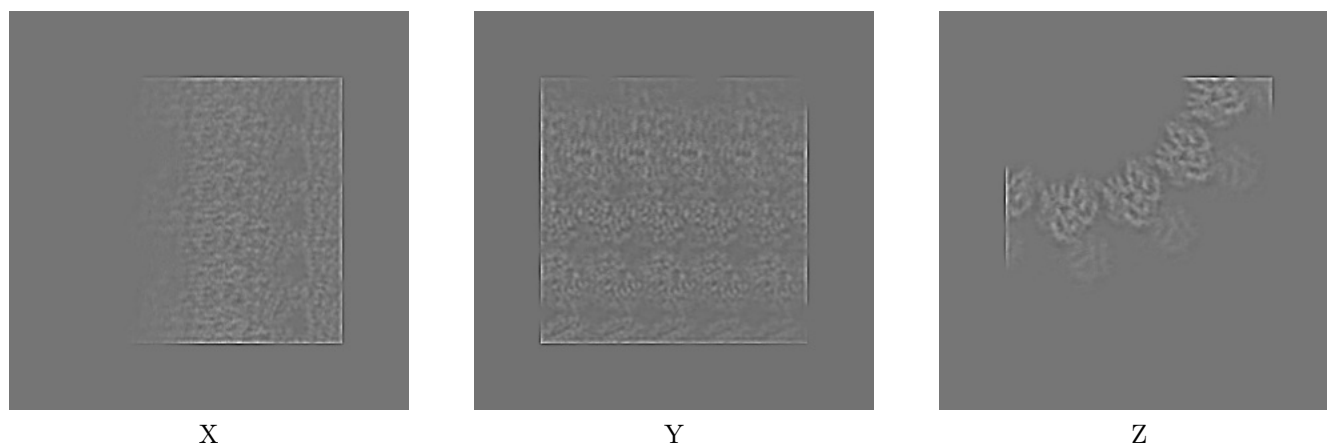
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24666. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

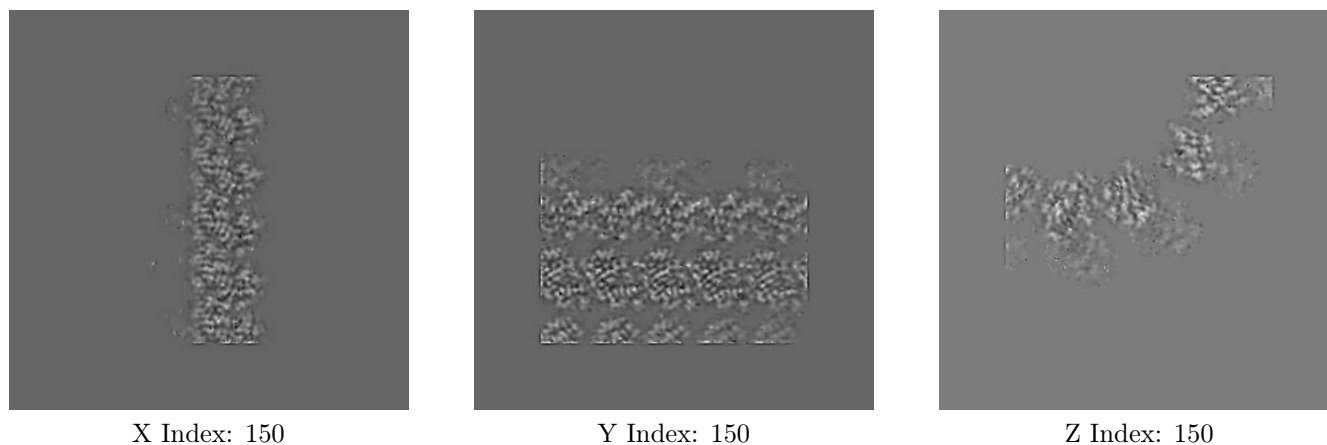
6.1.1 Primary map



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

6.2 Central slices [i](#)

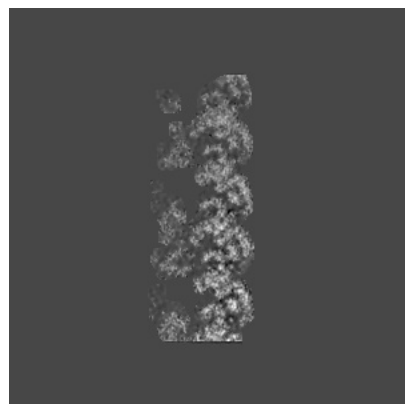
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

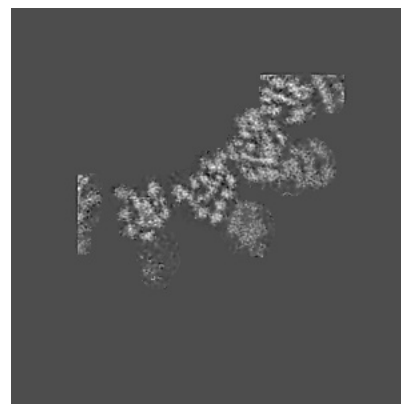
6.3.1 Primary map



X Index: 50



Y Index: 249

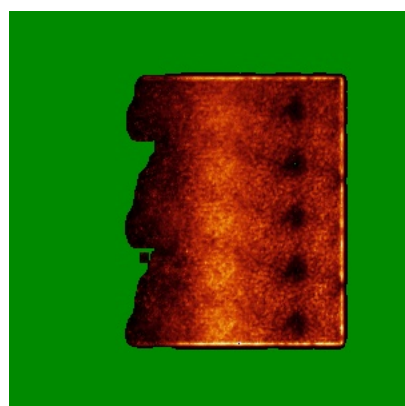


Z Index: 50

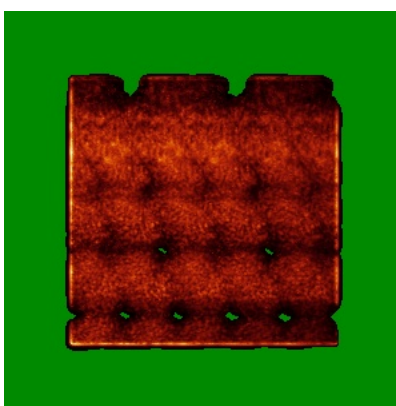
The images above show the largest variance slices of the map in three orthogonal directions.

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

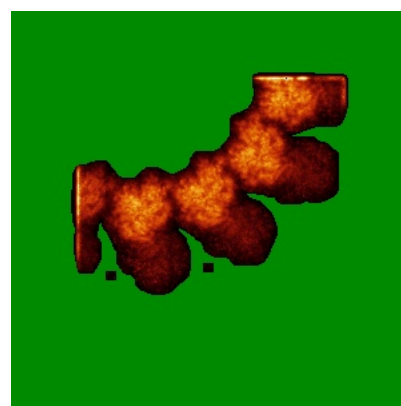
6.4.1 Primary map



X



Y

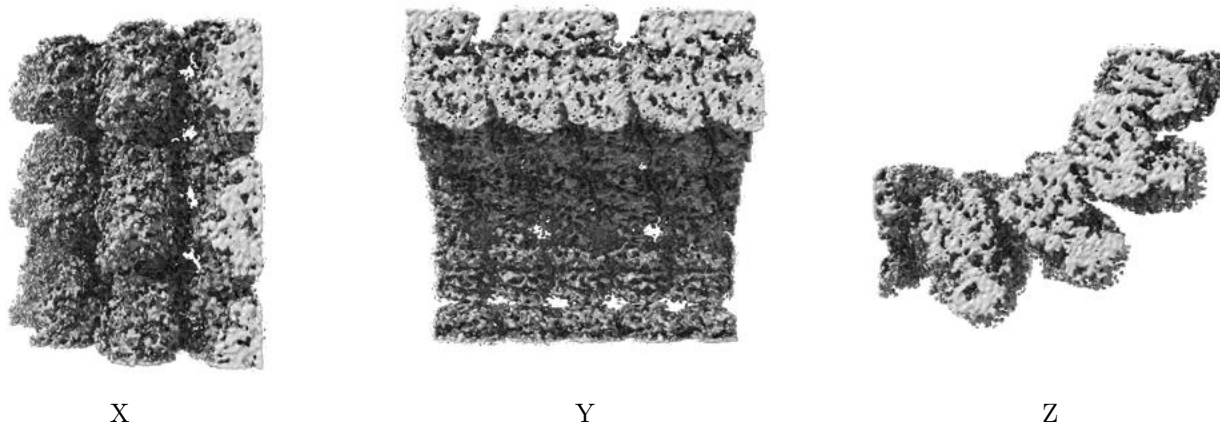


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

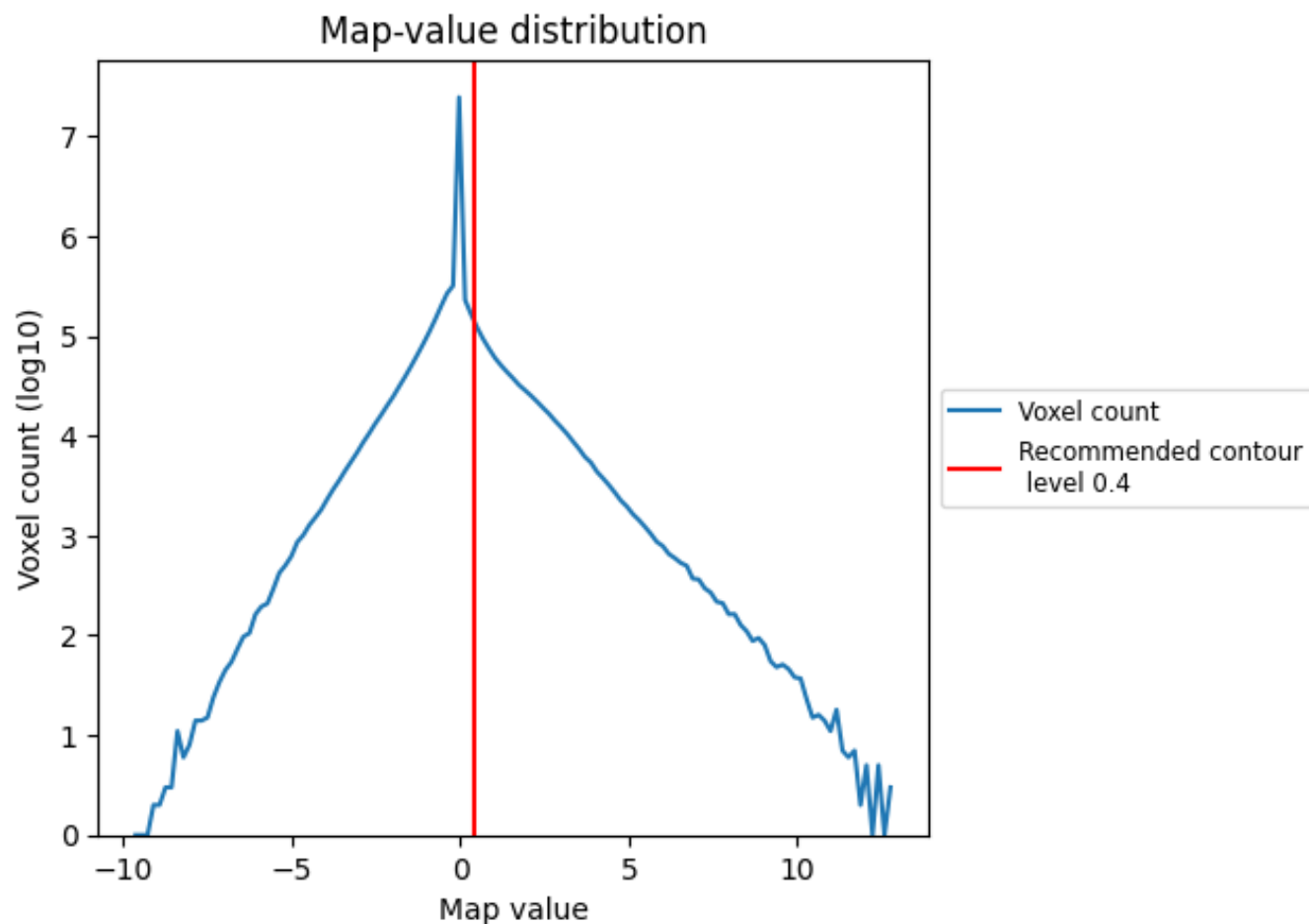
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

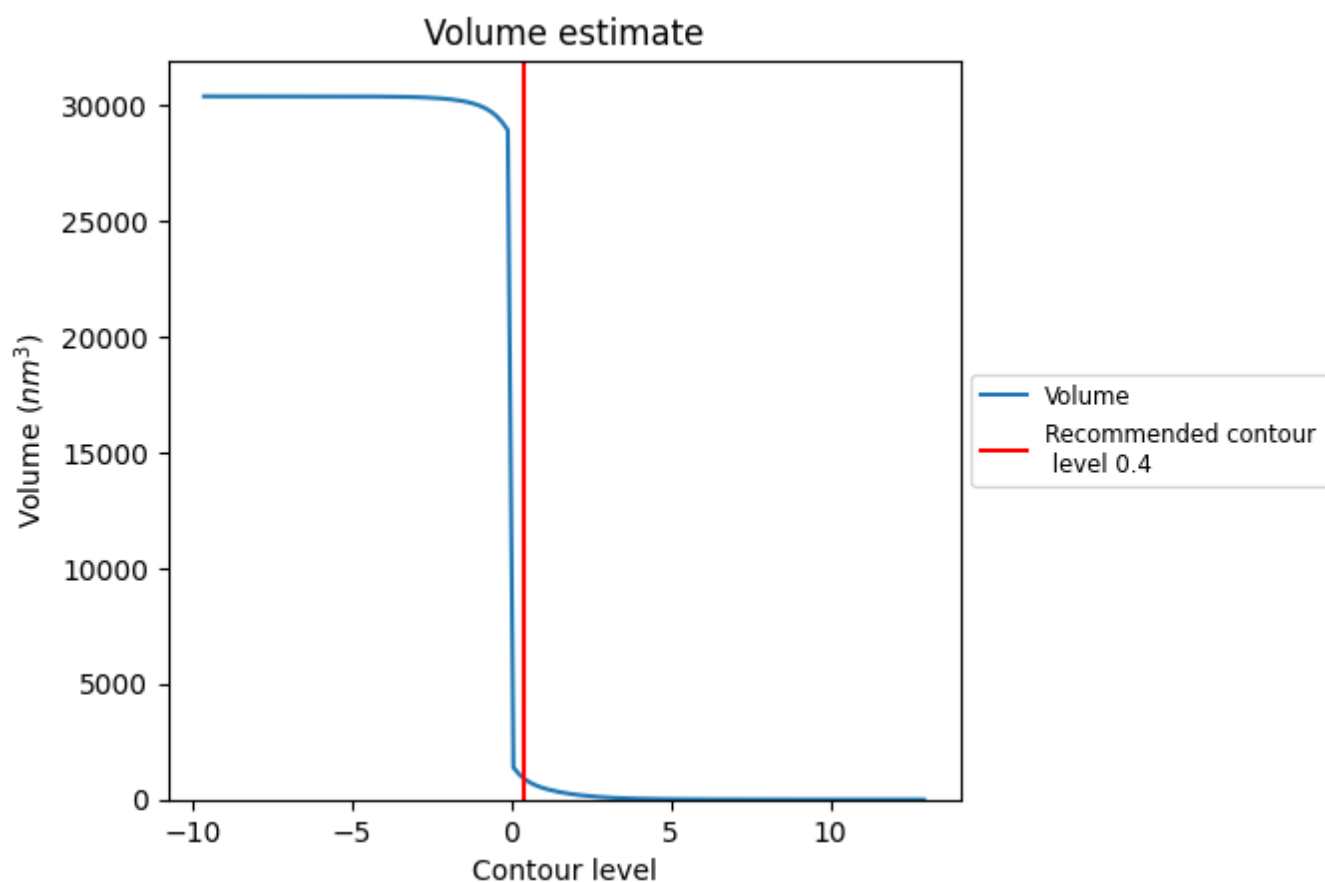
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

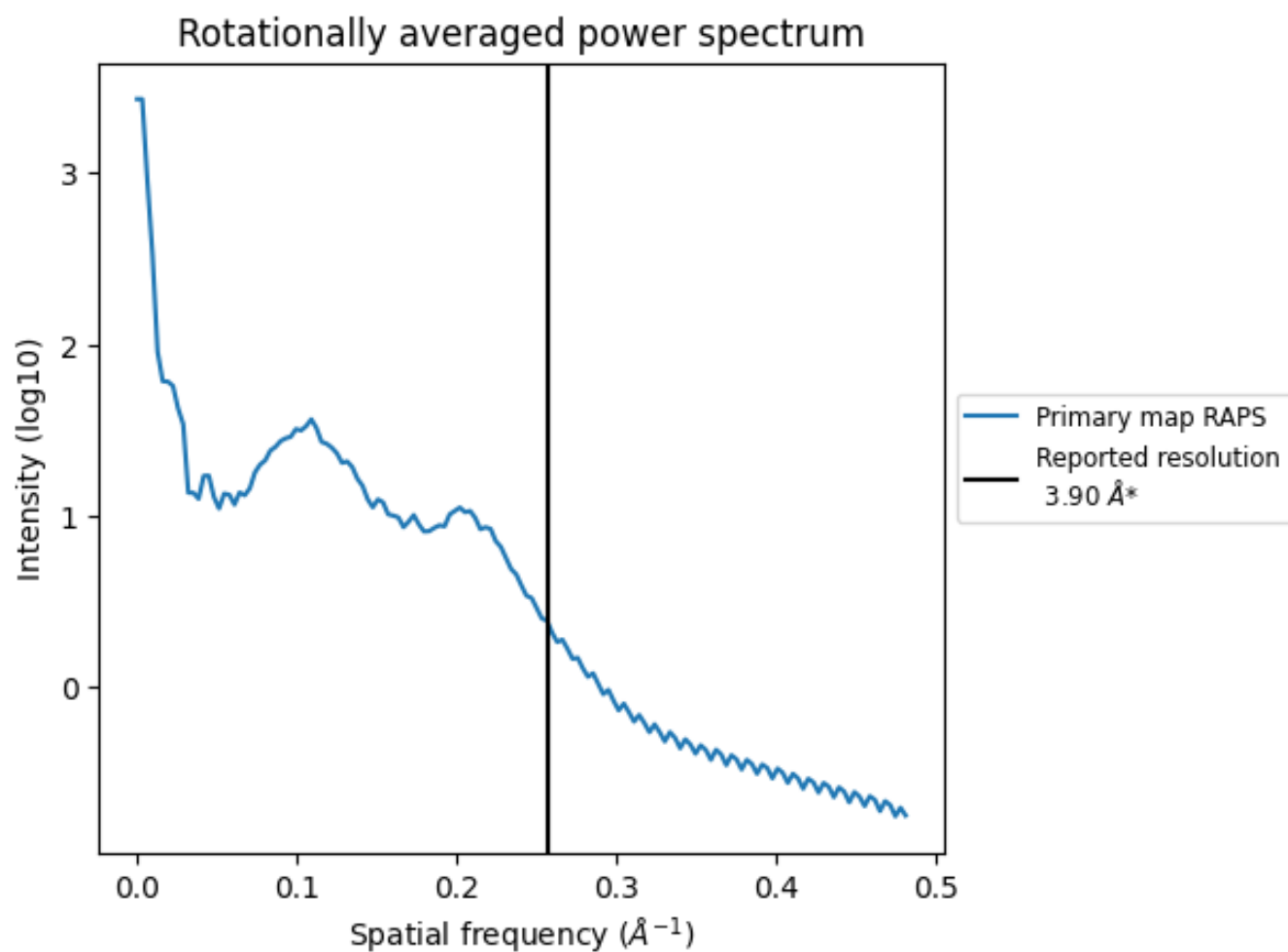
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 914 nm³; this corresponds to an approximate mass of 825 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

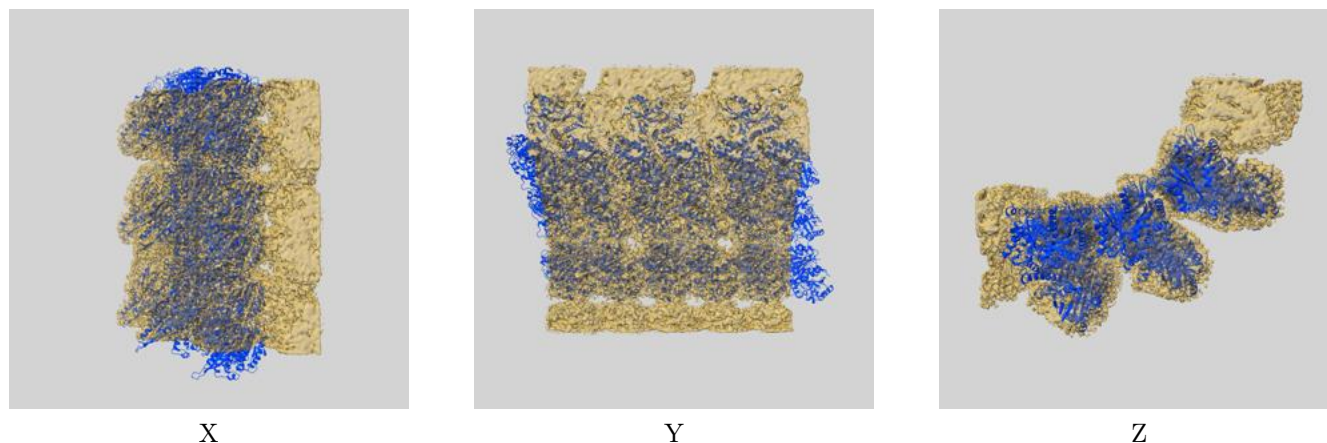
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

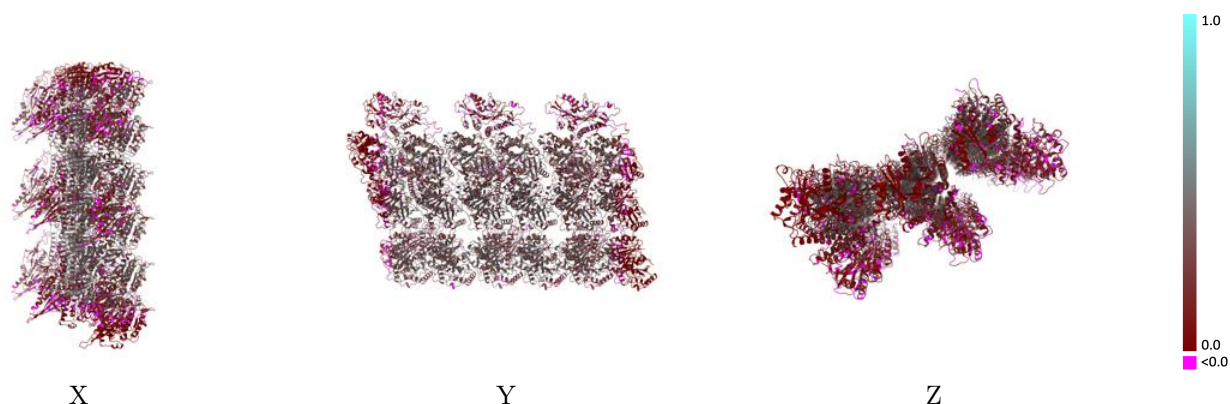
This section contains information regarding the fit between EMDB map EMD-24666 and PDB model 7RS5. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



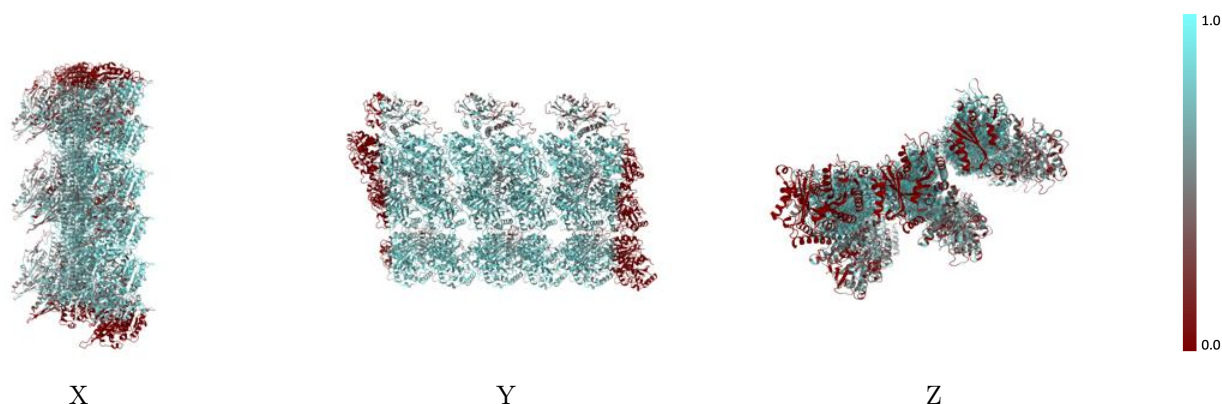
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



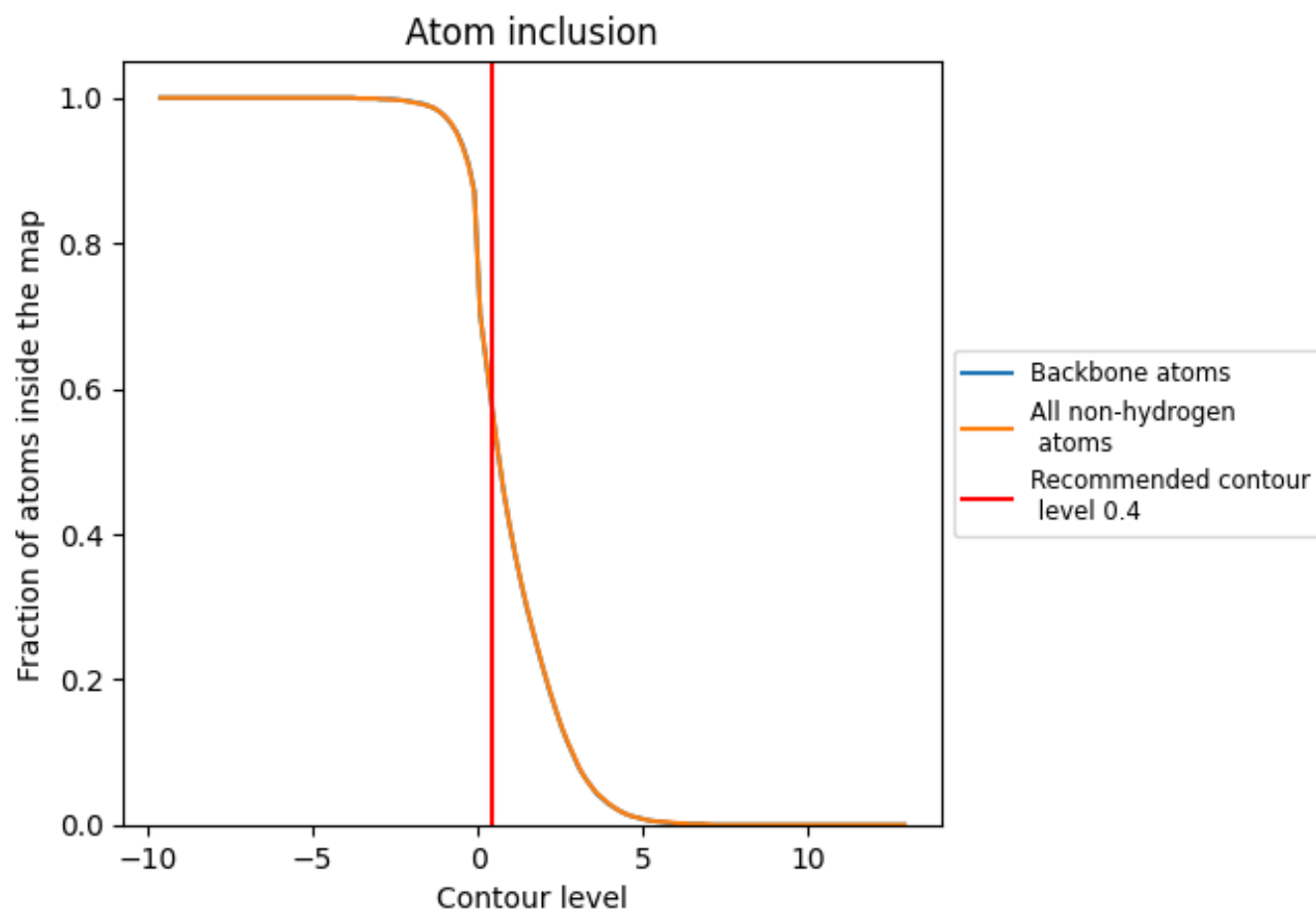
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 59% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5860	 0.2350
A	 0.7870	 0.3460
B	 0.7850	 0.3480
C	 0.7750	 0.3330
D	 0.7730	 0.3370
E	 0.7860	 0.3470
F	 0.7870	 0.3480
G	 0.7950	 0.3400
H	 0.5010	 0.2030
I	 0.3150	 0.1230
J	 0.7560	 0.3160
K	 0.4910	 0.1520
L	 0.7960	 0.3400
M	 0.3070	 0.1200
N	 0.5070	 0.1990
O	 0.7540	 0.3150
P	 0.7800	 0.3320
Q	 0.6550	 0.2690
R	 0.1420	 0.0560
S	 0.7440	 0.3050
a	 0.5060	 0.1490
b	 0.4880	 0.1540
c	 0.4640	 0.1270
d	 0.4360	 0.1210
e	 0.3620	 0.1000
f	 0.4440	 0.1190
g	 0.5310	 0.1540
h	 0.4030	 0.1030

