



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 2QL6 / pdb_00002ql6
Title : human nicotinamide riboside kinase (NRK1)
Authors : Khan, J.A.; Xiang, S.; Tong, L.
Deposited on : 2007-07-12
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

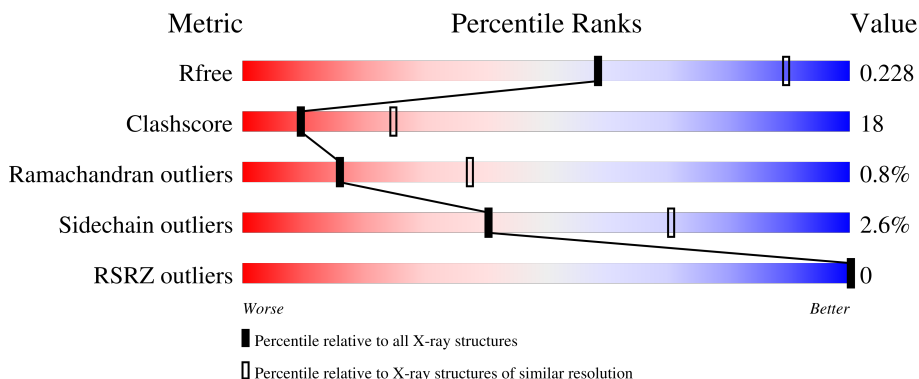
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	 57% 30% • 10%
1	B	199	 55% 31% • 10%
1	C	199	 55% 33% • 10%
1	D	199	 55% 33% • 10%
1	E	199	 59% 29% • 10%

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Mol	Chain	Length	Quality of chain			
1	F	199				
1	G	199				
1	H	199				
1	I	199				
1	J	199				
1	K	199				
1	L	199				
1	M	199				
1	N	199				
1	O	199				
1	P	199				

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24416 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

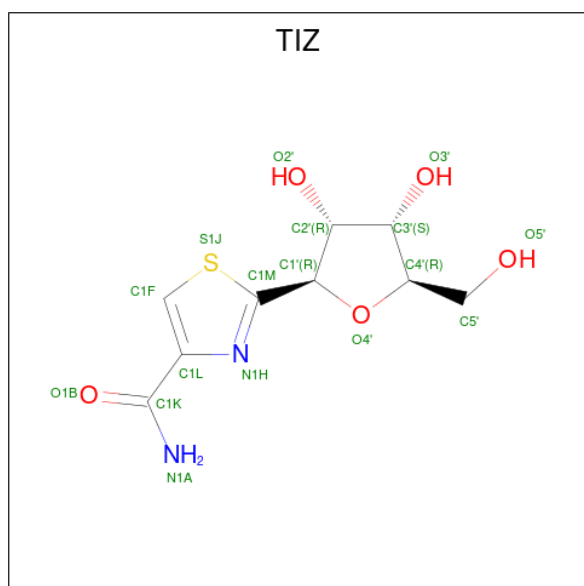
- Molecule 1 is a protein called nicotinamide riboside kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	179	1482	956	238	279	3	6	0	0	0
1	B	179	1482	956	238	279	3	6	0	0	0
1	C	179	1482	956	238	279	3	6	0	0	0
1	D	179	1482	956	238	279	3	6	0	0	0
1	E	179	1482	956	238	279	3	6	0	0	0
1	F	179	1482	956	238	279	3	6	0	0	0
1	G	179	1482	956	238	279	3	6	0	0	0
1	H	179	1482	956	238	279	3	6	0	0	0
1	I	179	1482	956	238	279	3	6	0	0	0
1	J	179	1482	956	238	279	3	6	0	0	0
1	K	179	1482	956	238	279	3	6	0	0	0
1	L	179	1482	956	238	279	3	6	0	0	0
1	M	179	1482	956	238	279	3	6	0	0	0
1	N	179	1482	956	238	279	3	6	0	0	0
1	O	179	1482	956	238	279	3	6	0	0	0
1	P	179	1482	956	238	279	3	6	0	0	0

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

- Molecule 3 is (1R)-1-[4-(AMINOCARBONYL)-1,3-THIAZOL-2-YL]-1,4-ANHYDRO-D-RIBITOL (CCD ID: TIZ) (formula: C₉H₁₂N₂O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	B	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	C	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	D	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	E	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	F	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	G	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	H	1	Total	C	N	O	S	0	0
			17	9	2	5	1		

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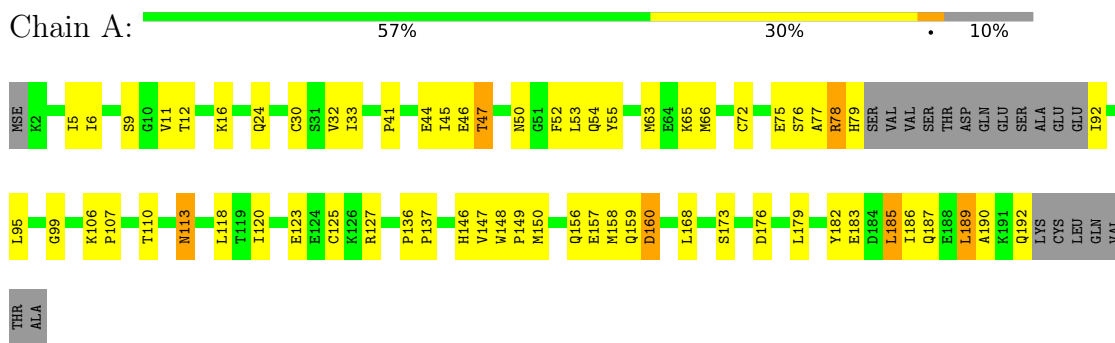
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	I	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	J	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	K	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	L	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	M	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	N	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	O	1	Total	C	N	O	S	0	0
			17	9	2	5	1		
3	P	1	Total	C	N	O	S	0	0
			17	9	2	5	1		

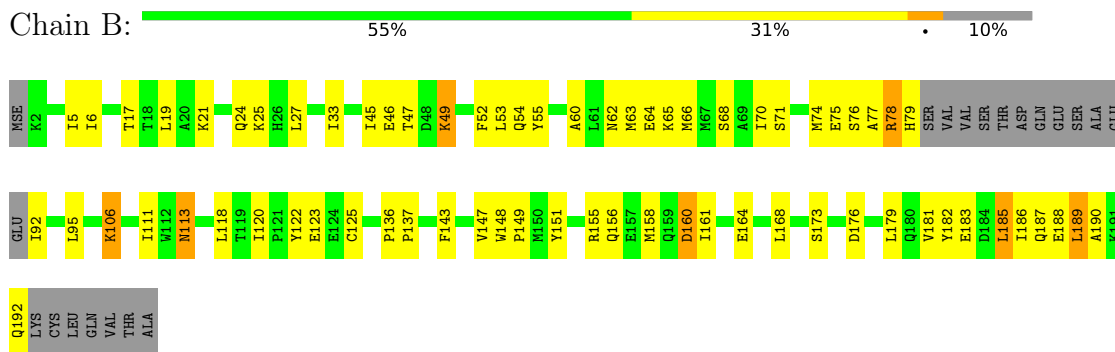
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

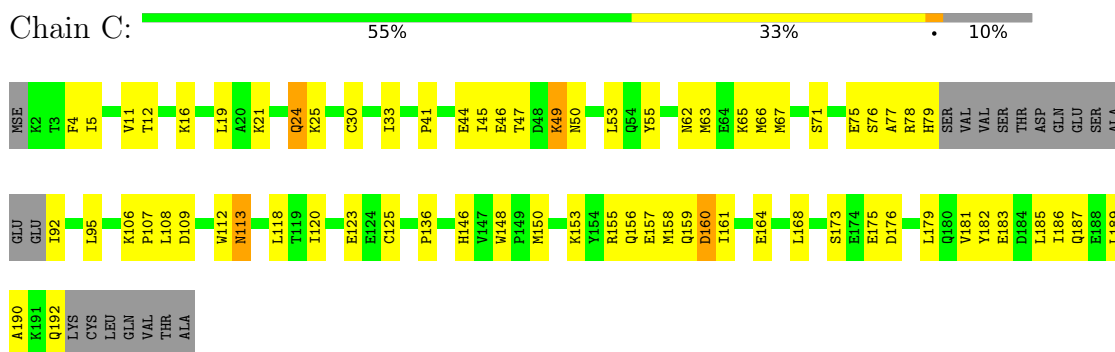
- Molecule 1: nicotinamide riboside kinase 1



- Molecule 1: nicotinamide riboside kinase 1

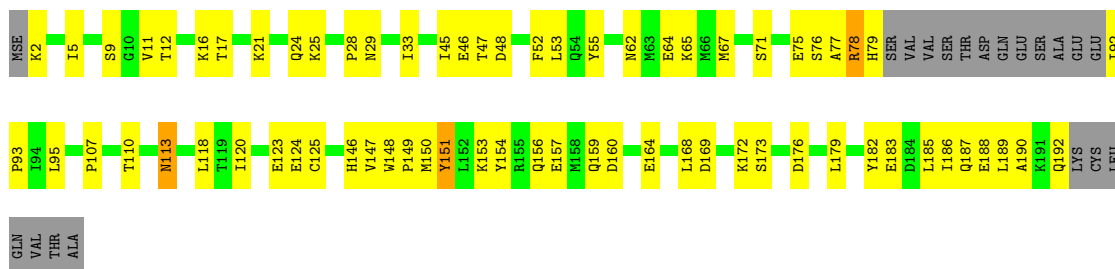


- Molecule 1: nicotinamide riboside kinase 1



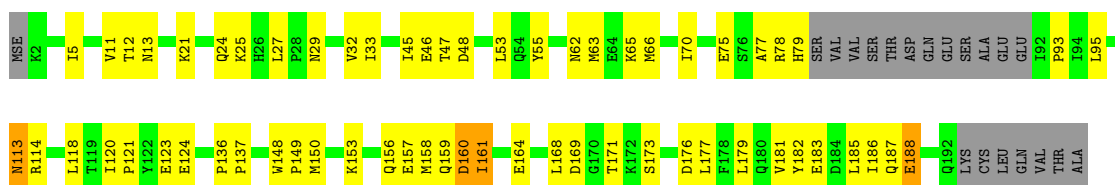
- Molecule 1: nicotinamide riboside kinase 1

Chain D:  55% 33% 10%



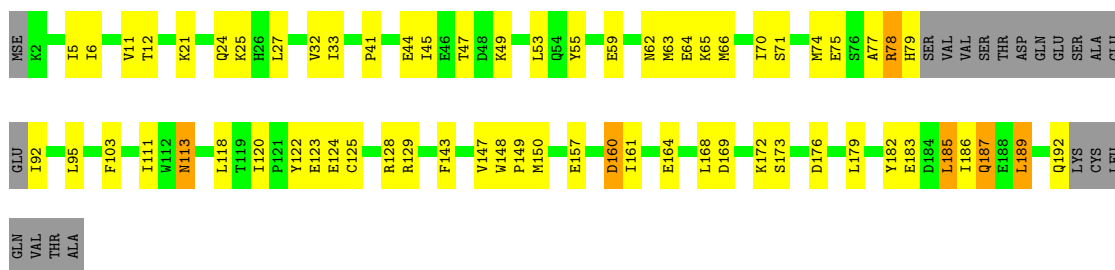
- Molecule 1: nicotinamide riboside kinase 1

Chain E:  59% 29% 10%



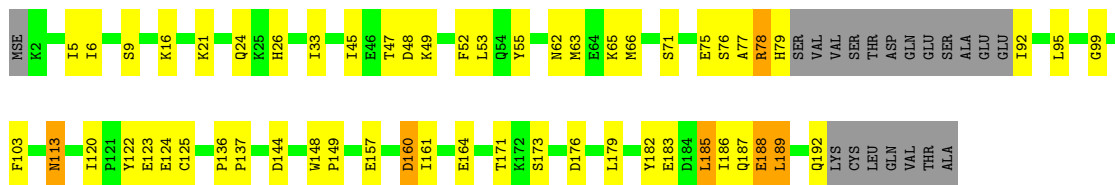
- Molecule 1: nicotinamide riboside kinase 1

Chain F:  57% 30% 10%



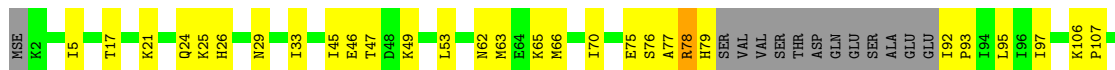
- Molecule 1: nicotinamide riboside kinase 1

Chain G:  62% 25% 10%



- Molecule 1: nicotinamide riboside kinase 1

Chain H:  58% 30% 10%





- Molecule 1: nicotinamide riboside kinase 1

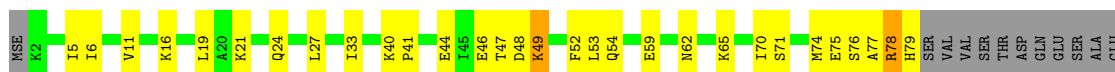
Chain I: 57% 29% 10%



VAL
THR
ALA

- Molecule 1: nicotinamide riboside kinase 1

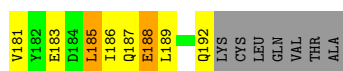
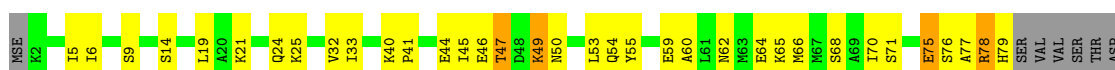
Chain J: 59% 29% 10%



ALA

- Molecule 1: nicotinamide riboside kinase 1

Chain K: 51% 34% 5% 10%



- Molecule 1: nicotinamide riboside kinase 1

Chain L: 56% 32% 10%



K191
Q192
LYS
CYS
LEU
GLN
VAL
THR
ALA

- Molecule 1: nicotinamide riboside kinase 1

Chain M: 55% 33% 10%

MSE
K2 I5 I6 V11 T12 K21 Q24 K25 P28 N29 V32 I33 P41 E44 I45 E46 T47 D48 K49 F52 L53 Q54 Y55 M62 M63 E64 K65 M66 I70 M74 E75 S76 A77 R78 R79 SER VAL VAL SER THR ASP GLN GLU SER ALA GLU

I92 L95 N113 L118 L119 L120 Y121 Y122 E123 E124 C125 K126 R127 F143 D144 G145 H146 W148 P149 M150 Y151 L152 K153 Y154 R155 Q156 E157 M158 Q159 D160 I161 E164 L168 D169 K172 S173 E174 E175 D176 L177 F178 L179 E183 D184 L185 I186 I187 E188 L189 K191

Q192
LYS
CYS
LEU
GLN
VAL
THR
ALA

- Molecule 1: nicotinamide riboside kinase 1

Chain N: 56% 30% 10%

MSE
K2 I5 I6 V11 T12 T18 L19 A20 K21 Q24 K25 N29 I33 D37 E44 T47 K49 F52 L53 Q54 A60 L61 M62 M63 K65 M66 I70 S71 M74 E75 S76 A77 R78 SER THR ASP GLN

GLU SER ALA GLU 192 P93 L94 L95 Y105 K106 P107 I111 W112 N113 L118 L119 L120 Y121 Y122 E123 E124 R128 F143 Q156 E157 M158 Q159 D160 I161 L168 T171 K172 S173 E174 E175 D176 L179 Q180 Y181 Y182 E183 D184 L185 I186 Q187 Q188 L189 Q192 LYS

CYS
LEU
VAL
THR
ALA

- Molecule 1: nicotinamide riboside kinase 1

Chain O: 54% 34% 10%

MSE
K2 I5 V11 T12 T17 K21 Q24 K25 H26 N29 I33 P41 E44 I45 E46 T47 D48 K49 L53 Q54 Y55 M62 M63 E64 A65 M66 M67 E75 S76 A77 R78 H79 SER VAL VAL THR ASP GLN GLU THR SER

L95 I96 I97 F103 L108 L112 N113 L118 L119 L120 Y121 Y122 E123 E124 C125 P136 P137 D144 G145 H146 V147 W148 P149 M150 Y151 R155 Q156 Q159 D160 K65 M66 I161 E164 L168 S173 E174 E175 D176 L179 Y182 Q183 L184 L185 L186 Q187 E188 L189

A190
K191
Q192
LYS
CYS
LEU
GLN
VAL
THR
ALA

- Molecule 1: nicotinamide riboside kinase 1

Chain P: 54% 34% 10%

MSE
K2 I5 I6 S9 G10 T12 K16 K21 Q24 K25 H26 L27 I33 P41 E44 I45 E46 T47 L53 Q54 Y55 M62 M63 E64 K65 M66 I70 M74 E75 S76 A77 R78 H79 SER VAL VAL THR ASP GLN GLU THR SER ALA GLU

P93 I94 L95 Y105 K106 P107 T110 V111 N113 L118 Y122 E123 E124 P136 P137 D144 G145 H146 W148 P149 M150 Y151 Q156 E157 M158 Q159 D160 L168 K172 S173 E174 E175 D176 L177 F178 L179 Y182 E183 D184 L185 I186 Q187 E188 L189 A190 K191 Q192 LYS CYS

LEU
GLN
VAL
THR
ALA

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.71Å 99.96Å 145.59Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-2.70) 96.5 (30.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.235 0.202 , 0.228	Depositor DCC
R_{free} test set	10338 reflections (8.87%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.431	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.196 for -l,k,h 0.199 for -h,-k,l 0.420 for l,-k,h	Xtrriage
Reported twinning fraction	0.370 for l,-k,h	Depositor
Outliers	0 of 116523 reflections	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24416	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TIZ, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.61	0/1513	1.00	6/2037 (0.3%)
1	B	0.66	0/1513	1.02	7/2037 (0.3%)
1	C	0.61	0/1513	1.01	6/2037 (0.3%)
1	D	0.62	0/1513	0.98	6/2037 (0.3%)
1	E	0.64	0/1513	0.99	5/2037 (0.2%)
1	F	0.60	0/1513	0.97	5/2037 (0.2%)
1	G	0.65	0/1513	0.99	5/2037 (0.2%)
1	H	0.62	0/1513	0.97	2/2037 (0.1%)
1	I	0.67	1/1513 (0.1%)	1.27	11/2037 (0.5%)
1	J	0.61	0/1513	0.98	4/2037 (0.2%)
1	K	0.66	0/1513	1.06	10/2037 (0.5%)
1	L	0.61	0/1513	1.01	7/2037 (0.3%)
1	M	0.63	0/1513	0.98	5/2037 (0.2%)
1	N	0.60	0/1513	1.01	5/2037 (0.2%)
1	O	0.60	0/1513	0.97	8/2037 (0.4%)
1	P	0.61	0/1513	1.00	7/2037 (0.3%)
All	All	0.62	1/24208 (0.0%)	1.02	99/32592 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	135	GLN	C-O	-5.24	1.17	1.24

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	135	GLN	CA-C-N	-22.63	97.07	120.38
1	I	135	GLN	C-N-CA	-22.63	97.07	120.38
1	L	113	ASN	N-CA-C	-9.56	102.19	114.04
1	K	188	GLU	N-CA-C	-9.16	104.17	114.62
1	O	113	ASN	N-CA-C	-8.68	103.27	114.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	135	GLN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1482	0	1449	64	0
1	B	1482	0	1449	59	0
1	C	1482	0	1449	58	0
1	D	1482	0	1449	61	0
1	E	1482	0	1449	49	0
1	F	1482	0	1449	55	0
1	G	1482	0	1449	44	0
1	H	1482	0	1449	51	0
1	I	1482	0	1449	75	0
1	J	1482	0	1449	60	0
1	K	1482	0	1449	65	0
1	L	1482	0	1449	53	0
1	M	1482	0	1449	51	0
1	N	1482	0	1449	58	0
1	O	1482	0	1449	50	0
1	P	1482	0	1449	58	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	0	0
2	H	27	0	12	1	0
2	I	27	0	12	1	0
2	J	27	0	12	0	0
2	K	27	0	12	0	0
2	L	27	0	12	0	0
2	M	27	0	12	0	0
2	N	27	0	12	0	0
2	O	27	0	12	0	0
2	P	27	0	12	0	0
3	A	17	0	12	0	0
3	B	17	0	12	0	0
3	C	17	0	12	0	0
3	D	17	0	12	0	0
3	E	17	0	12	0	0
3	F	17	0	12	1	0
3	G	17	0	12	0	0
3	H	17	0	12	0	0
3	I	17	0	12	1	0
3	J	17	0	12	0	0
3	K	17	0	12	0	0
3	L	17	0	12	0	0
3	M	17	0	12	0	0
3	N	17	0	12	0	0
3	O	17	0	12	0	0
3	P	17	0	12	0	0
All	All	24416	0	23568	853	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 18.

The worst 5 of 853 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:D:110:THR:HG21	1:F:111:ILE:HD11	1.21	1.10
1:I:78:ARG:CZ	1:J:160:ASP:HB3	1.81	1.09
1:A:110:THR:HG21	1:B:111:ILE:HD11	1.28	1.08
1:P:47:THR:HG22	1:P:53:LEU:HD23	1.36	1.07
1:G:5:ILE:H	1:G:113:ASN:HD22	1.03	1.00

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 X-ray entries followed by that with respect to entries of similar resolution.

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	175/199 (88%)	163 (93%)	11 (6%)	1 (1%)	21	44
1	B	175/199 (88%)	162 (93%)	12 (7%)	1 (1%)	21	44
1	C	175/199 (88%)	161 (92%)	13 (7%)	1 (1%)	21	44
1	D	175/199 (88%)	163 (93%)	11 (6%)	1 (1%)	21	44
1	E	175/199 (88%)	162 (93%)	11 (6%)	2 (1%)	11	29
1	F	175/199 (88%)	162 (93%)	12 (7%)	1 (1%)	21	44
1	G	175/199 (88%)	164 (94%)	10 (6%)	1 (1%)	21	44
1	H	175/199 (88%)	168 (96%)	6 (3%)	1 (1%)	21	44
1	I	175/199 (88%)	161 (92%)	9 (5%)	5 (3%)	3	9
1	J	175/199 (88%)	159 (91%)	15 (9%)	1 (1%)	21	44
1	K	175/199 (88%)	161 (92%)	12 (7%)	2 (1%)	11	29
1	L	175/199 (88%)	163 (93%)	11 (6%)	1 (1%)	21	44
1	M	175/199 (88%)	163 (93%)	12 (7%)	0	100	100
1	N	175/199 (88%)	164 (94%)	9 (5%)	2 (1%)	11	29
1	O	175/199 (88%)	165 (94%)	9 (5%)	1 (1%)	21	44
1	P	175/199 (88%)	161 (92%)	13 (7%)	1 (1%)	21	44
All	All	2800/3184 (88%)	2602 (93%)	176 (6%)	22 (1%)	16	37

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	78	ARG
1	I	136	PRO
1	D	78	ARG
1	F	78	ARG

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Mol	Chain	Res	Type
1	I	135	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	B	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	C	166/177 (94%)	161 (97%)	5 (3%)	36 66
1	D	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	E	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	F	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	G	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	H	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	I	166/177 (94%)	161 (97%)	5 (3%)	36 66
1	J	166/177 (94%)	161 (97%)	5 (3%)	36 66
1	K	166/177 (94%)	160 (96%)	6 (4%)	31 60
1	L	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	M	166/177 (94%)	161 (97%)	5 (3%)	36 66
1	N	166/177 (94%)	162 (98%)	4 (2%)	43 72
1	O	166/177 (94%)	161 (97%)	5 (3%)	36 66
1	P	166/177 (94%)	163 (98%)	3 (2%)	51 78
All	All	2656/2832 (94%)	2586 (97%)	70 (3%)	40 70

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	185	LEU
1	N	49	LYS
1	O	160	ASP
1	F	185	LEU

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Mol	Chain	Res	Type
1	F	160	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	156	GLN
1	O	13	ASN
1	P	113	ASN
1	F	26	HIS
1	F	13	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	E	301	-	28,29,29	1.16	4 (14%)	43,45,45	1.76	9 (20%)
3	TIZ	M	302	-	17,18,18	1.18	2 (11%)	25,26,26	1.99	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	D	301	-	28,29,29	1.18	4 (14%)	43,45,45	1.84	10 (23%)
2	ADP	K	301	-	28,29,29	1.16	3 (10%)	43,45,45	1.69	7 (16%)
3	TIZ	D	302	-	17,18,18	1.17	2 (11%)	25,26,26	2.06	9 (36%)
2	ADP	P	301	-	28,29,29	1.16	3 (10%)	43,45,45	1.75	8 (18%)
3	TIZ	E	302	-	17,18,18	1.20	2 (11%)	25,26,26	1.97	8 (32%)
3	TIZ	I	302	-	17,18,18	1.18	2 (11%)	25,26,26	2.01	8 (32%)
3	TIZ	F	302	-	17,18,18	1.19	2 (11%)	25,26,26	1.90	7 (28%)
2	ADP	F	301	-	28,29,29	1.17	3 (10%)	43,45,45	1.69	7 (16%)
2	ADP	B	301	-	28,29,29	1.16	3 (10%)	43,45,45	1.76	9 (20%)
3	TIZ	K	302	-	17,18,18	1.19	2 (11%)	25,26,26	1.92	7 (28%)
3	TIZ	H	302	-	17,18,18	1.20	2 (11%)	25,26,26	2.02	8 (32%)
3	TIZ	G	302	-	17,18,18	1.19	2 (11%)	25,26,26	2.06	7 (28%)
2	ADP	J	301	-	28,29,29	1.16	3 (10%)	43,45,45	1.70	7 (16%)
2	ADP	N	301	-	28,29,29	1.16	3 (10%)	43,45,45	1.75	7 (16%)
3	TIZ	O	302	-	17,18,18	1.17	2 (11%)	25,26,26	1.96	8 (32%)
2	ADP	I	301	-	28,29,29	1.17	4 (14%)	43,45,45	1.79	9 (20%)
3	TIZ	L	302	-	17,18,18	1.20	2 (11%)	25,26,26	2.10	9 (36%)
3	TIZ	C	302	-	17,18,18	1.20	2 (11%)	25,26,26	1.90	7 (28%)
2	ADP	A	301	-	28,29,29	1.17	4 (14%)	43,45,45	1.76	9 (20%)
3	TIZ	B	302	-	17,18,18	1.18	2 (11%)	25,26,26	1.91	7 (28%)
3	TIZ	P	302	-	17,18,18	1.23	2 (11%)	25,26,26	2.08	11 (44%)
2	ADP	H	301	-	28,29,29	1.17	3 (10%)	43,45,45	1.78	8 (18%)
2	ADP	G	301	-	28,29,29	1.15	3 (10%)	43,45,45	1.73	9 (20%)
2	ADP	M	301	-	28,29,29	1.17	4 (14%)	43,45,45	1.74	8 (18%)
3	TIZ	A	302	-	17,18,18	1.20	2 (11%)	25,26,26	2.07	8 (32%)
2	ADP	C	301	-	28,29,29	1.17	3 (10%)	43,45,45	1.76	9 (20%)
2	ADP	O	301	-	28,29,29	1.17	3 (10%)	43,45,45	1.75	9 (20%)
2	ADP	L	301	-	28,29,29	1.17	2 (7%)	43,45,45	1.78	9 (20%)
3	TIZ	J	302	-	17,18,18	1.21	2 (11%)	25,26,26	1.94	7 (28%)
3	TIZ	N	302	-	17,18,18	1.20	2 (11%)	25,26,26	1.98	7 (28%)

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
2	ADP	E	301	-	-	1/16/32/32	0/3/3/3
3	TIZ	M	302	-	-	3/10/26/26	0/2/2/2
2	ADP	D	301	-	-	0/16/32/32	0/3/3/3
2	ADP	K	301	-	-	1/16/32/32	0/3/3/3
3	TIZ	D	302	-	-	3/10/26/26	0/2/2/2
2	ADP	P	301	-	-	0/16/32/32	0/3/3/3
3	TIZ	E	302	-	-	5/10/26/26	0/2/2/2
3	TIZ	I	302	-	-	4/10/26/26	0/2/2/2
3	TIZ	F	302	-	-	3/10/26/26	0/2/2/2
2	ADP	F	301	-	-	0/16/32/32	0/3/3/3
2	ADP	B	301	-	-	0/16/32/32	0/3/3/3
3	TIZ	K	302	-	-	4/10/26/26	0/2/2/2
3	TIZ	H	302	-	-	3/10/26/26	0/2/2/2
3	TIZ	G	302	-	-	3/10/26/26	0/2/2/2
2	ADP	J	301	-	-	0/16/32/32	0/3/3/3
2	ADP	N	301	-	-	0/16/32/32	0/3/3/3
3	TIZ	O	302	-	-	3/10/26/26	0/2/2/2
2	ADP	I	301	-	-	0/16/32/32	0/3/3/3
3	TIZ	L	302	-	-	4/10/26/26	0/2/2/2
3	TIZ	C	302	-	-	4/10/26/26	0/2/2/2
2	ADP	A	301	-	-	0/16/32/32	0/3/3/3
3	TIZ	B	302	-	-	4/10/26/26	0/2/2/2
3	TIZ	P	302	-	-	3/10/26/26	0/2/2/2
2	ADP	H	301	-	-	1/16/32/32	0/3/3/3
2	ADP	G	301	-	-	0/16/32/32	0/3/3/3
2	ADP	M	301	-	-	1/16/32/32	0/3/3/3
3	TIZ	A	302	-	-	3/10/26/26	0/2/2/2
2	ADP	C	301	-	-	0/16/32/32	0/3/3/3
2	ADP	O	301	-	-	0/16/32/32	0/3/3/3
2	ADP	L	301	-	-	0/16/32/32	0/3/3/3
3	TIZ	J	302	-	-	3/10/26/26	0/2/2/2
3	TIZ	N	302	-	-	3/10/26/26	0/2/2/2

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	302	TIZ	C1L-C1K	3.90	1.53	1.48
3	L	302	TIZ	C1L-C1K	3.83	1.53	1.48
3	A	302	TIZ	C1L-C1K	3.82	1.53	1.48
3	H	302	TIZ	C1L-C1K	3.82	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	TIZ	C1L-C1K	3.82	1.53	1.48

The worst 5 of 259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	ADP	C5-C4-N3	-5.52	119.11	126.72
2	H	301	ADP	C5-C4-N3	-5.45	119.21	126.72
2	N	301	ADP	C5-C4-N3	-5.45	119.22	126.72
2	L	301	ADP	C5-C4-N3	-5.44	119.23	126.72
2	D	301	ADP	C5-C4-N3	-5.41	119.26	126.72

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	TIZ	O4'-C1'-C1M-N1H
3	A	302	TIZ	O4'-C1'-C1M-S1J
3	A	302	TIZ	O1B-C1K-C1L-C1F
3	B	302	TIZ	O4'-C1'-C1M-N1H
3	B	302	TIZ	O4'-C1'-C1M-S1J

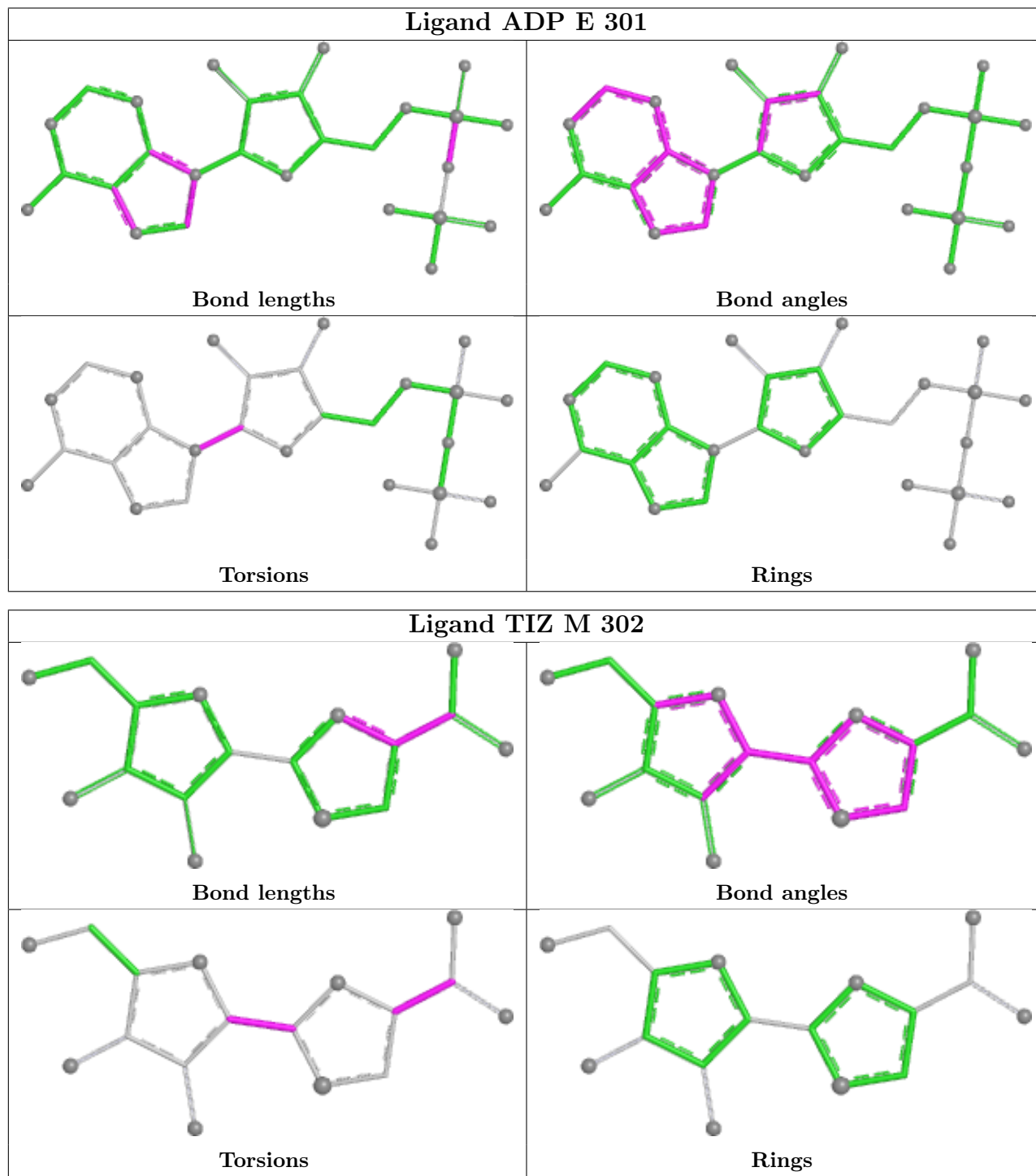
There are no ring outliers.

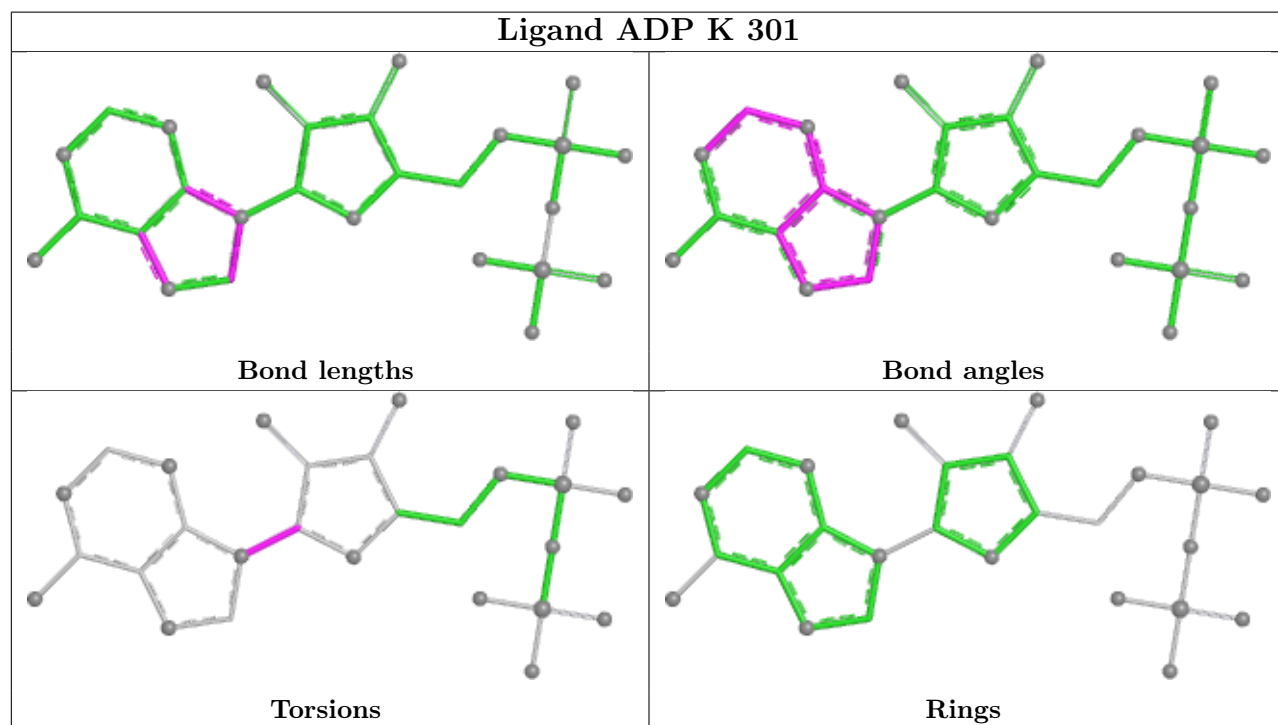
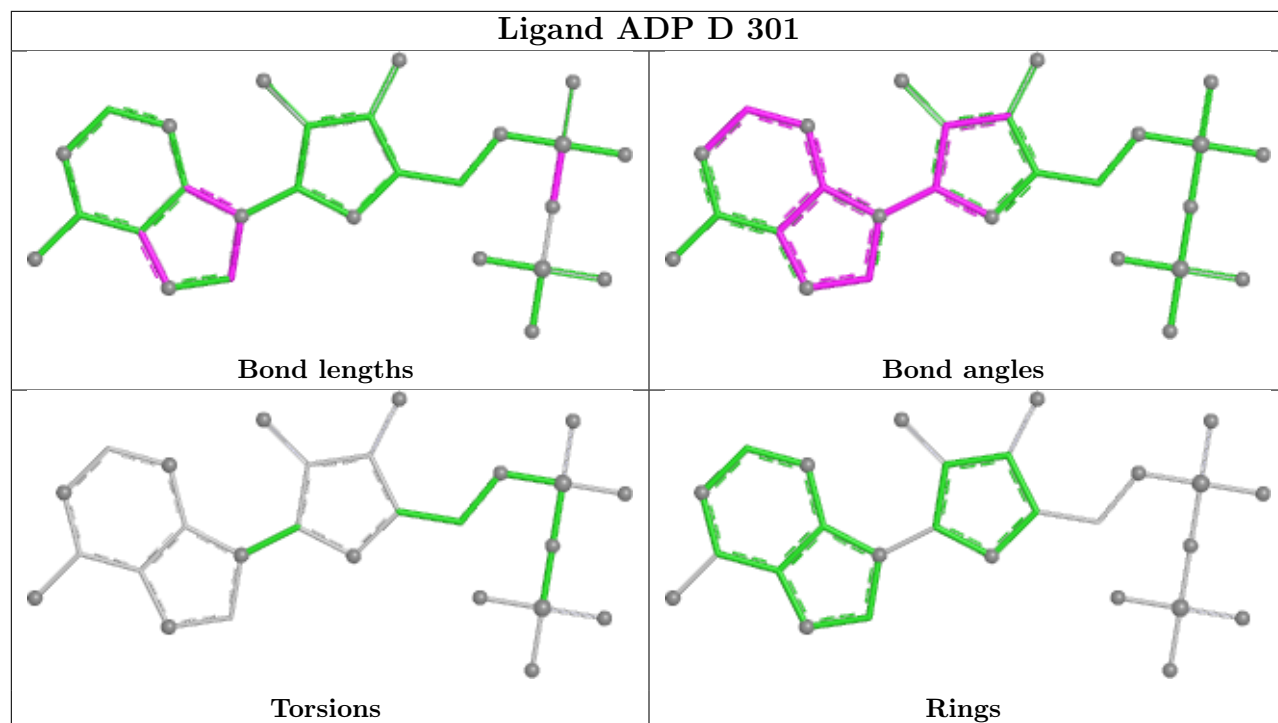
9 monomers are involved in 9 short contacts:

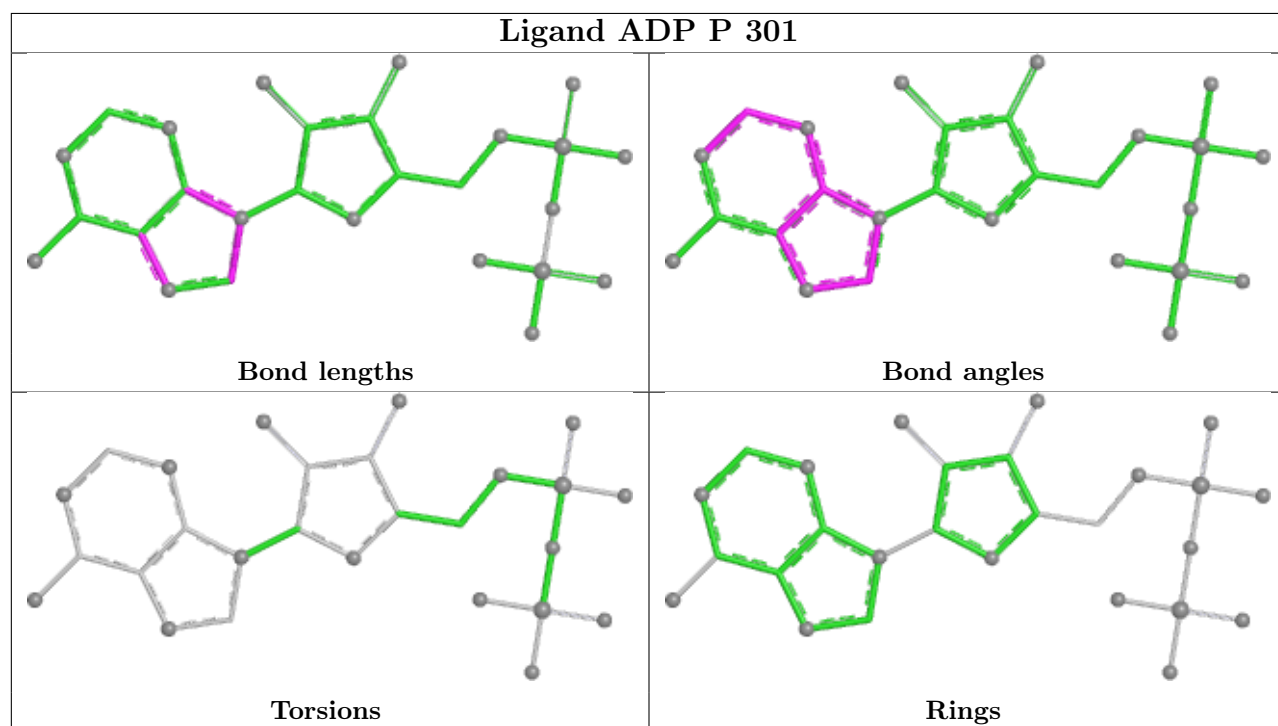
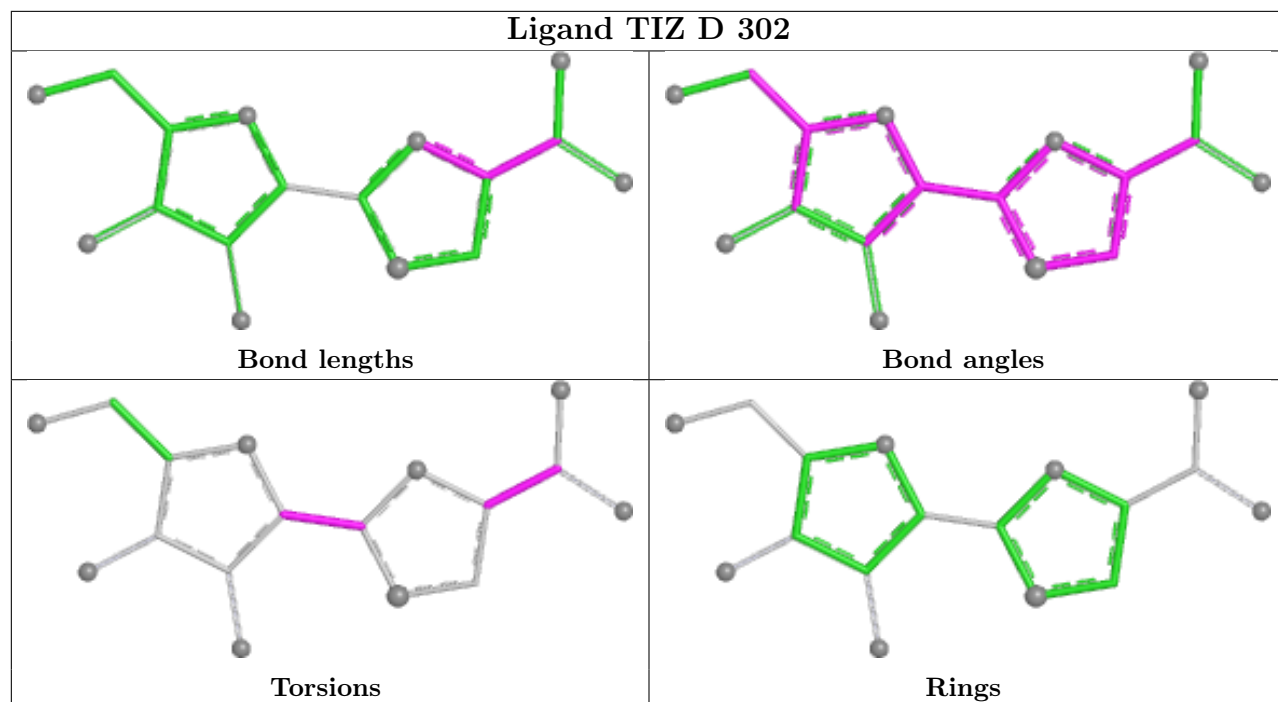
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	ADP	1	0
2	D	301	ADP	1	0
3	I	302	TIZ	1	0
3	F	302	TIZ	1	0
2	F	301	ADP	1	0
2	I	301	ADP	1	0
2	A	301	ADP	1	0
2	H	301	ADP	1	0
2	C	301	ADP	1	0

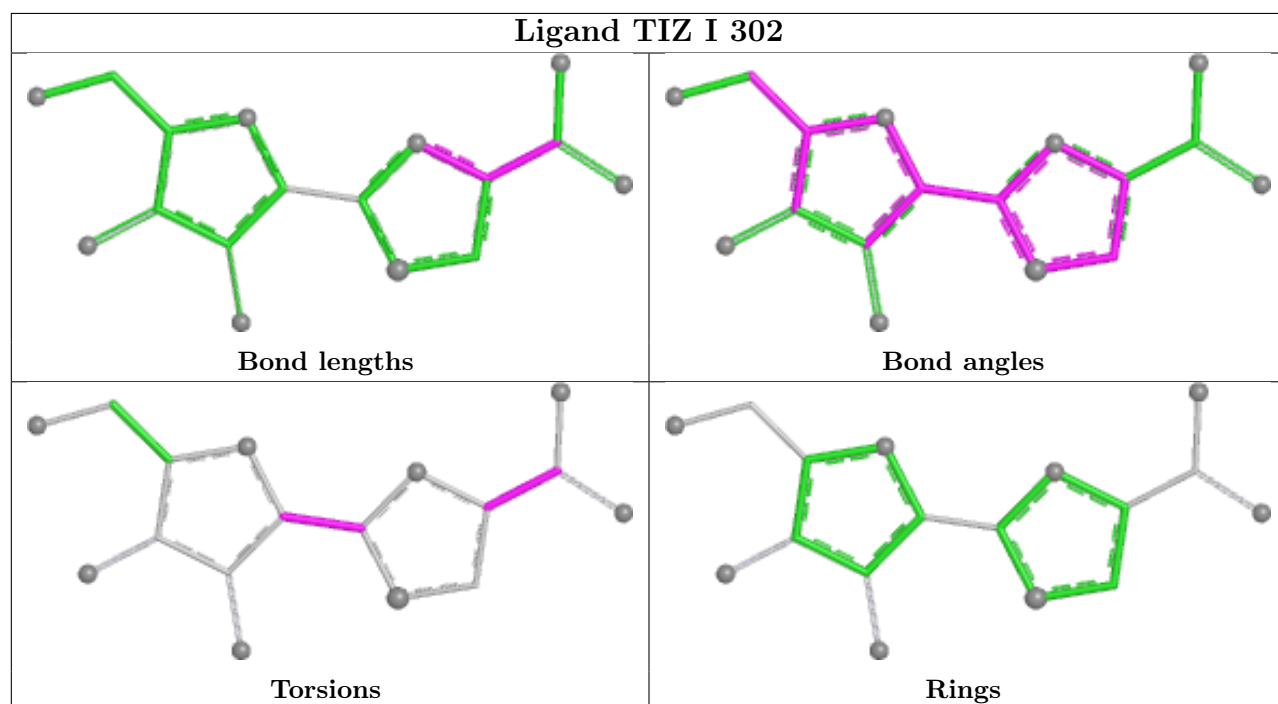
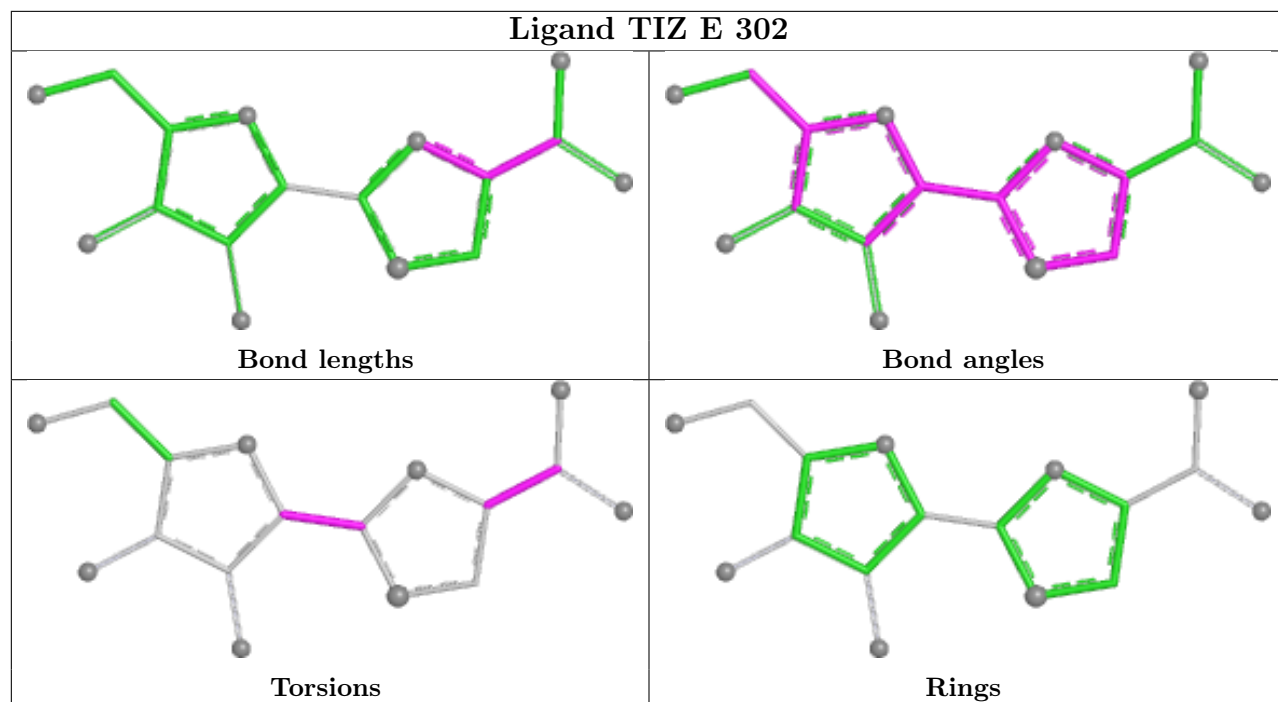
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

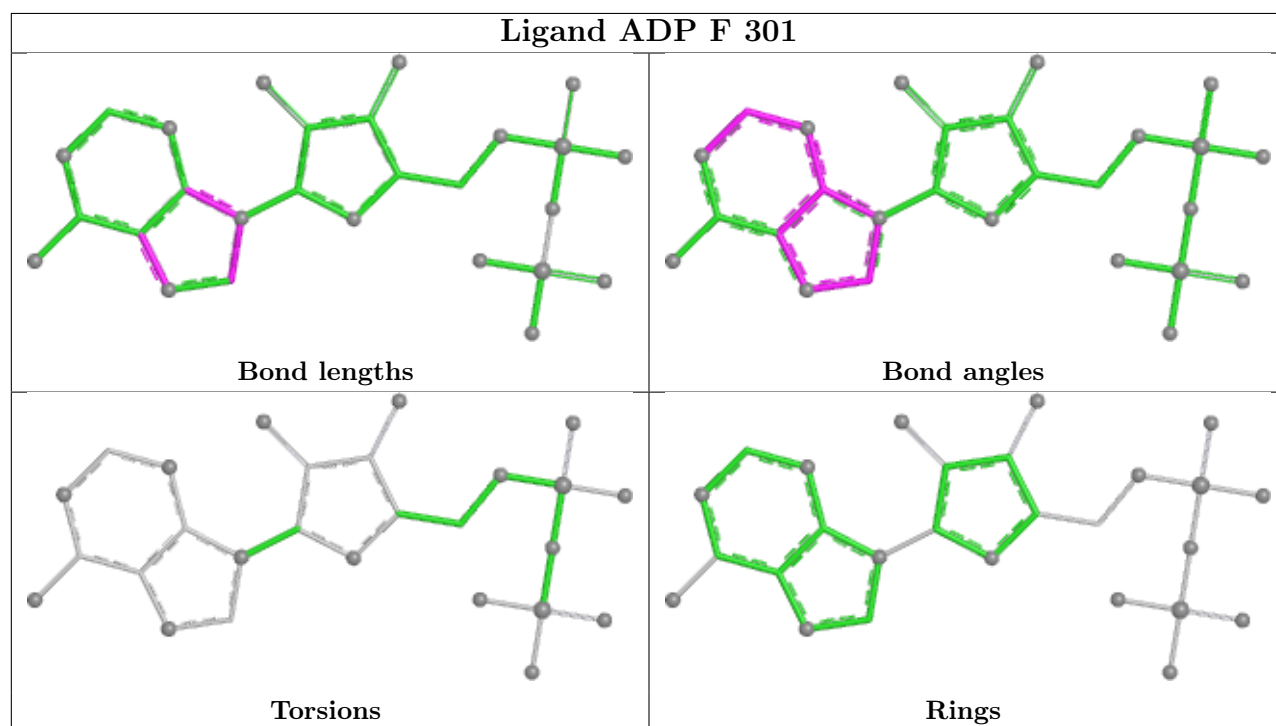
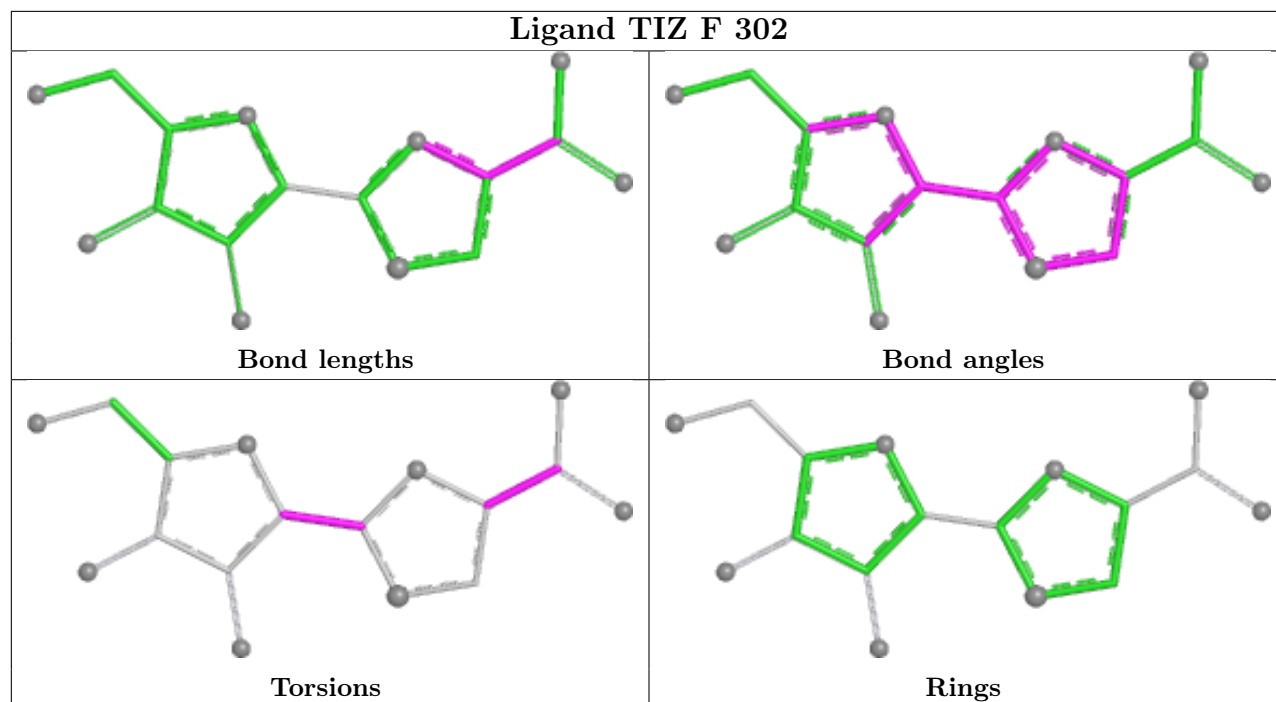
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

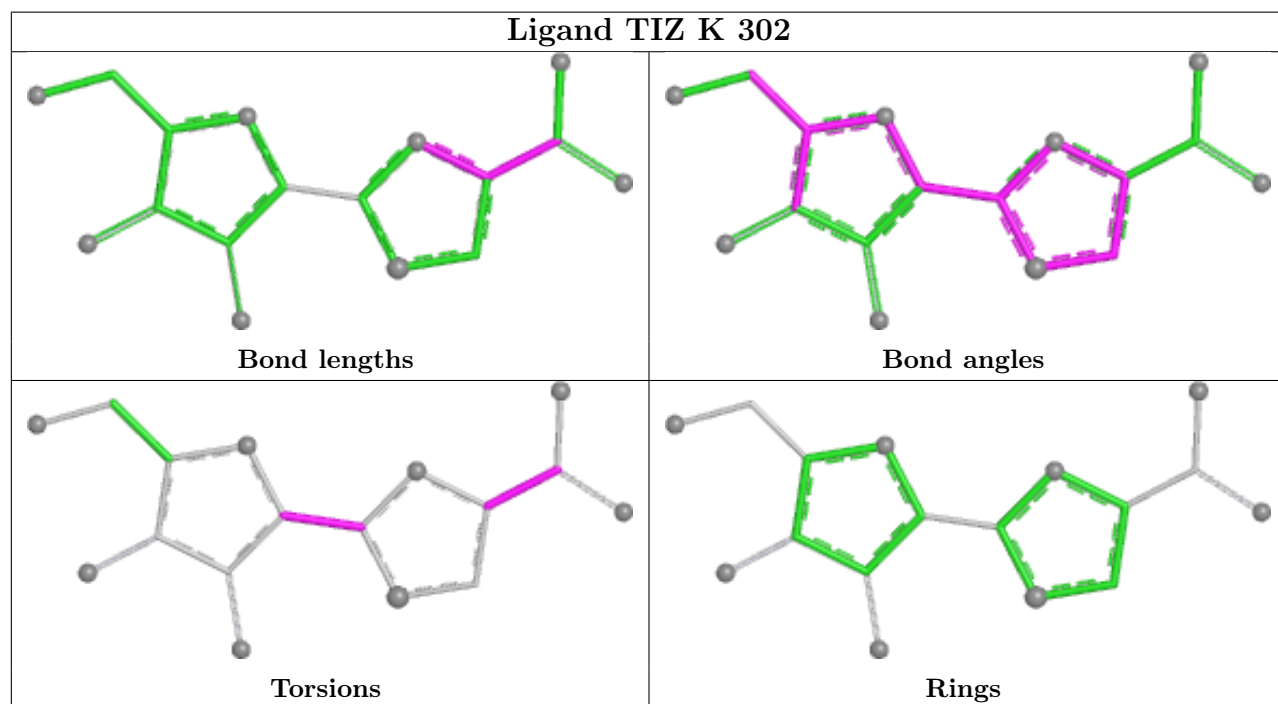
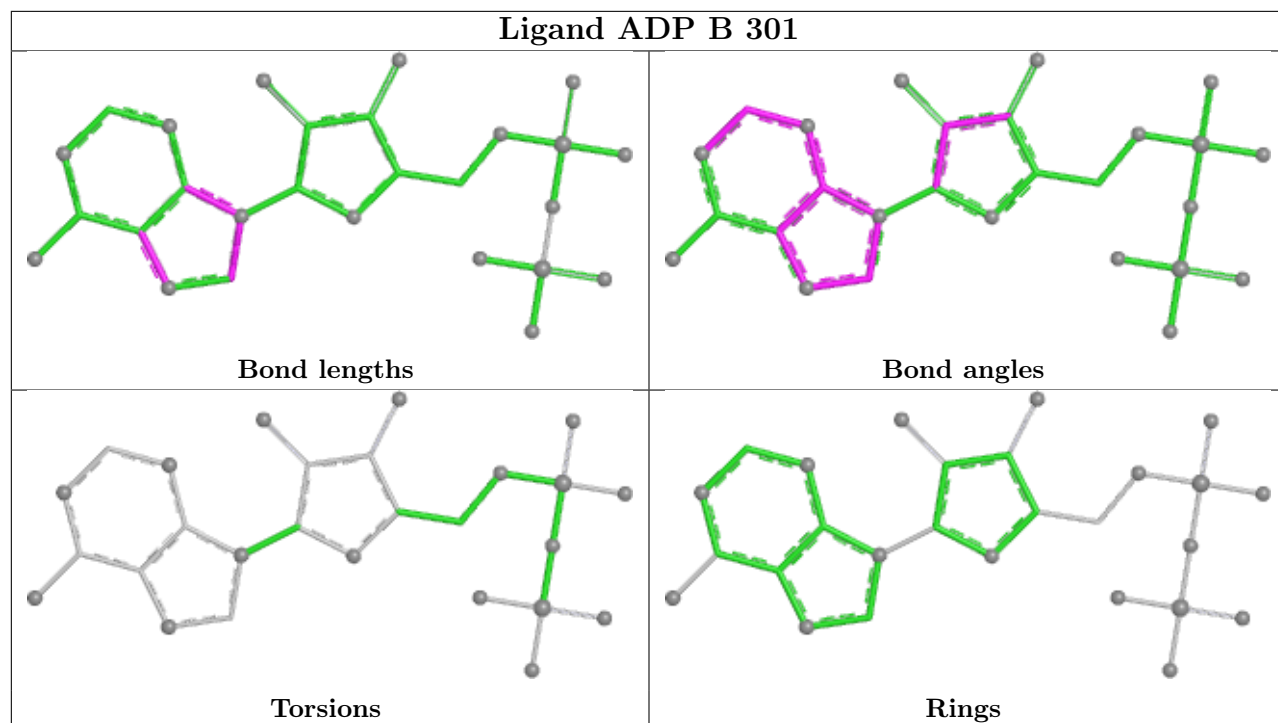


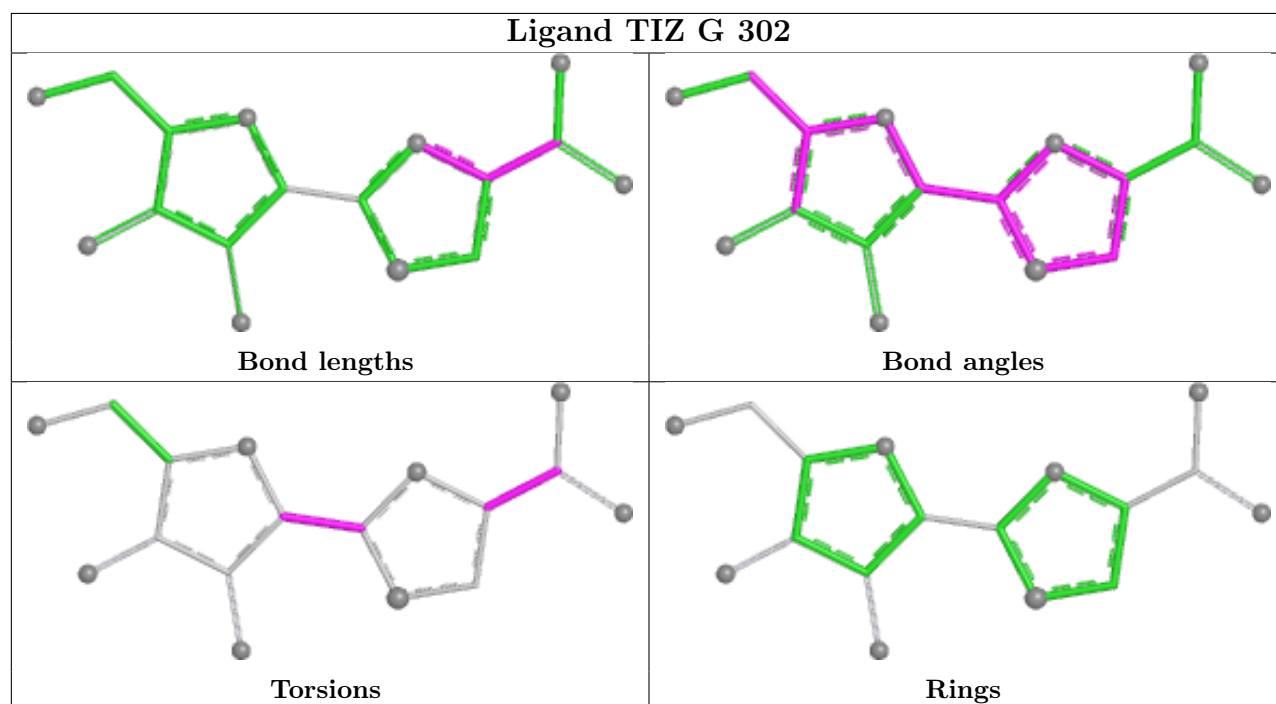
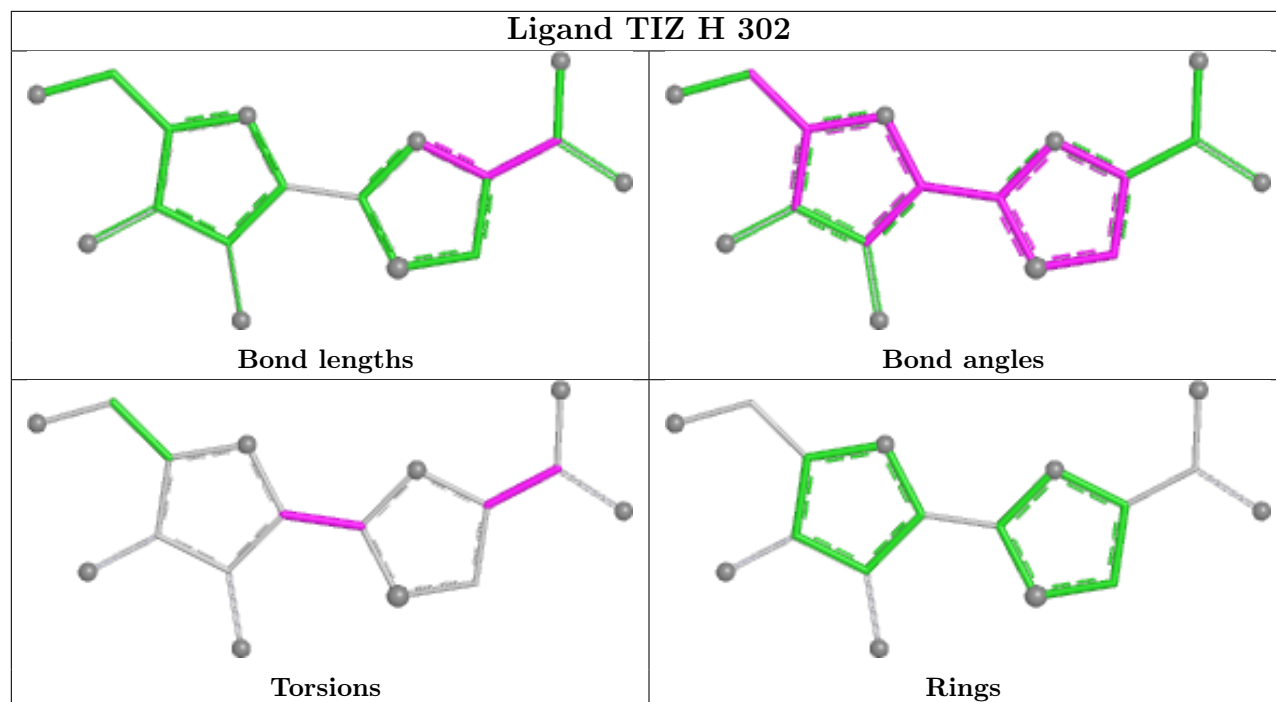


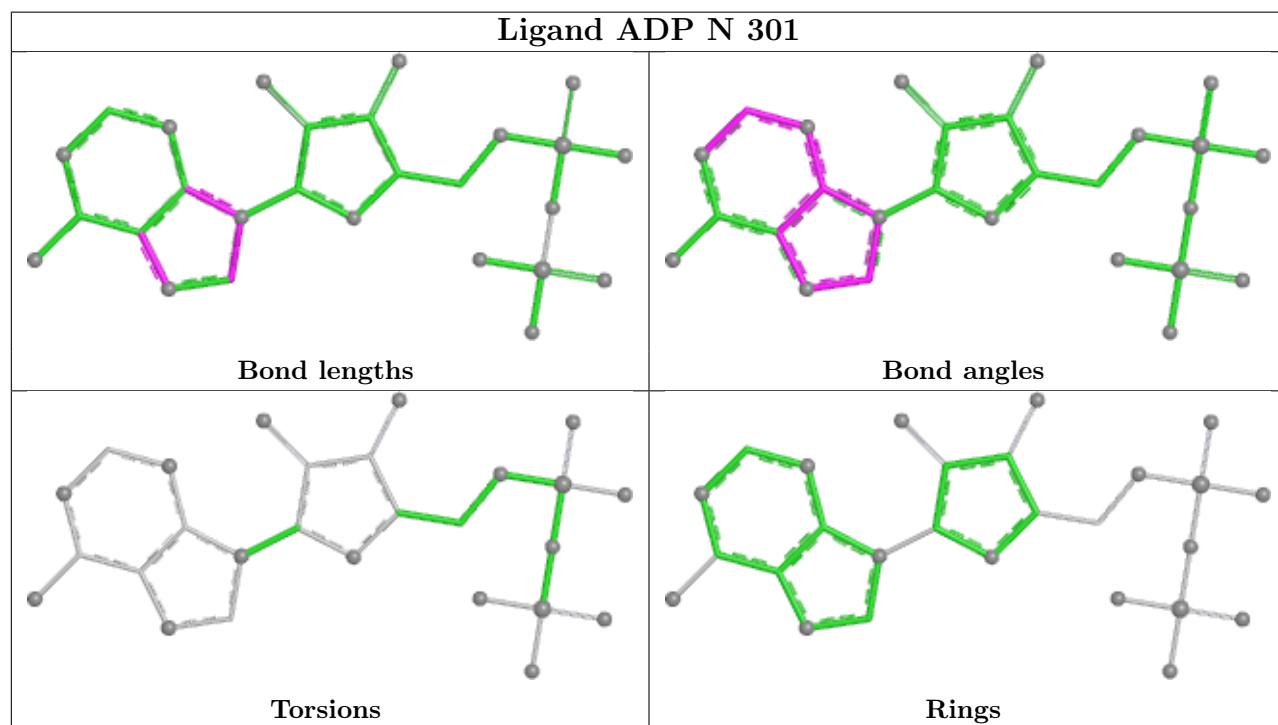
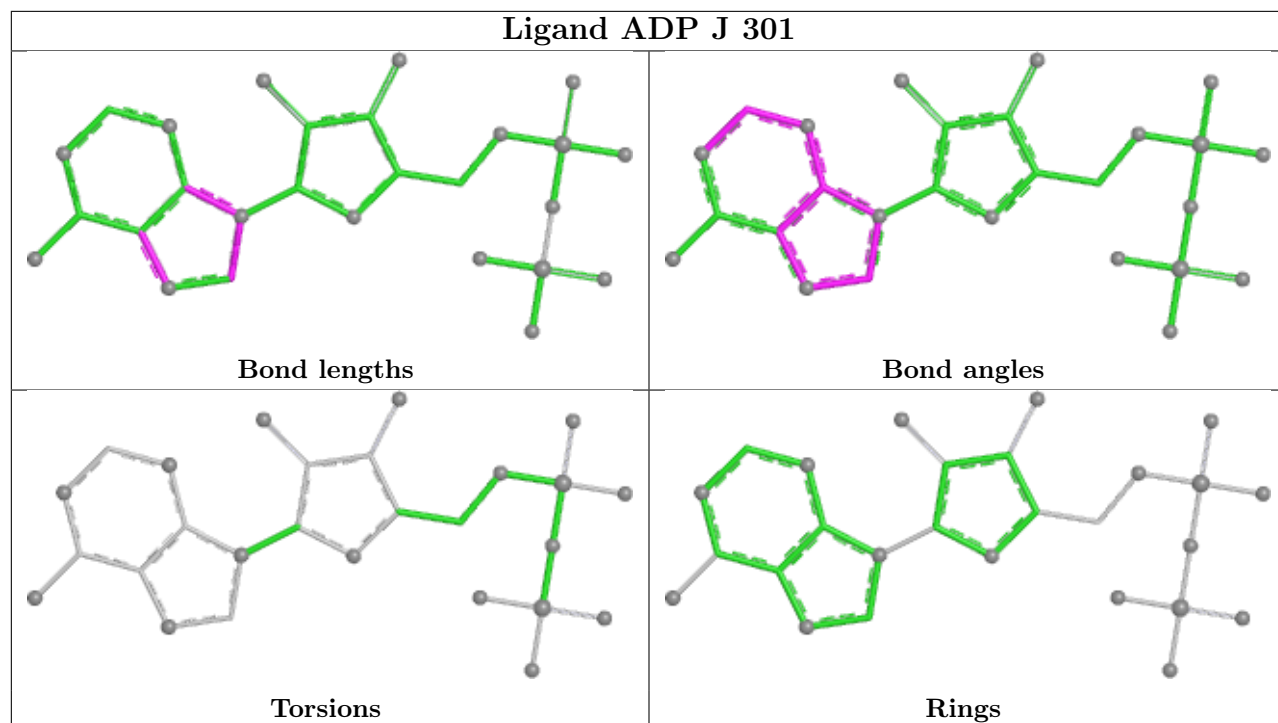


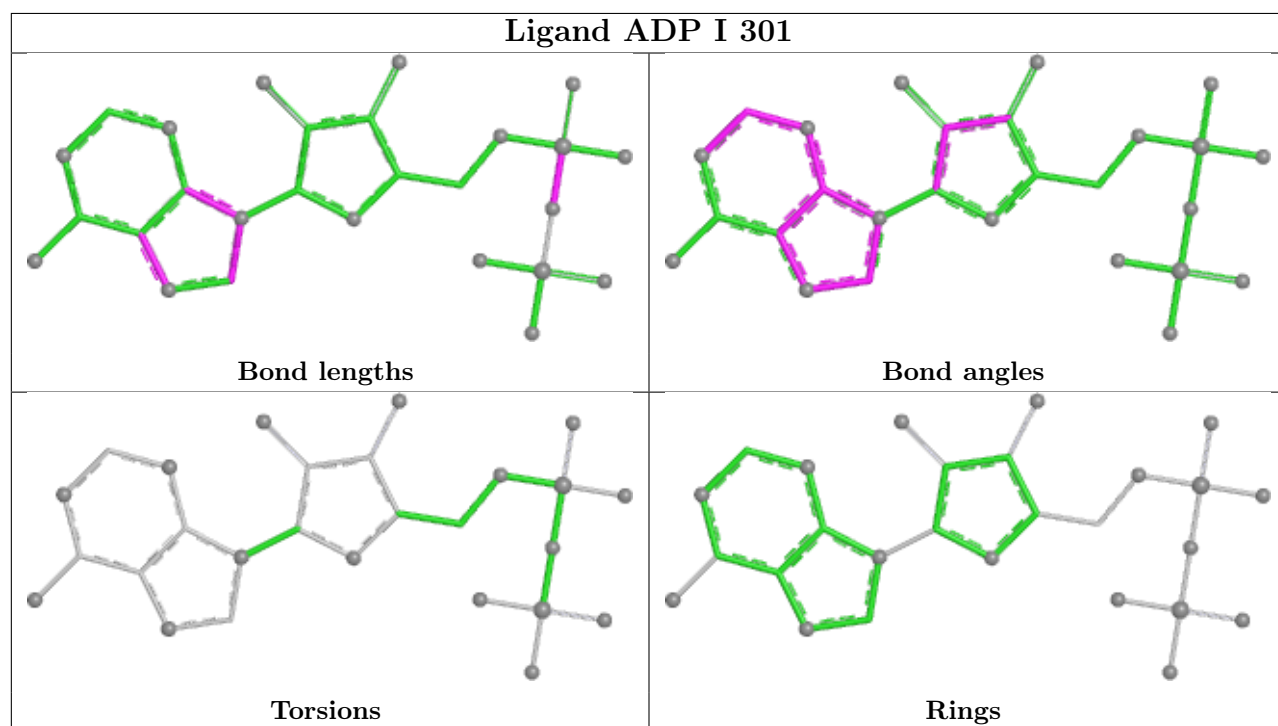
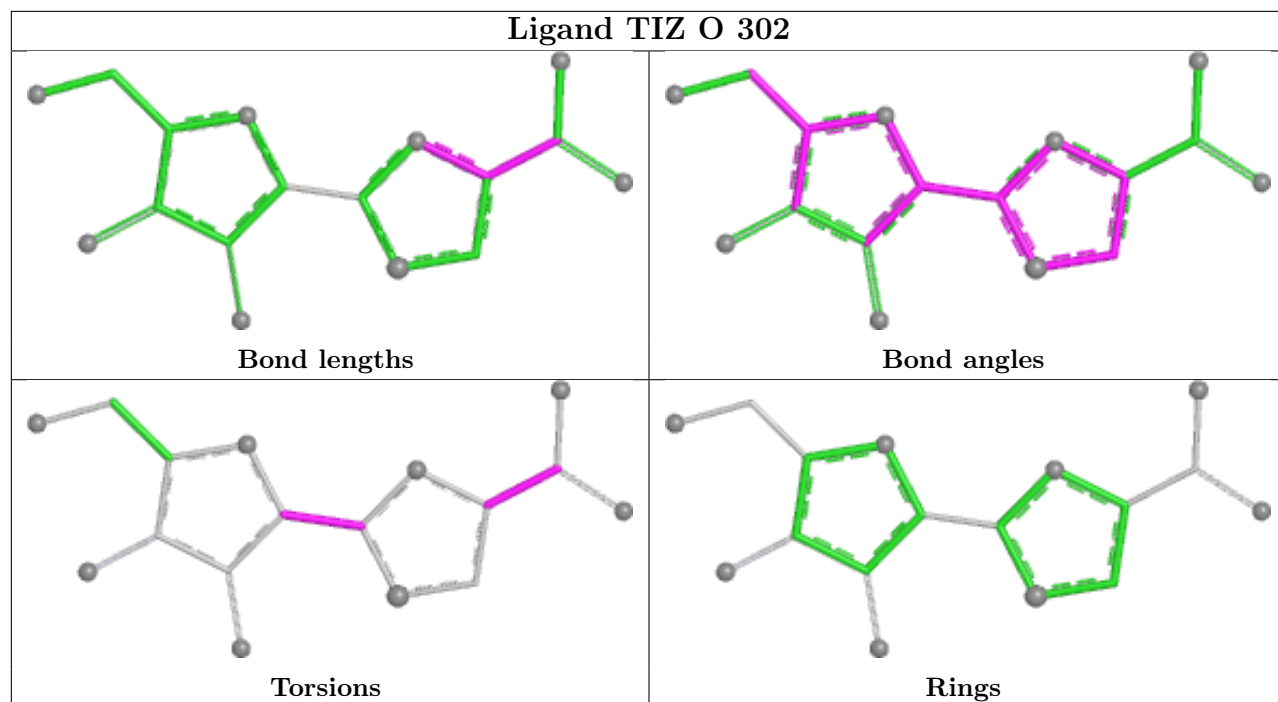


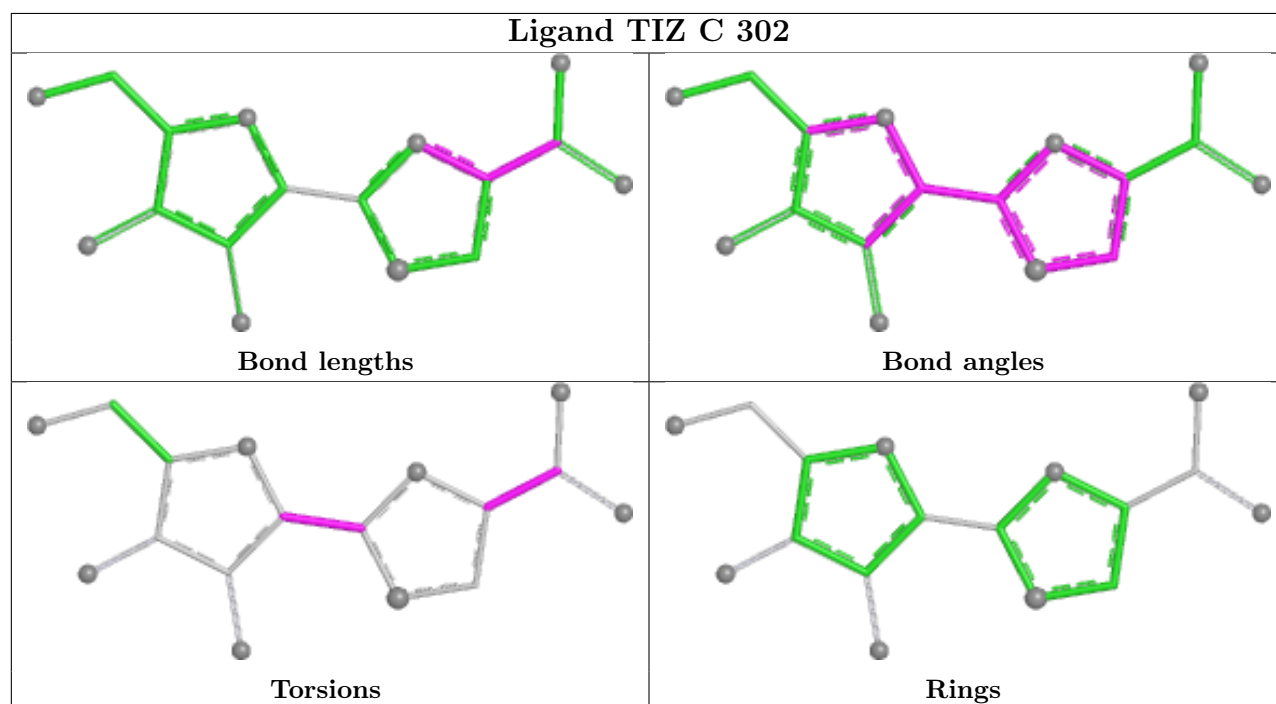
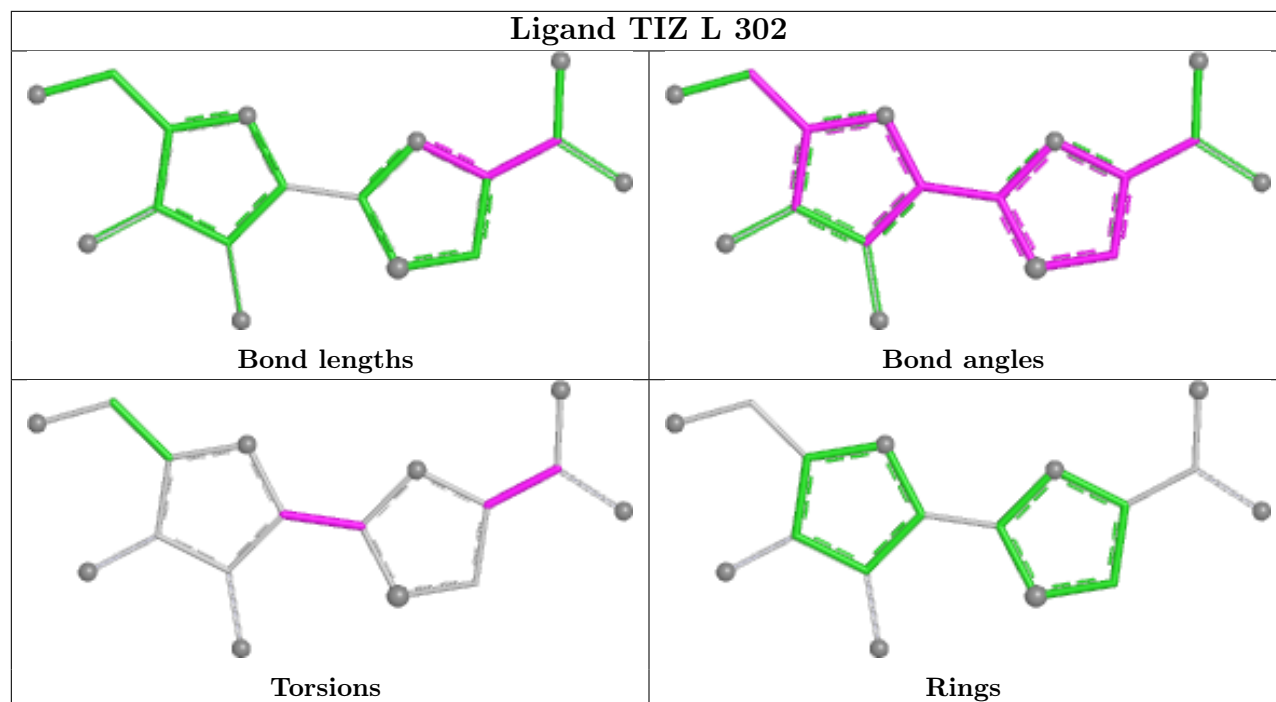


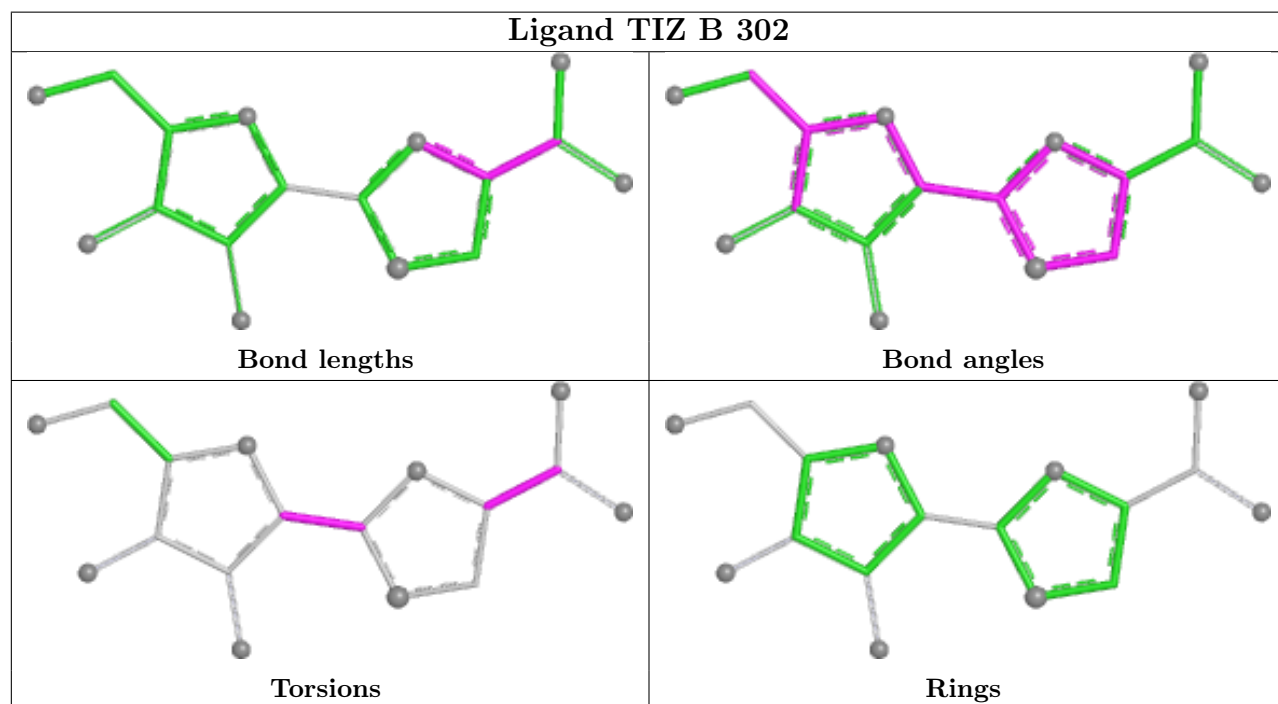
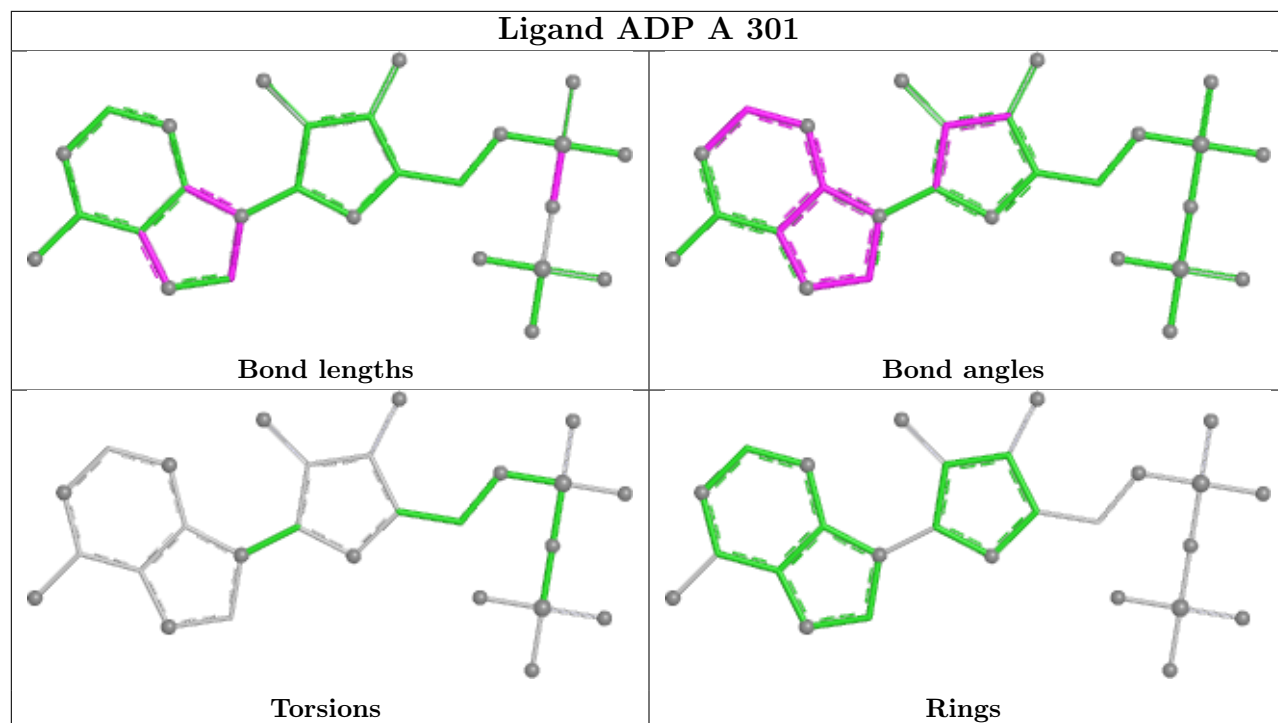


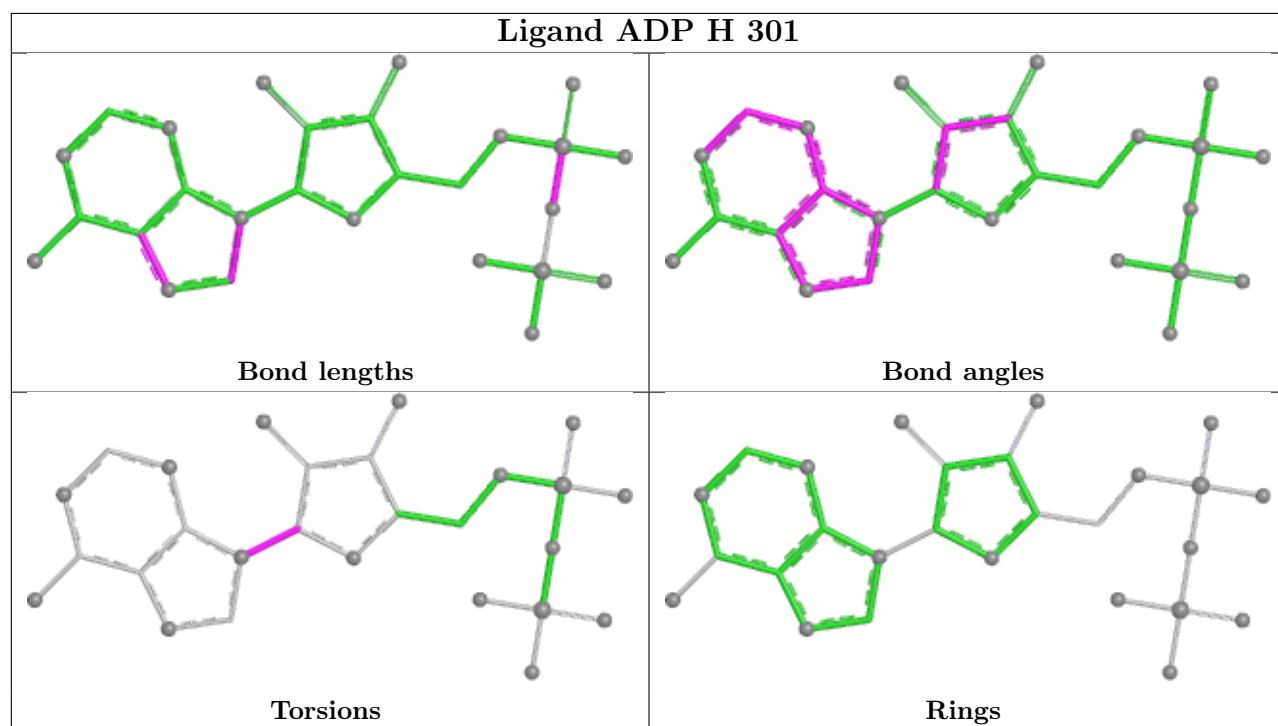
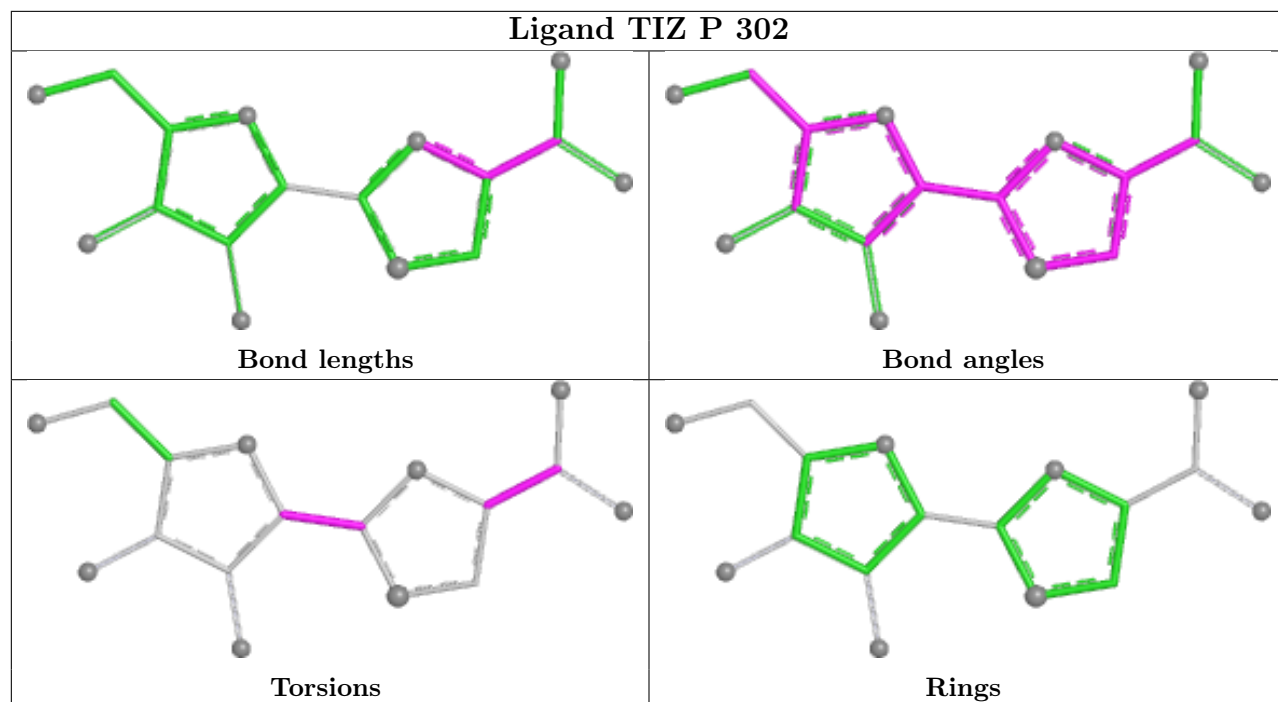


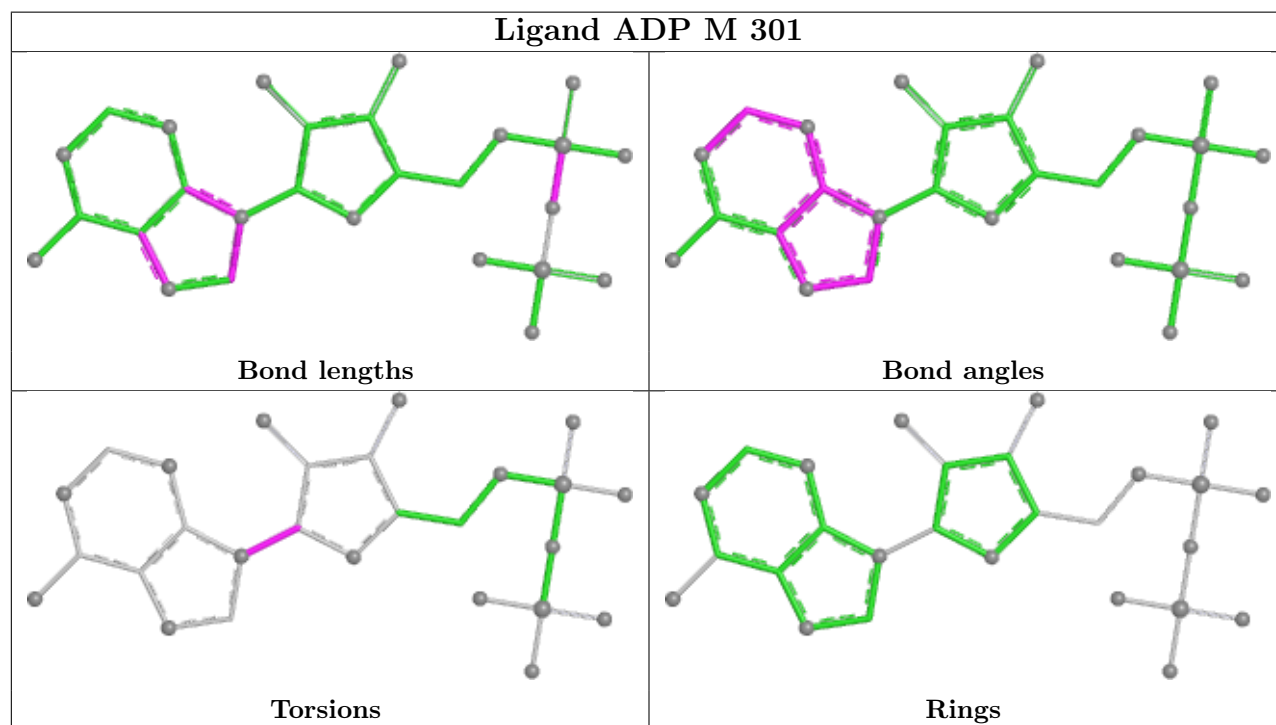
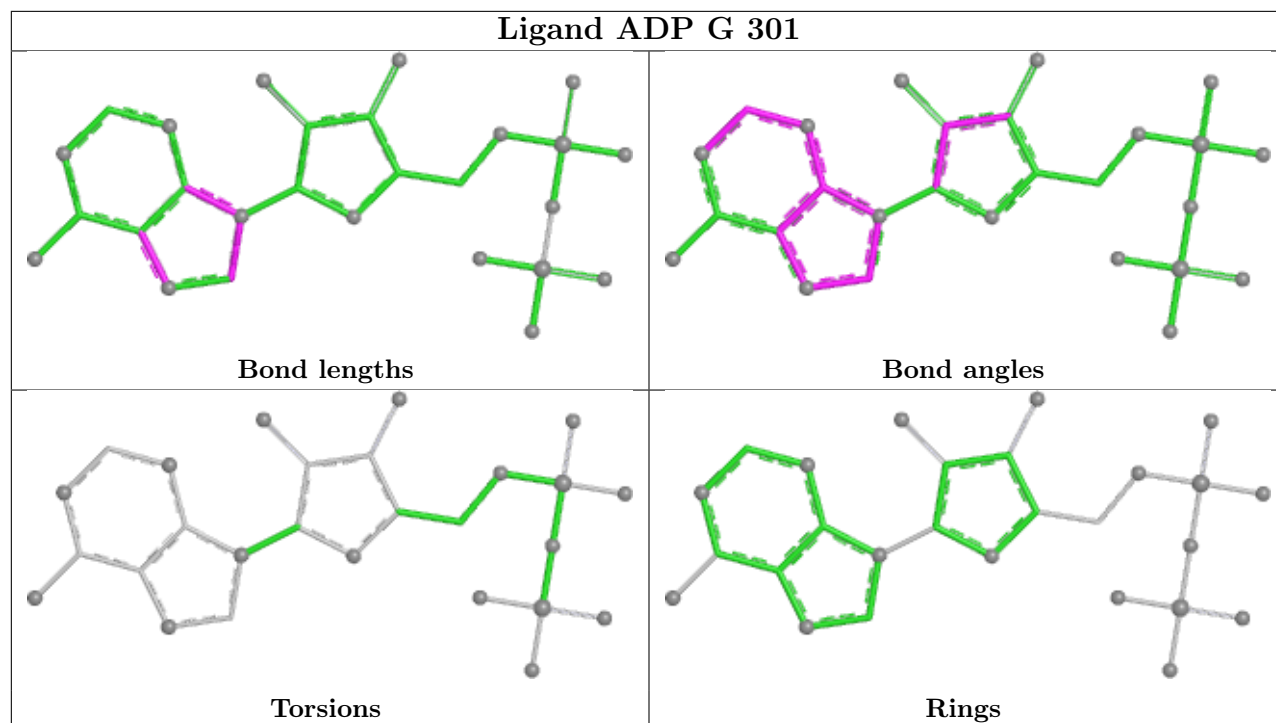


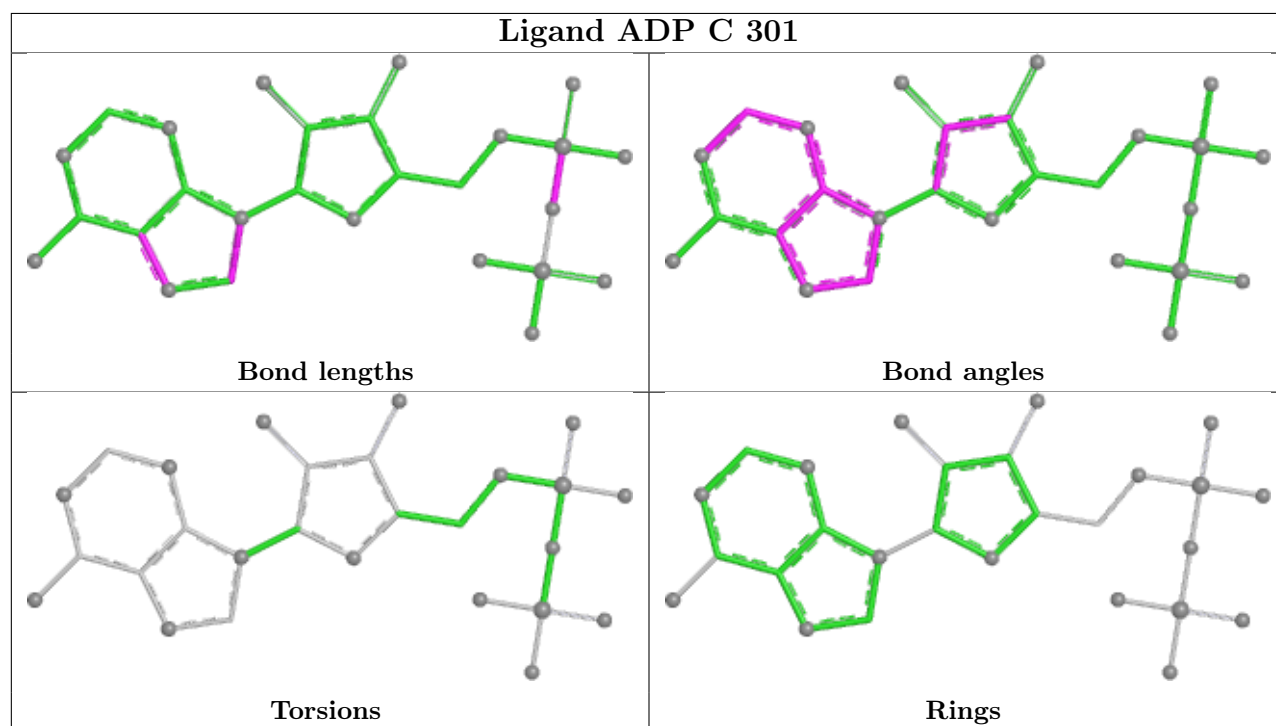
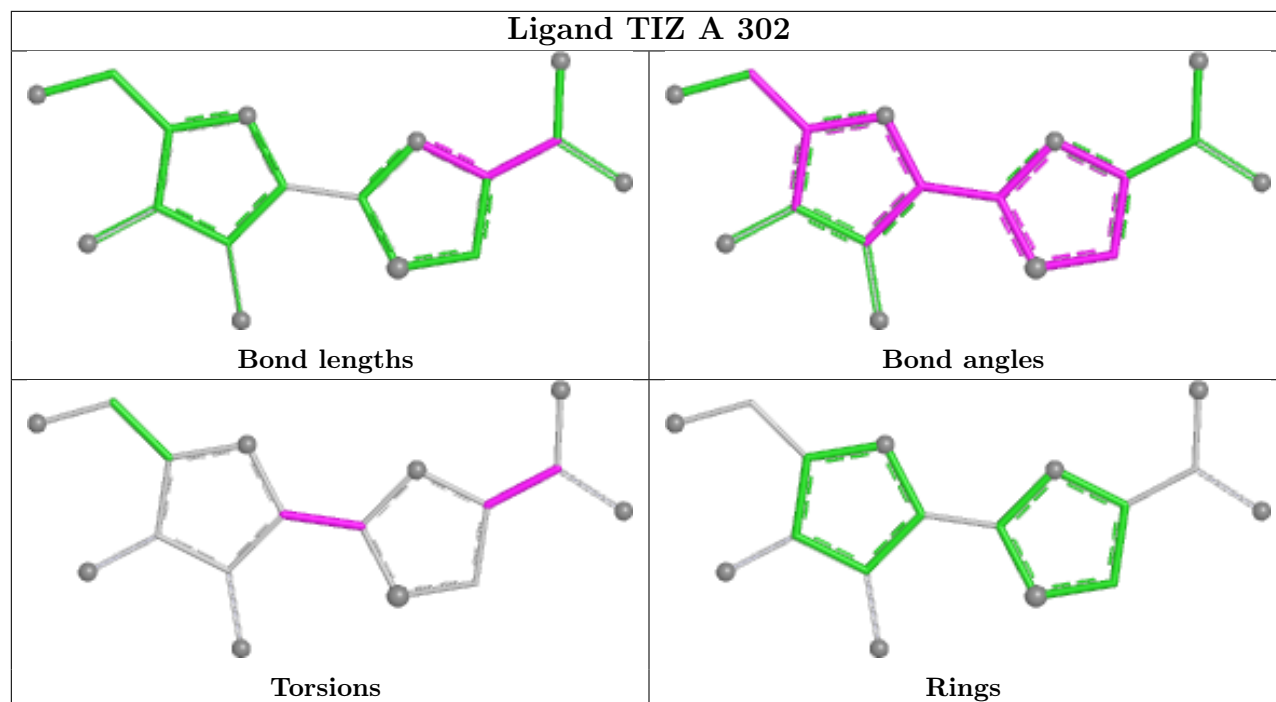


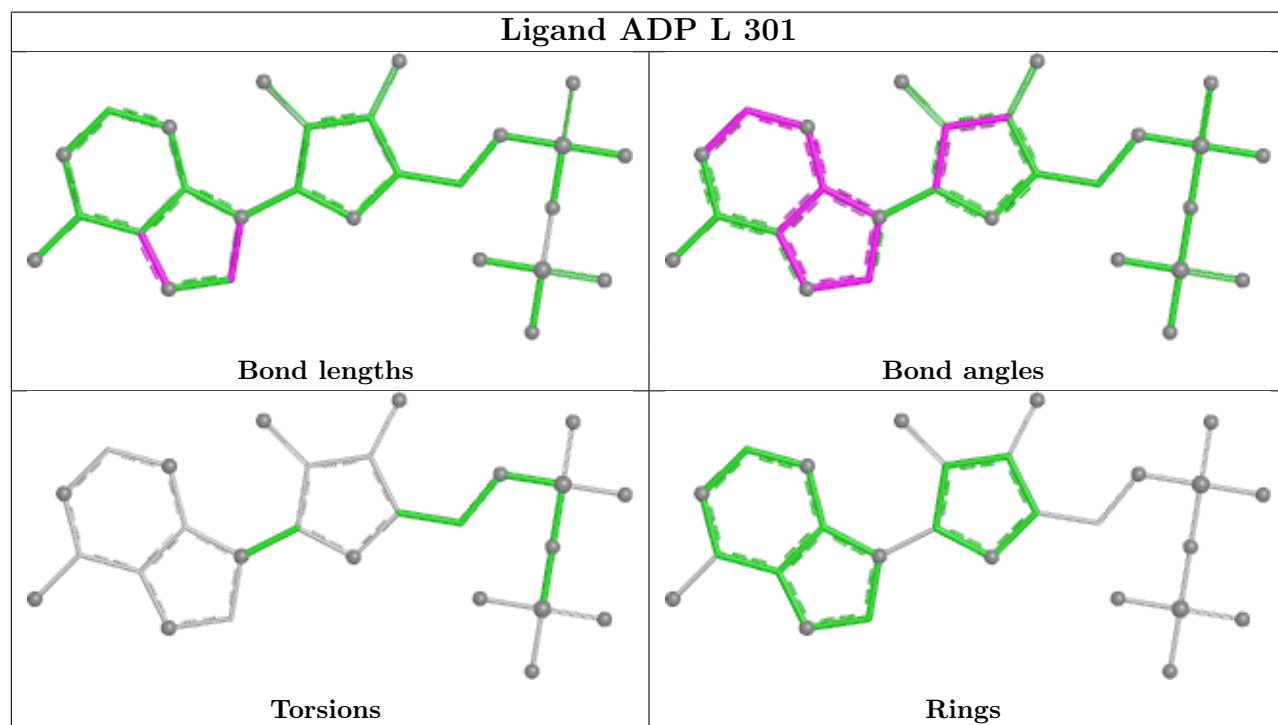
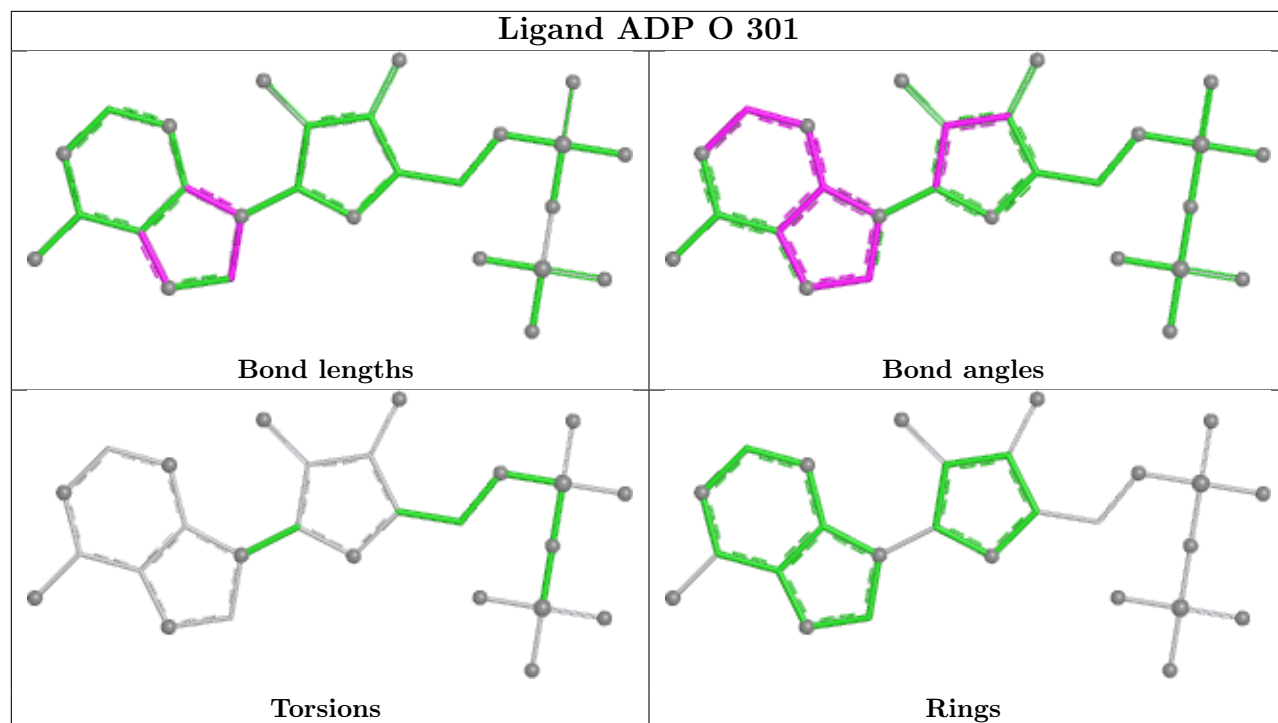


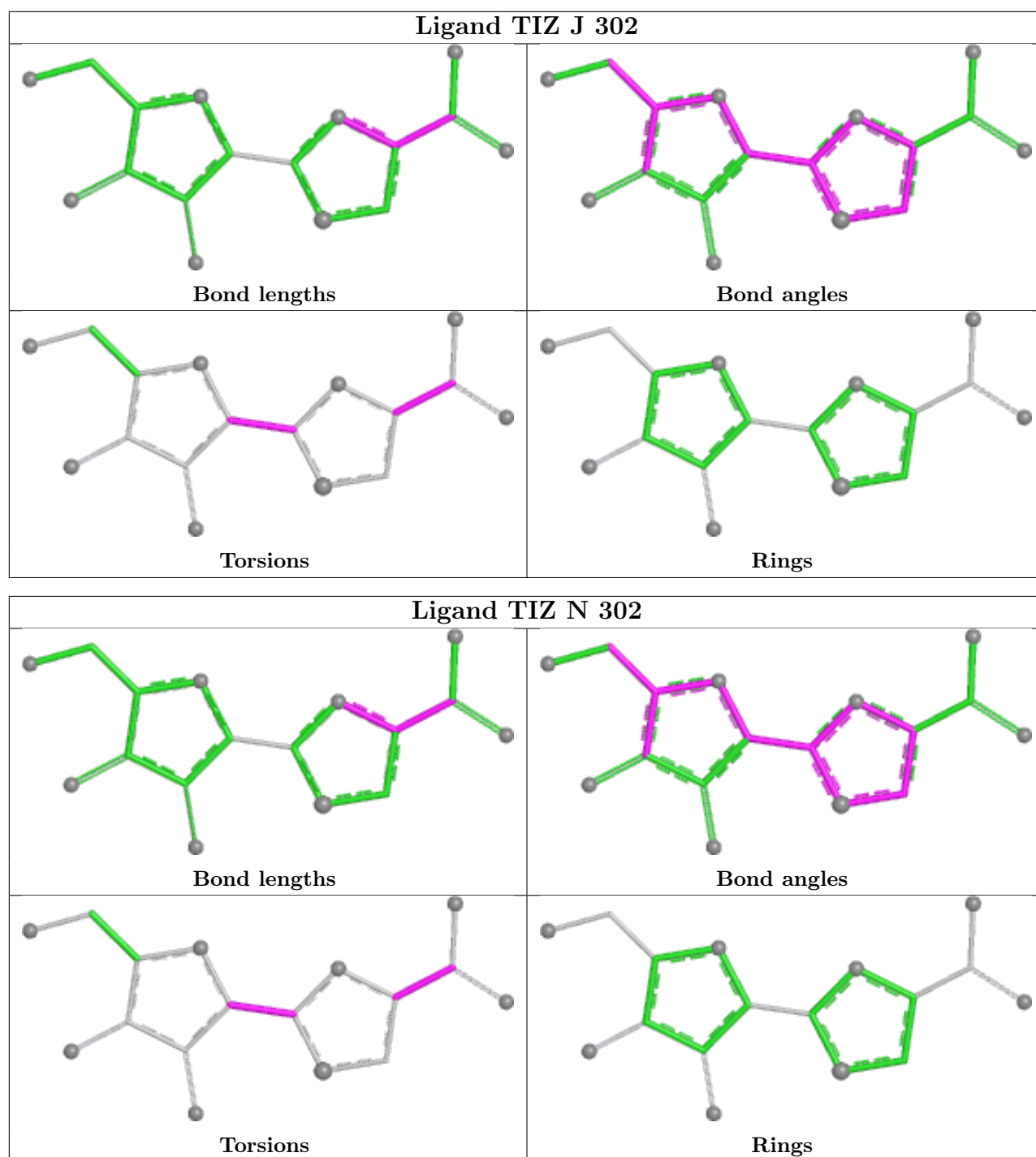












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	173/199 (86%)	-1.32	0 100 100	22, 22, 22, 22	0
1	B	173/199 (86%)	-1.34	0 100 100	22, 22, 22, 22	0
1	C	173/199 (86%)	-1.36	0 100 100	22, 22, 22, 22	0
1	D	173/199 (86%)	-1.35	0 100 100	22, 22, 22, 22	0
1	E	173/199 (86%)	-1.39	0 100 100	22, 22, 22, 22	0
1	F	173/199 (86%)	-1.36	0 100 100	22, 22, 22, 22	0
1	G	173/199 (86%)	-1.36	0 100 100	22, 22, 22, 22	0
1	H	173/199 (86%)	-1.33	0 100 100	22, 22, 22, 22	0
1	I	173/199 (86%)	-1.31	0 100 100	22, 22, 22, 22	0
1	J	173/199 (86%)	-1.30	0 100 100	22, 22, 22, 22	0
1	K	173/199 (86%)	-1.29	0 100 100	22, 22, 22, 22	0
1	L	173/199 (86%)	-1.34	0 100 100	22, 22, 22, 22	0
1	M	173/199 (86%)	-1.36	0 100 100	22, 22, 22, 22	0
1	N	173/199 (86%)	-1.26	0 100 100	22, 22, 22, 22	0
1	O	173/199 (86%)	-1.38	0 100 100	22, 22, 22, 22	0
1	P	173/199 (86%)	-1.33	0 100 100	22, 22, 22, 22	0
All	All	2768/3184 (86%)	-1.34	0 100 100	22, 22, 22, 22	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

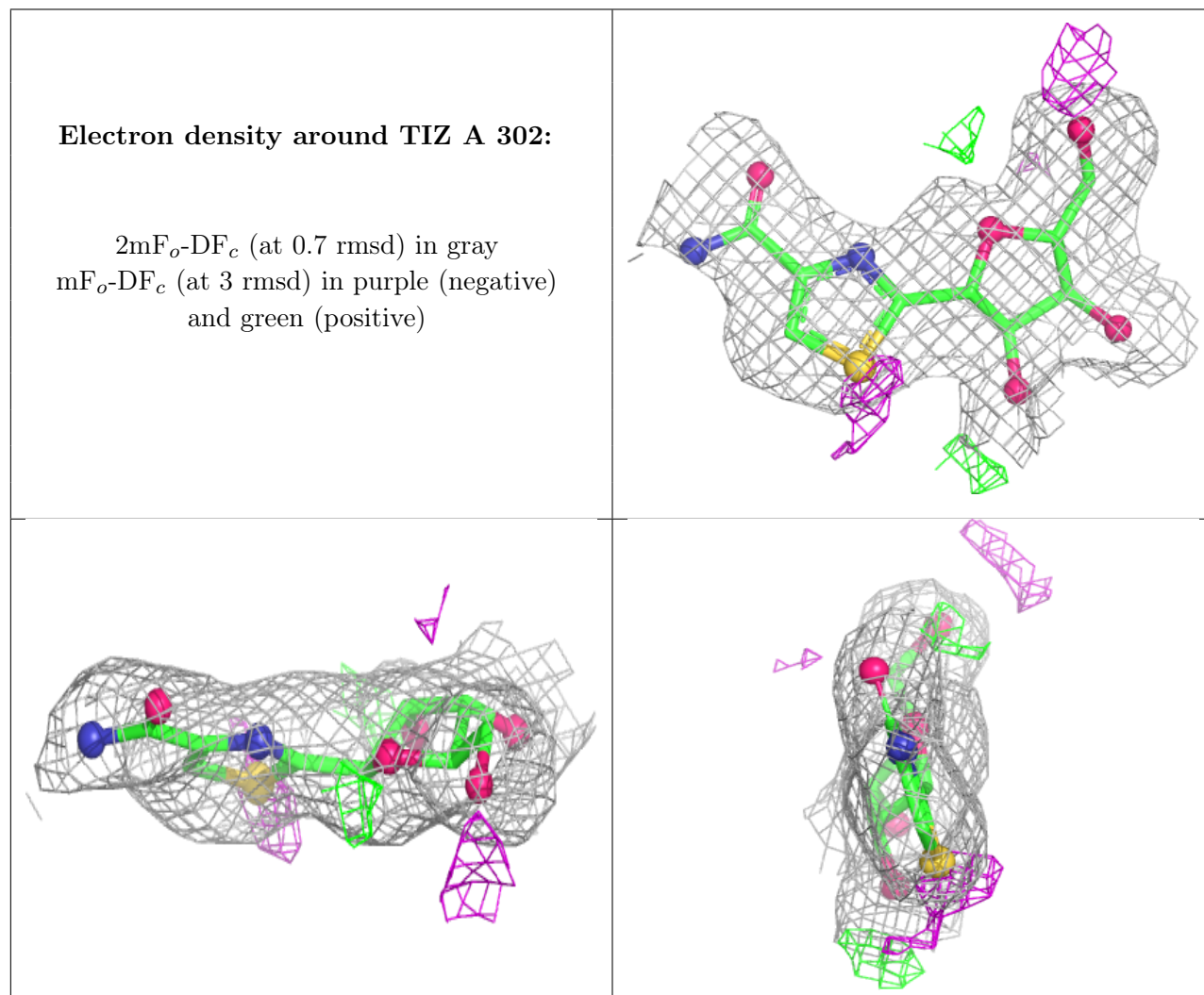
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

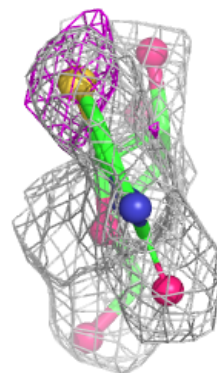
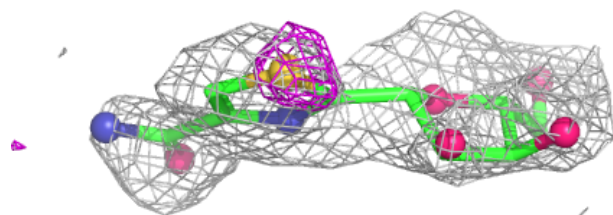
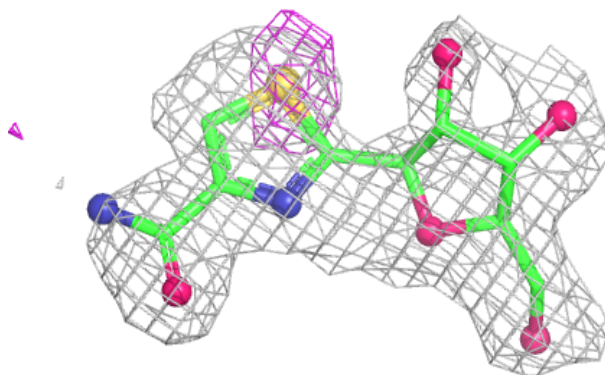
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TIZ	A	302	17/17	0.98	0.04	16,16,16,16	0
3	TIZ	H	302	17/17	0.98	0.09	16,16,16,16	0
3	TIZ	J	302	17/17	0.98	0.06	16,16,16,16	0
3	TIZ	K	302	17/17	0.98	0.07	16,16,16,16	0
3	TIZ	L	302	17/17	0.98	0.08	16,16,16,16	0
3	TIZ	N	302	17/17	0.98	0.06	16,16,16,16	0
3	TIZ	O	302	17/17	0.98	0.07	16,16,16,16	0
2	ADP	H	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	I	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	J	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	K	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	L	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	N	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	O	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	P	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	A	301	27/27	0.99	0.04	16,16,16,16	0
3	TIZ	B	302	17/17	0.99	0.05	16,16,16,16	0
3	TIZ	C	302	17/17	0.99	0.06	16,16,16,16	0
3	TIZ	D	302	17/17	0.99	0.04	16,16,16,16	0
3	TIZ	E	302	17/17	0.99	0.05	16,16,16,16	0
3	TIZ	F	302	17/17	0.99	0.05	16,16,16,16	0
3	TIZ	G	302	17/17	0.99	0.04	16,16,16,16	0
2	ADP	B	301	27/27	0.99	0.04	16,16,16,16	0
3	TIZ	I	302	17/17	0.99	0.05	16,16,16,16	0
2	ADP	C	301	27/27	0.99	0.04	16,16,16,16	0
2	ADP	D	301	27/27	0.99	0.03	16,16,16,16	0
2	ADP	E	301	27/27	0.99	0.04	16,16,16,16	0
3	TIZ	M	302	17/17	0.99	0.04	16,16,16,16	0
2	ADP	F	301	27/27	0.99	0.03	16,16,16,16	0
2	ADP	G	301	27/27	0.99	0.04	16,16,16,16	0
3	TIZ	P	302	17/17	0.99	0.04	16,16,16,16	0
2	ADP	M	301	27/27	1.00	0.03	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



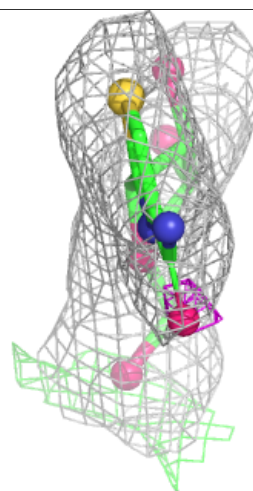
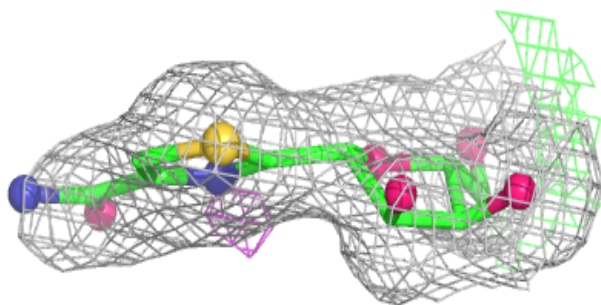
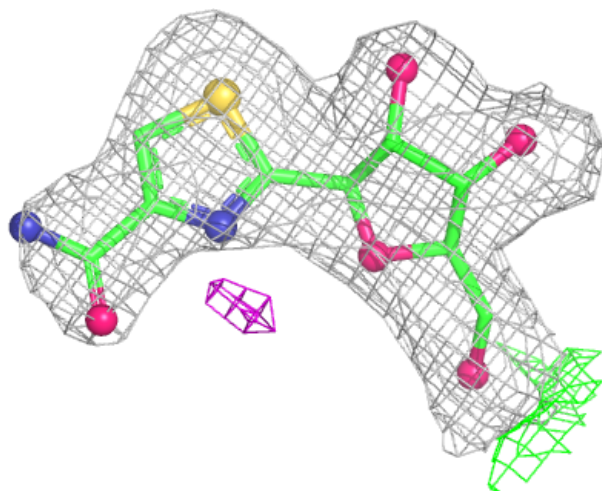
Electron density around TIZ H 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



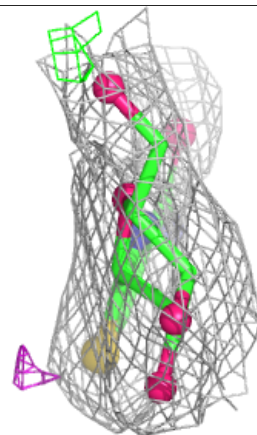
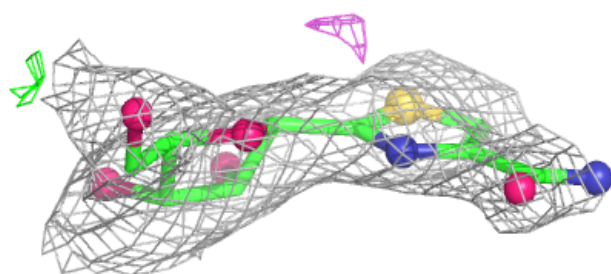
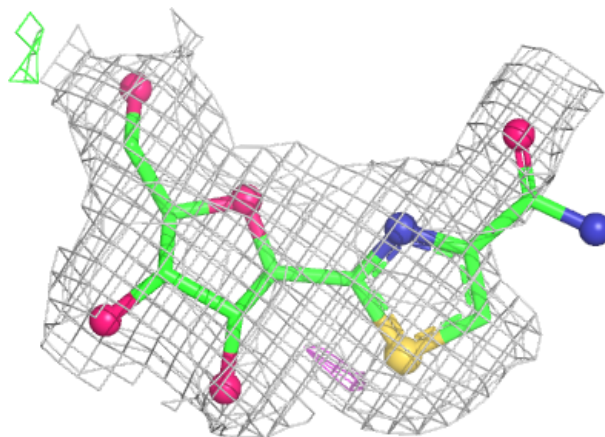
Electron density around TIZ J 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



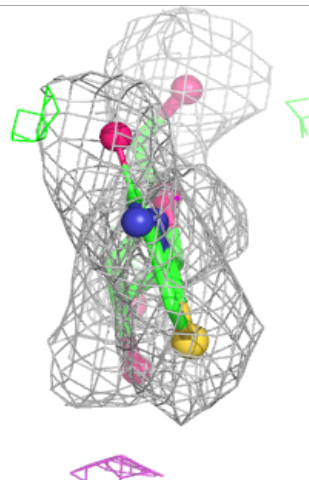
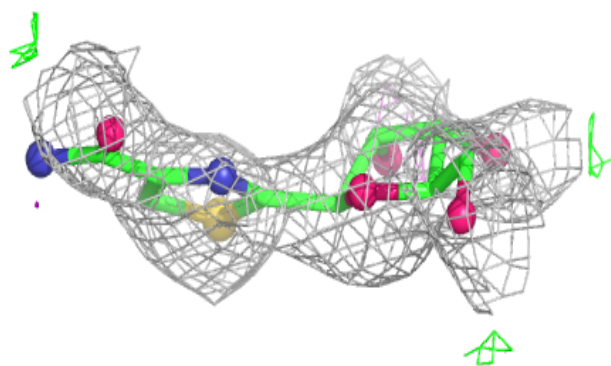
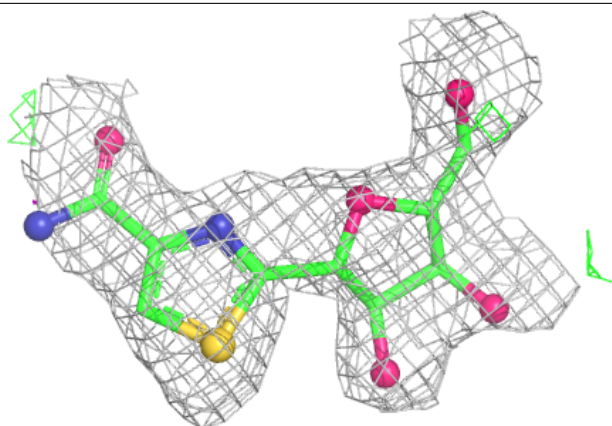
Electron density around TIZ K 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



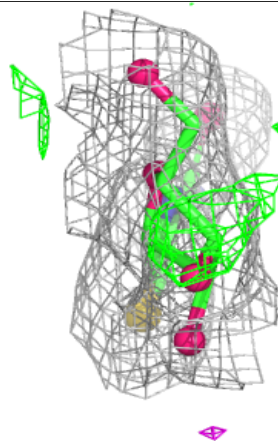
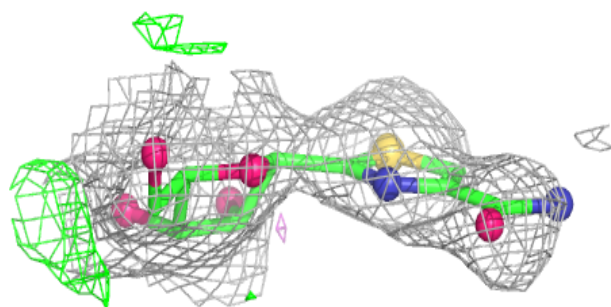
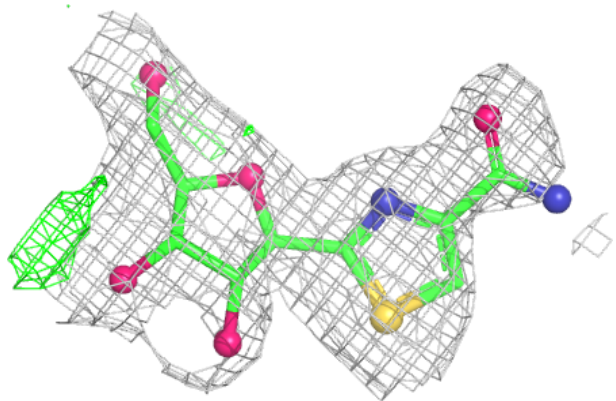
Electron density around TIZ L 302:

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and green (positive)

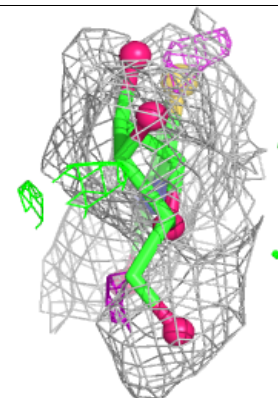
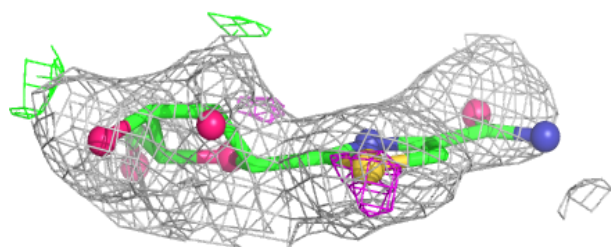
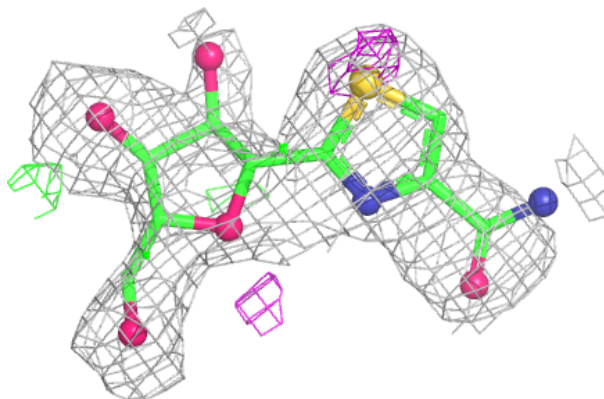


Electron density around TIZ N 302:

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and green (positive)

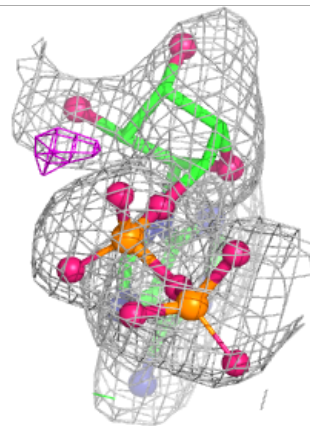
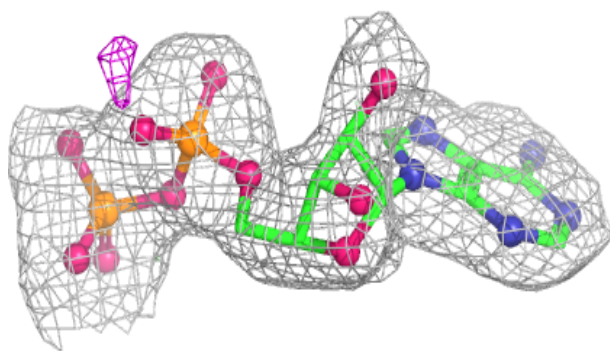
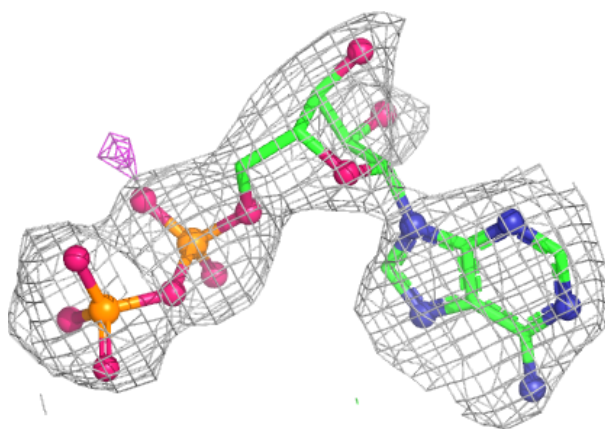
**Electron density around TIZ O 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



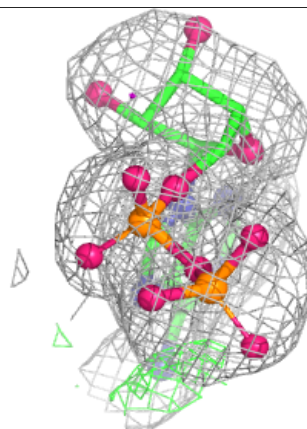
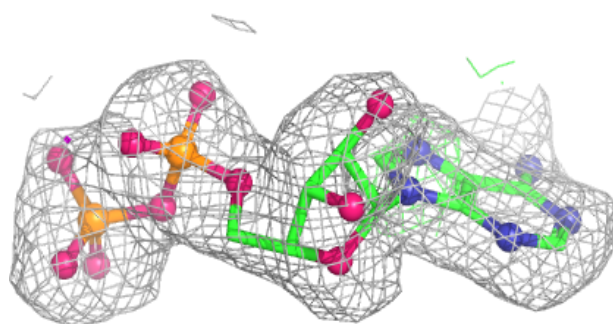
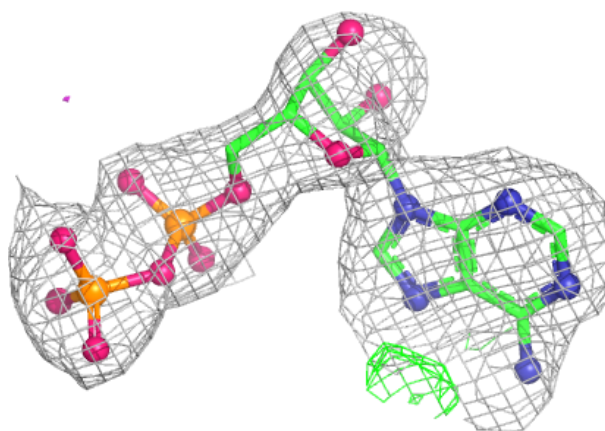
Electron density around ADP H 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



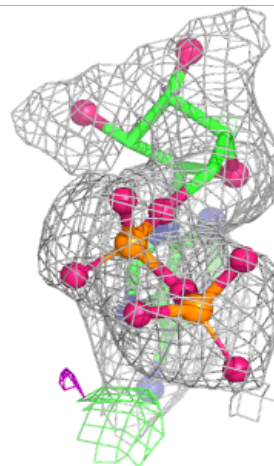
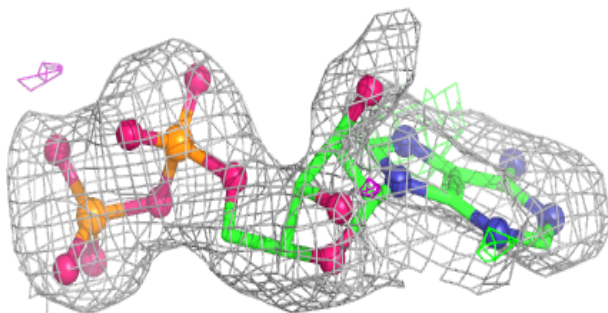
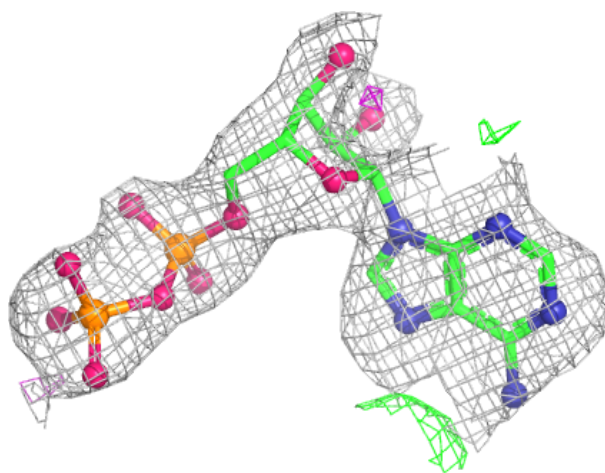
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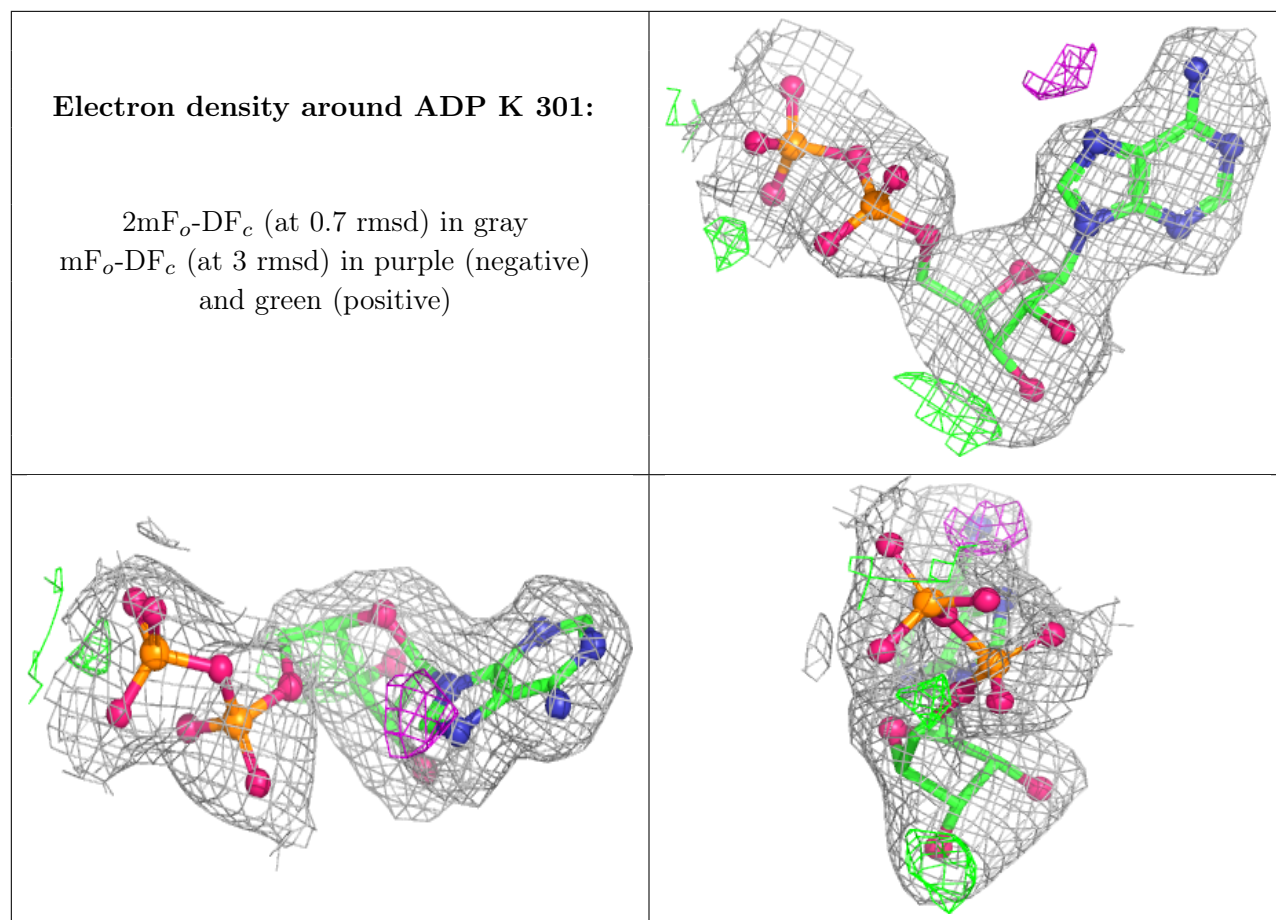
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and green (positive)



Electron density around ADP J 301:

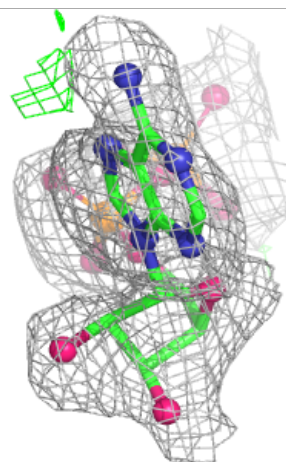
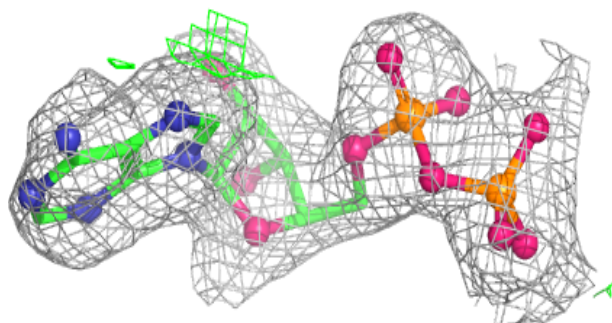
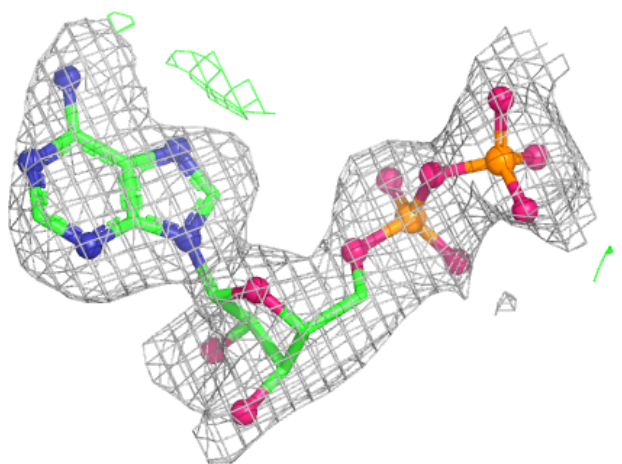
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





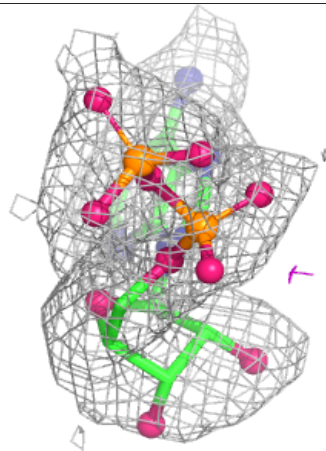
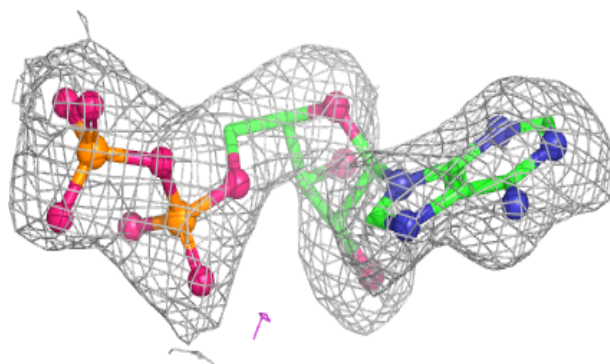
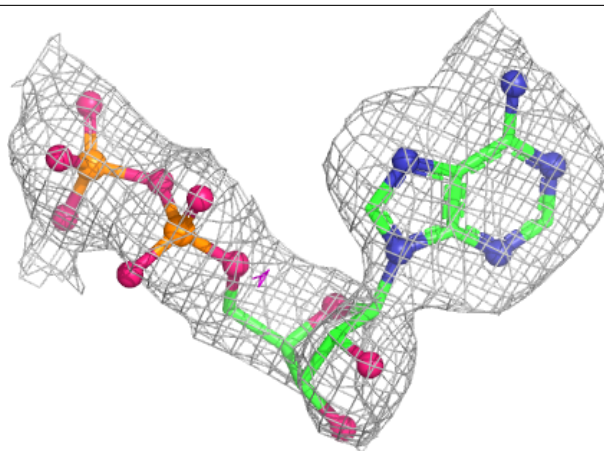
Electron density around ADP L 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

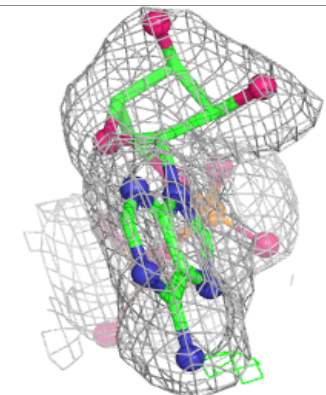
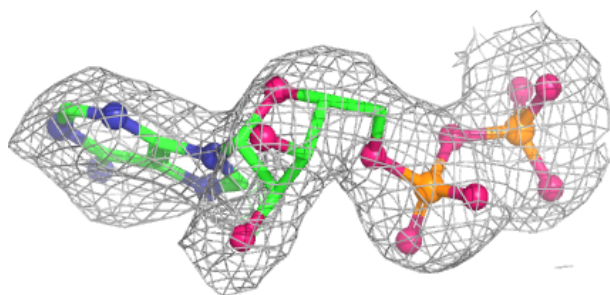
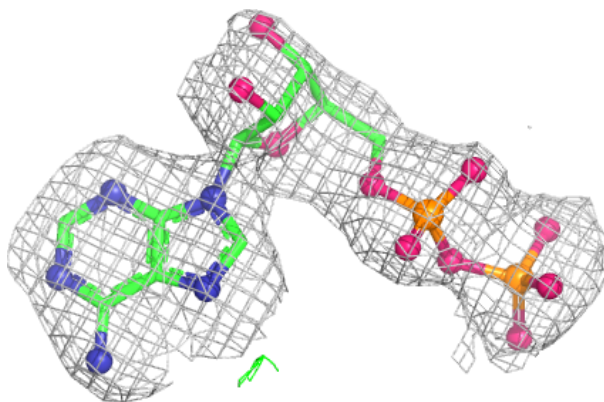


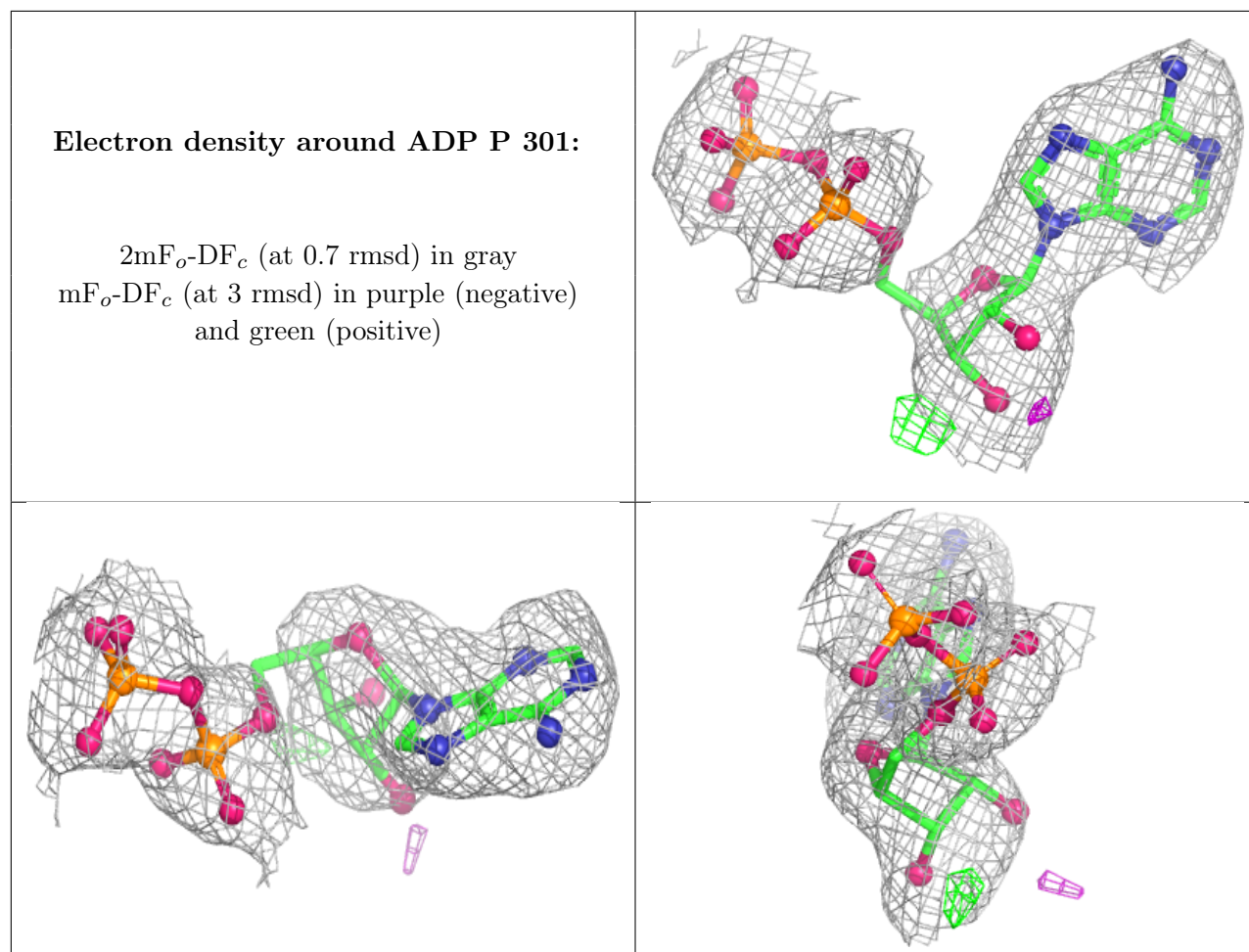
Electron density around ADP N 301:

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and green (positive)

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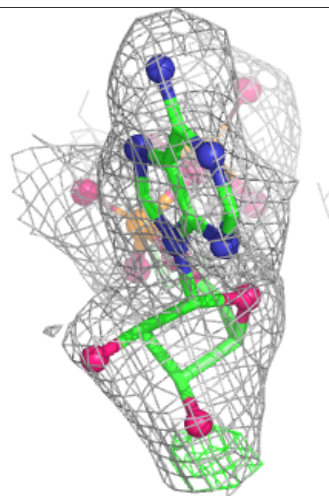
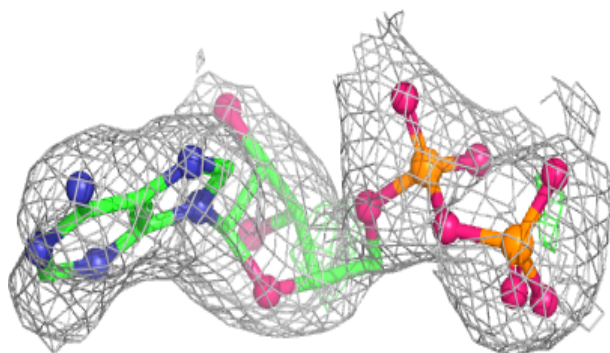
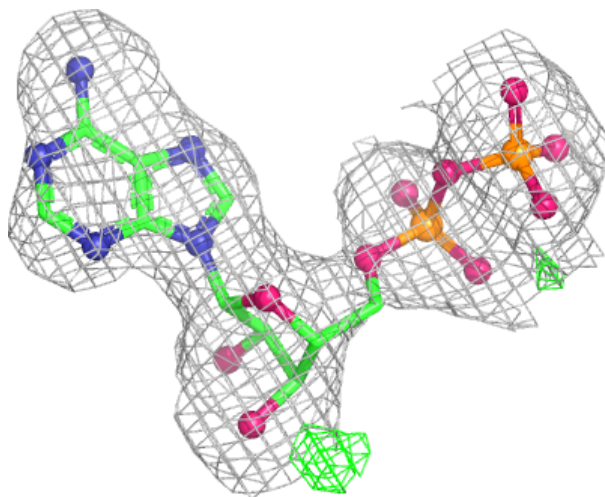
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





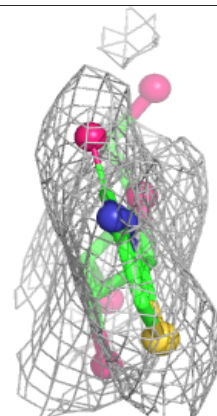
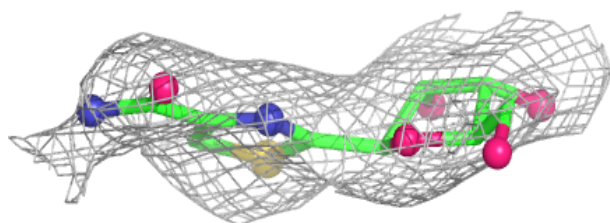
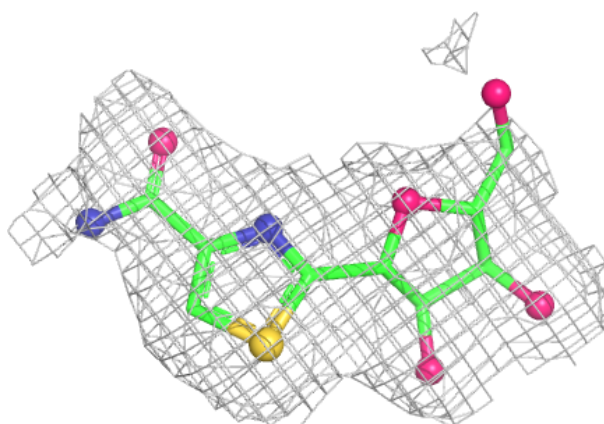
Electron density around ADP A 301:

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and green (positive)



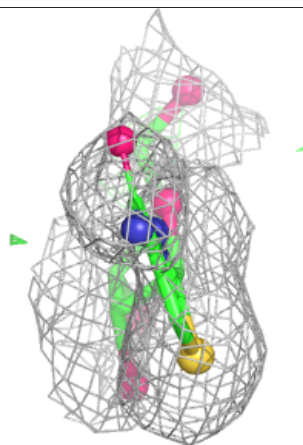
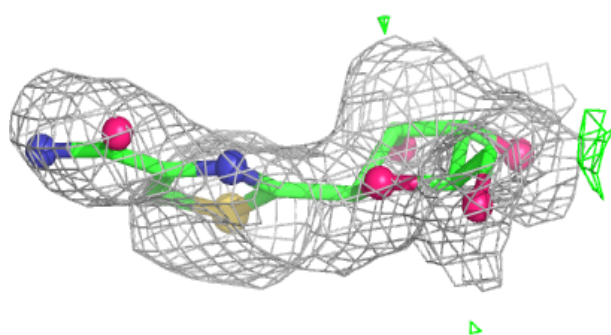
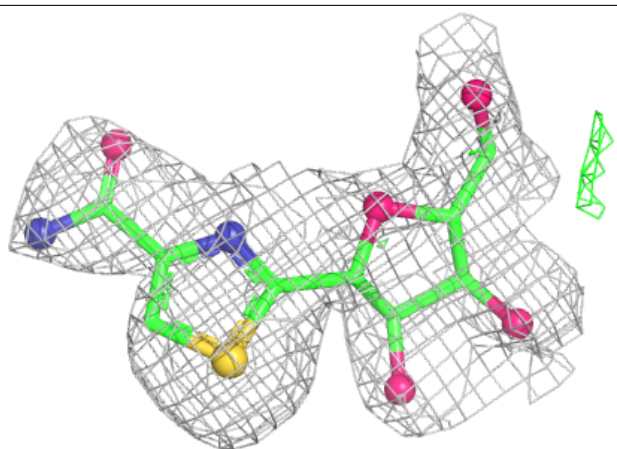
Electron density around TIZ B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



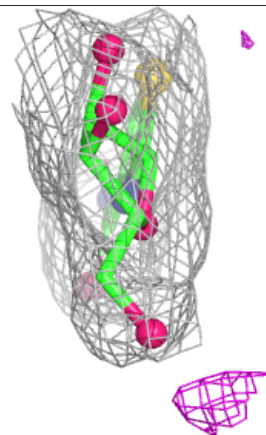
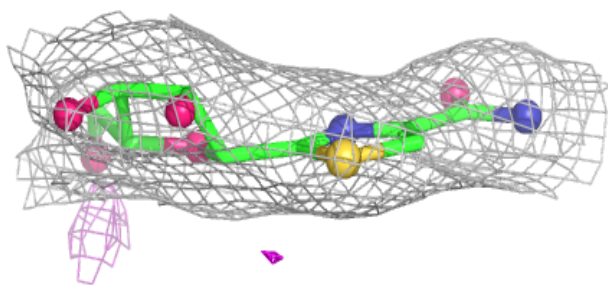
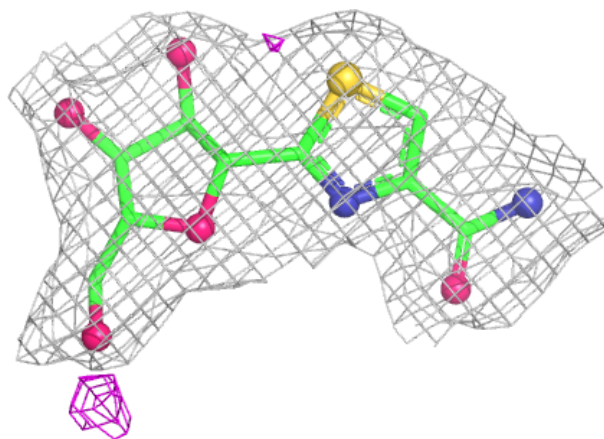
Electron density around TIZ C 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



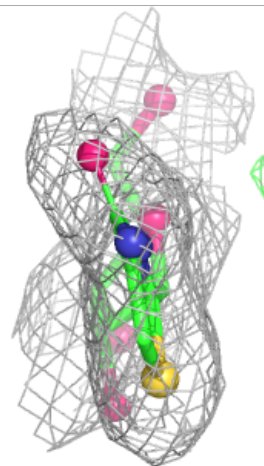
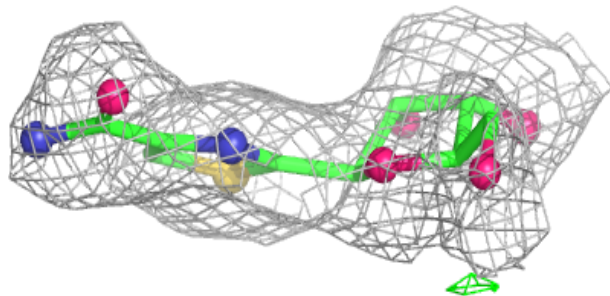
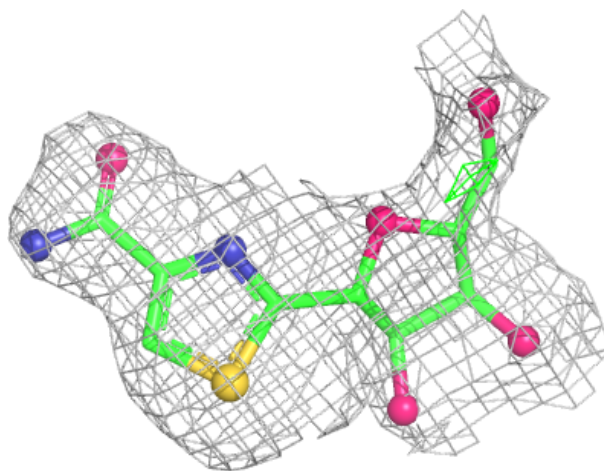
Electron density around TIZ D 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



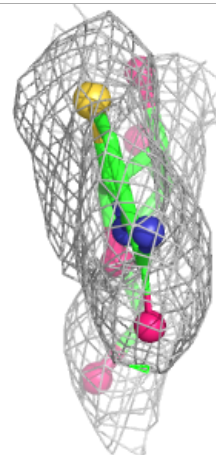
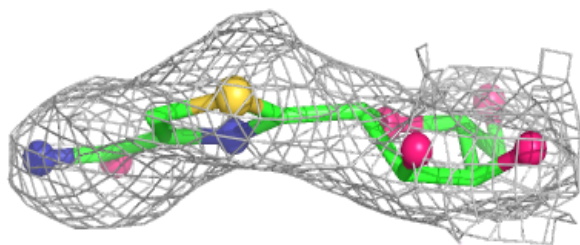
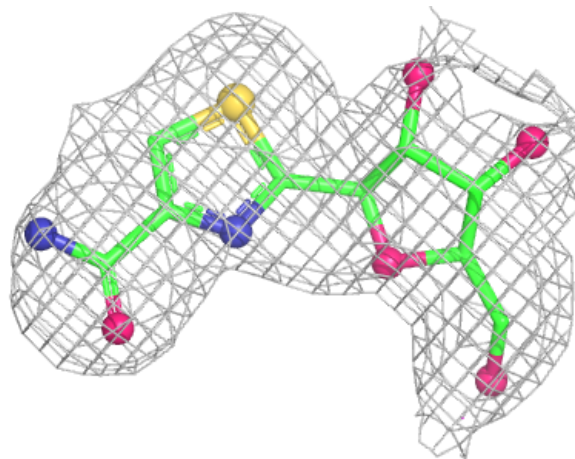
Electron density around TIZ E 302:

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and green (positive)



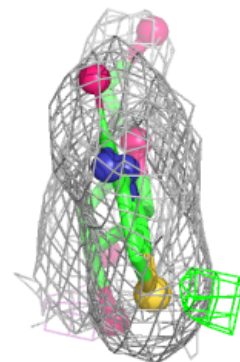
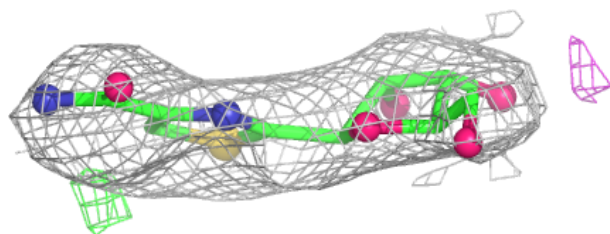
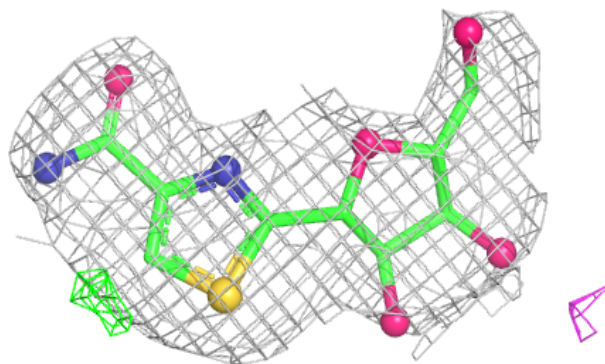
Electron density around TIZ F 302:

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and green (positive)

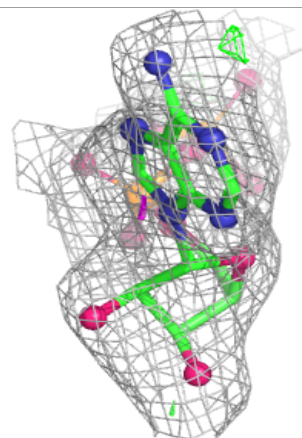
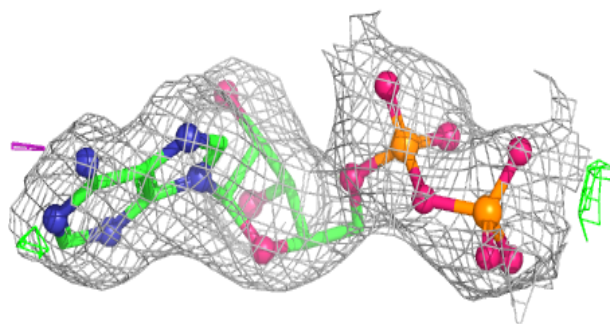
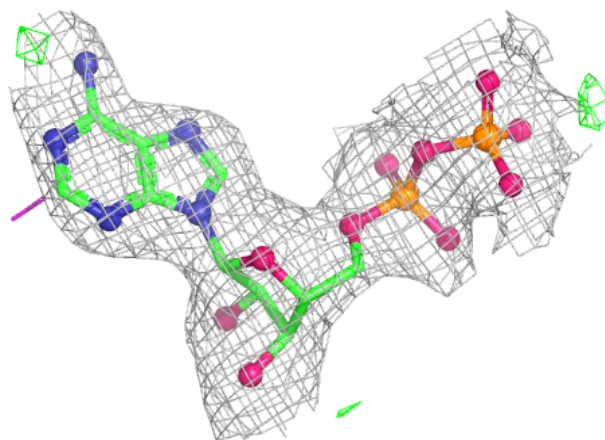


Electron density around TIZ G 302:

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and green (positive)

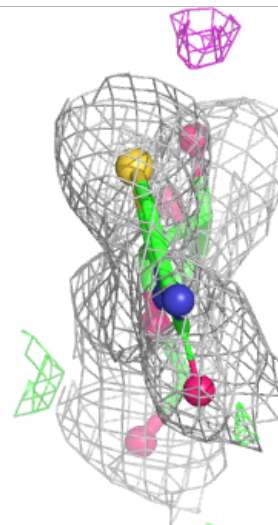
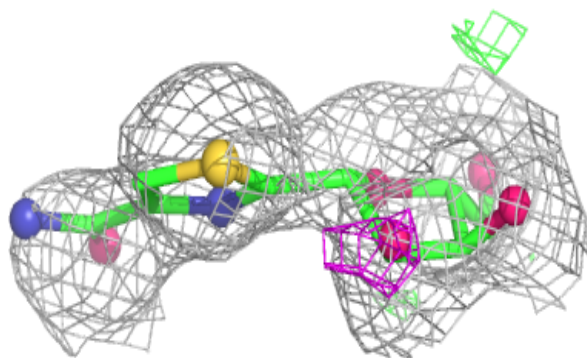
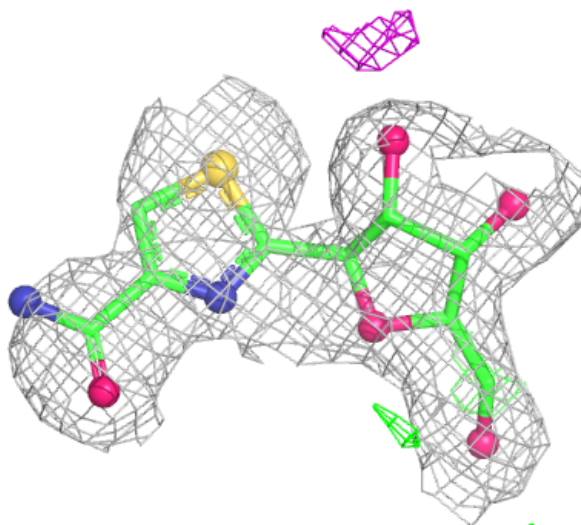
**Electron density around ADP B 301:**

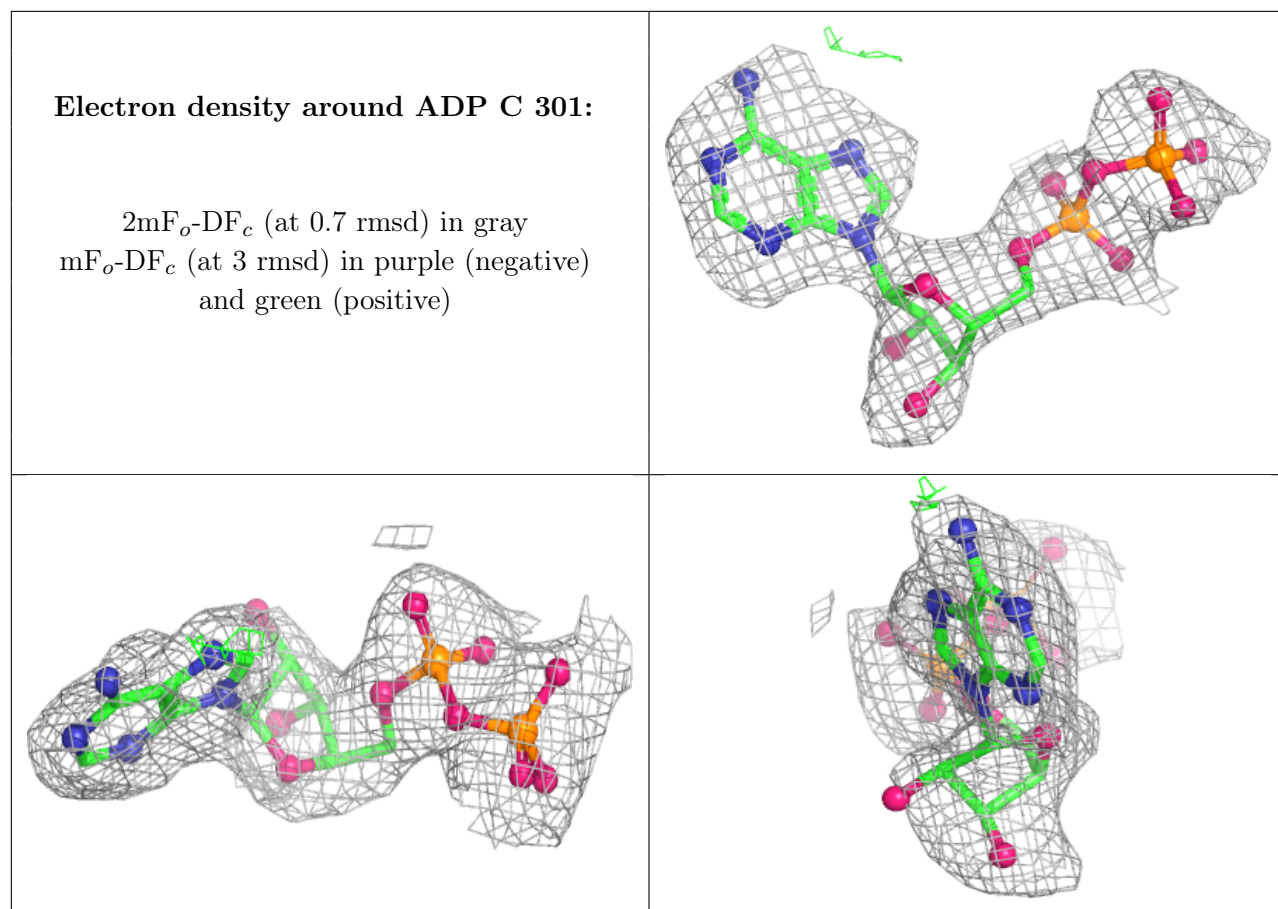
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TIZ I 302:

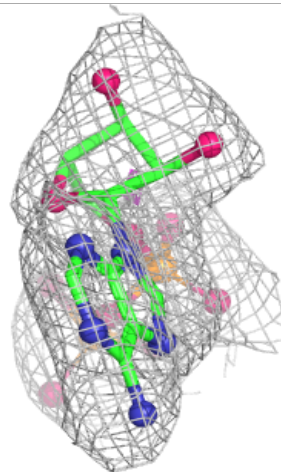
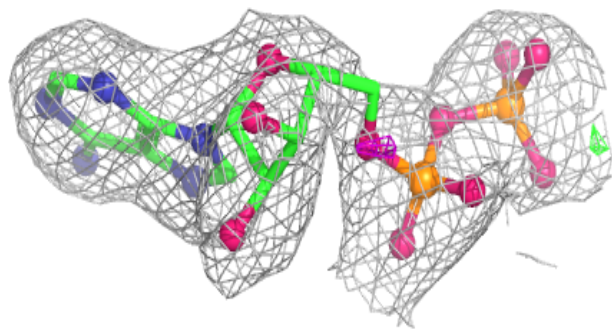
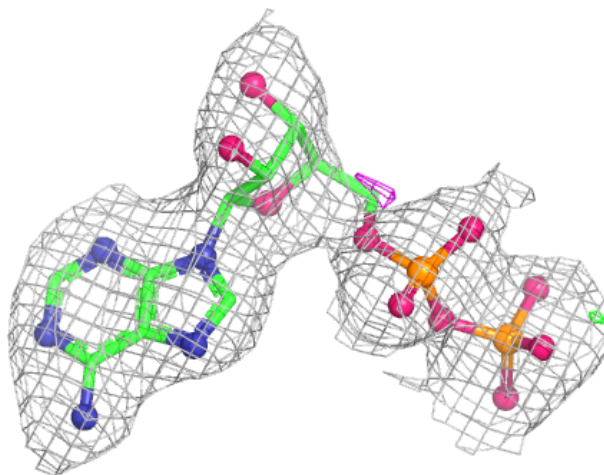
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





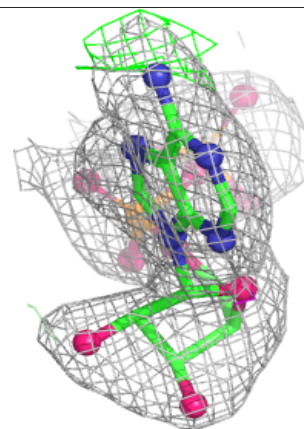
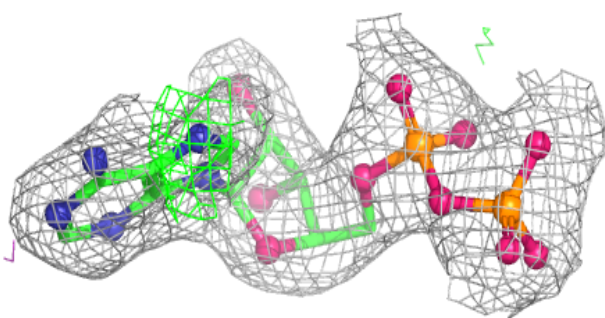
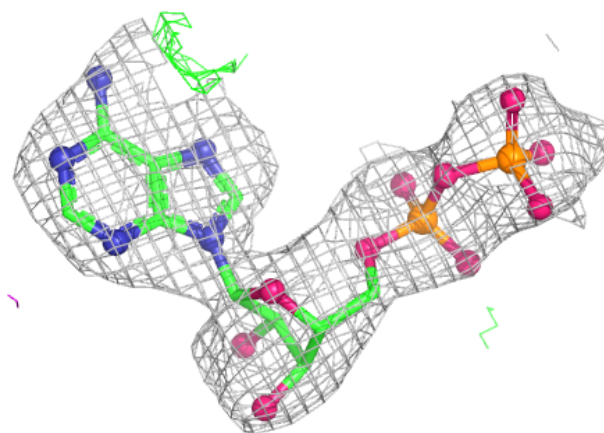
Electron density around ADP D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

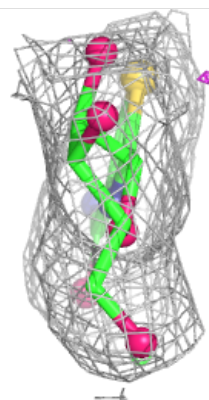
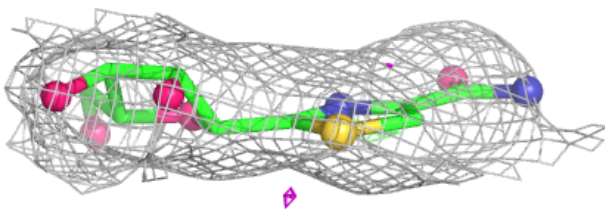
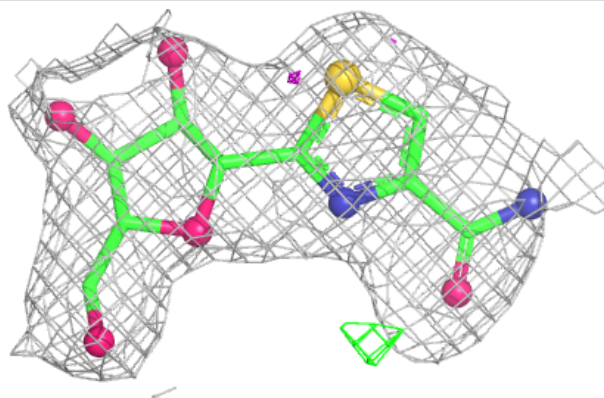


Electron density around ADP E 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

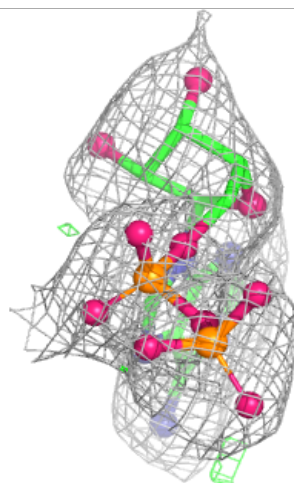
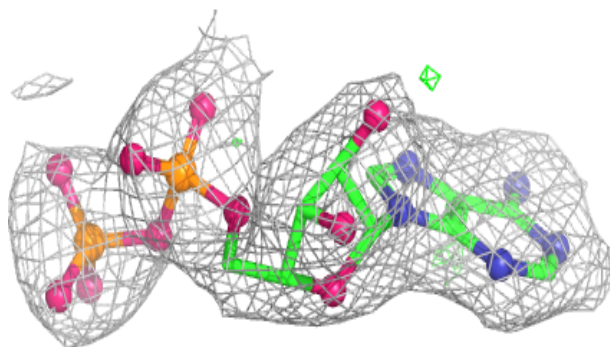
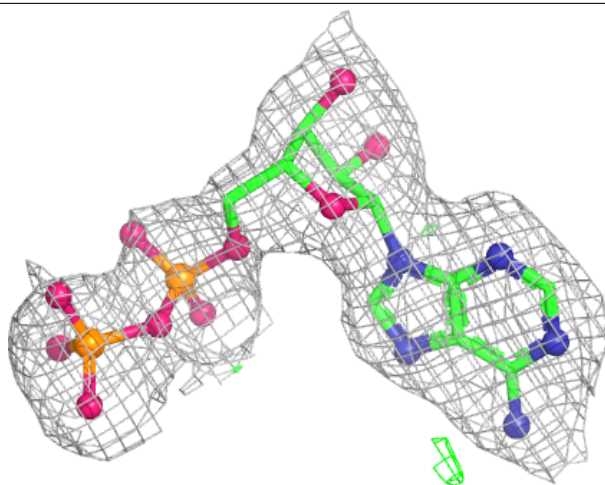
**Electron density around TIZ M 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



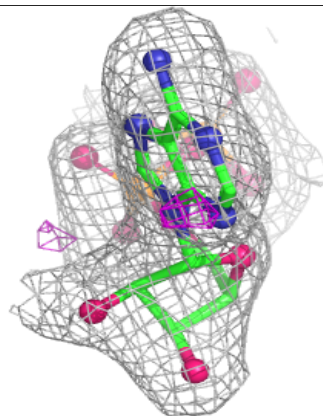
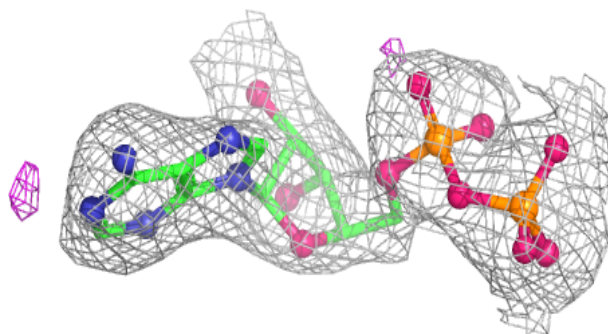
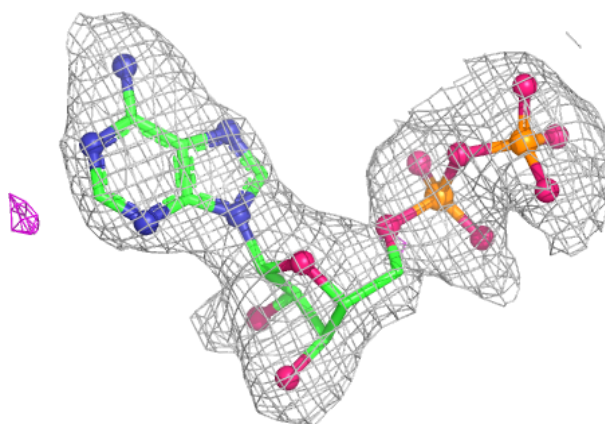
Electron density around ADP F 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

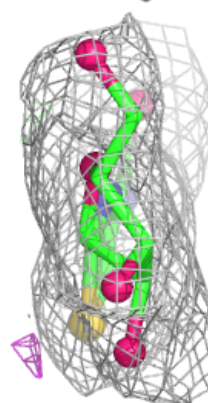
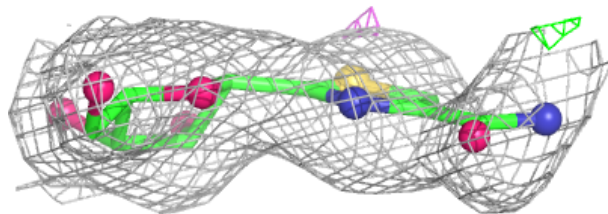
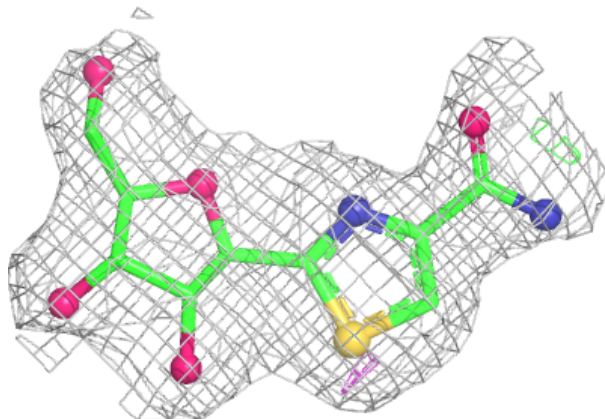


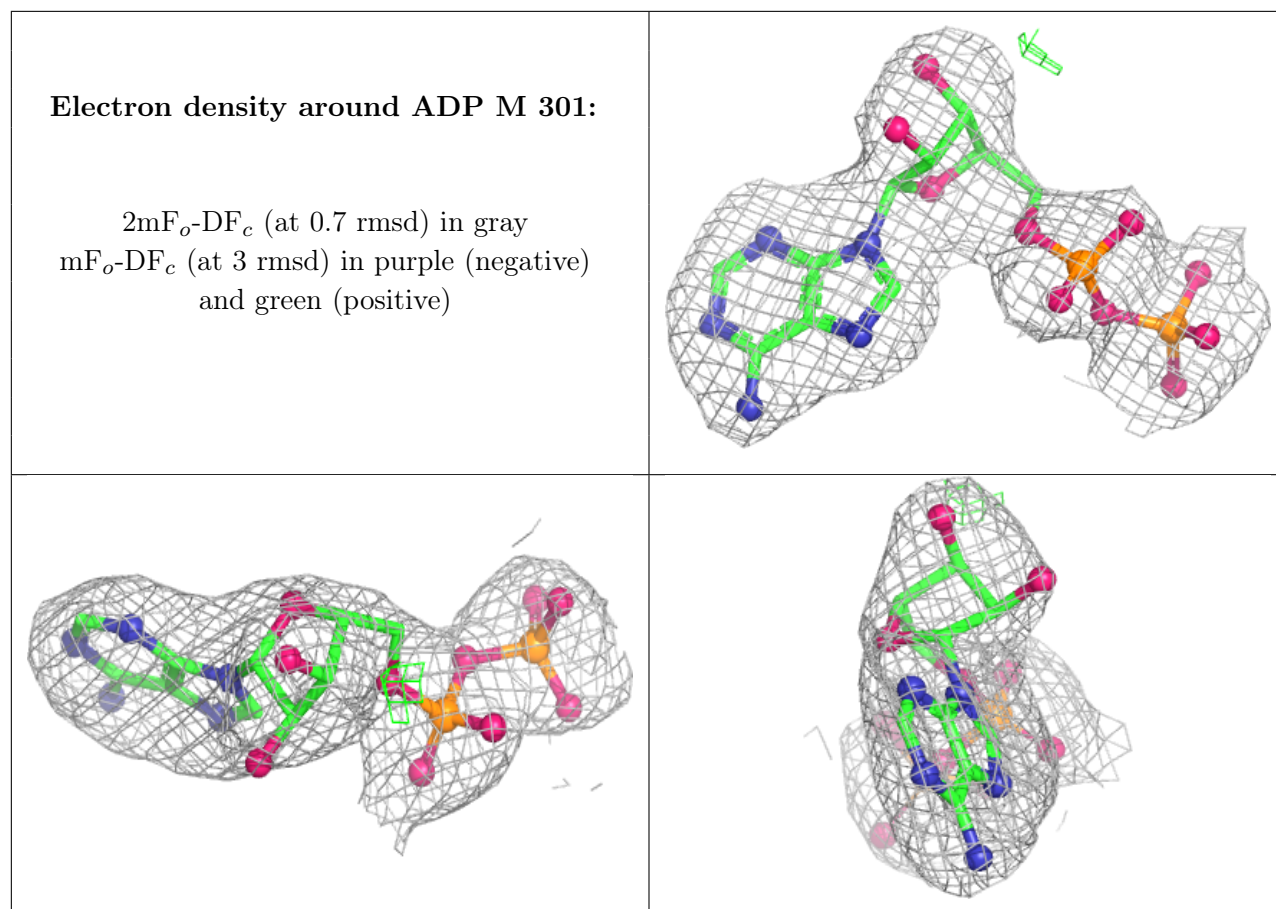
Electron density around ADP G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TIZ P 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.