



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:01 AM UTC

PDB ID : 9NLR / pdb_00009nlr
Title : Crystal structure of human glutamine synthetase in complex with ADP and phosphate
Authors : Lovell, S.; Battaile, K.P.; Jeitner, T.M.
Deposited on : 2025-03-03
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure 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/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:

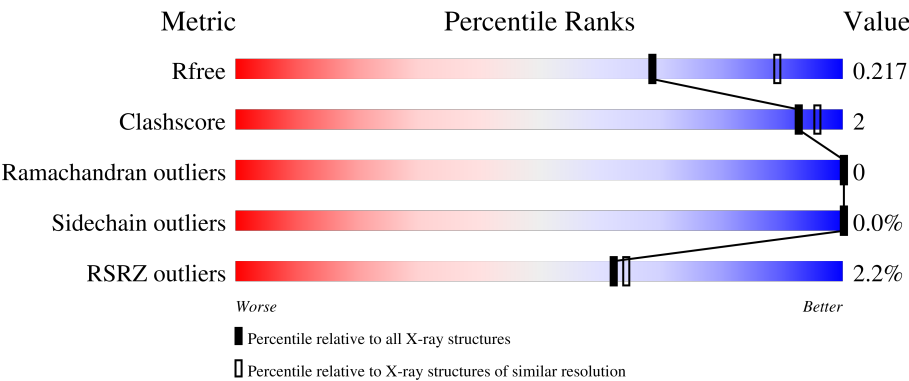
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	373	<div><div>2%</div><div>96%</div><div>..</div></div>
1	B	373	<div><div>%</div><div>95%</div><div>..</div></div>
1	C	373	<div><div>2%</div><div>96%</div><div>..</div></div>
1	D	373	<div><div>%</div><div>95%</div><div>..</div></div>
1	E	373	<div><div>2%</div><div>96%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	373	
1	G	373	
1	H	373	
1	I	373	
1	J	373	
1	K	373	
1	L	373	
1	M	373	
1	N	373	
1	O	373	
1	P	373	
1	Q	373	
1	R	373	
1	S	373	
1	T	373	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59088 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 Glutamine synthetase.

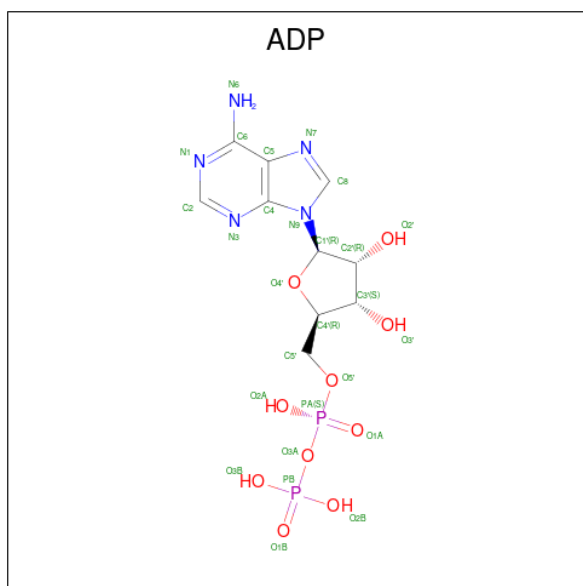
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2846	1794	502	528	22			
1	B	370	Total	C	N	O	S	0	0	0
			2897	1822	512	541	22			
1	C	370	Total	C	N	O	S	0	0	0
			2908	1828	514	544	22			
1	D	370	Total	C	N	O	S	0	0	0
			2903	1824	515	542	22			
1	E	368	Total	C	N	O	S	0	0	0
			2882	1813	508	539	22			
1	F	366	Total	C	N	O	S	0	0	0
			2864	1799	510	533	22			
1	G	363	Total	C	N	O	S	0	0	0
			2837	1779	505	531	22			
1	H	366	Total	C	N	O	S	0	0	0
			2857	1798	505	532	22			
1	I	370	Total	C	N	O	S	0	0	0
			2884	1813	512	537	22			
1	J	359	Total	C	N	O	S	0	0	0
			2791	1756	502	511	22			
1	K	356	Total	C	N	O	S	0	0	0
			2775	1743	494	516	22			
1	L	368	Total	C	N	O	S	0	0	0
			2842	1785	503	532	22			
1	M	369	Total	C	N	O	S	0	0	0
			2814	1767	502	523	22			
1	N	367	Total	C	N	O	S	0	0	0
			2829	1778	499	530	22			
1	O	365	Total	C	N	O	S	0	0	0
			2853	1791	511	529	22			
1	P	362	Total	C	N	O	S	0	0	0
			2806	1765	494	525	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	359	Total	C	N	O	S	0	0	0
			2762	1744	487	509	22			
1	R	364	Total	C	N	O	S	0	0	0
			2766	1740	490	514	22			
1	S	356	Total	C	N	O	S	0	0	0
			2695	1699	477	497	22			
1	T	367	Total	C	N	O	S	0	0	0
			2831	1783	502	524	22			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
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		
2	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	R	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	S	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

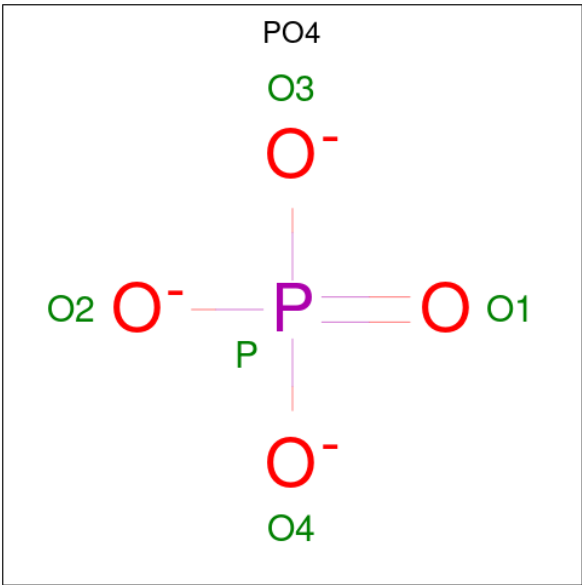
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mn	0	0
			3	3		
3	B	3	Total	Mn	0	0
			3	3		
3	C	3	Total	Mn	0	0
			3	3		
3	D	3	Total	Mn	0	0
			3	3		
3	E	3	Total	Mn	0	0
			3	3		
3	F	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Mn 3	0	0
3	H	3	Total 3	Mn 3	0	0
3	I	3	Total 3	Mn 3	0	0
3	J	3	Total 3	Mn 3	0	0
3	K	3	Total 3	Mn 3	0	0
3	L	3	Total 3	Mn 3	0	0
3	M	3	Total 3	Mn 3	0	0
3	N	3	Total 3	Mn 3	0	0
3	O	3	Total 3	Mn 3	0	0
3	P	3	Total 3	Mn 3	0	0
3	Q	3	Total 3	Mn 3	0	0
3	R	3	Total 3	Mn 3	0	0
3	S	3	Total 3	Mn 3	0	0
3	T	3	Total 3	Mn 3	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	L	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		
4	N	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total	O	P	0	0
			5	4	1		
4	P	1	Total	O	P	0	0
			5	4	1		
4	Q	1	Total	O	P	0	0
			5	4	1		
4	R	1	Total	O	P	0	0
			5	4	1		
4	S	1	Total	O	P	0	0
			5	4	1		
4	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	C	2	Total	Na	0	0
			2	2		
5	D	1	Total	Na	0	0
			1	1		
5	E	1	Total	Na	0	0
			1	1		
5	F	1	Total	Na	0	0
			1	1		
5	G	1	Total	Na	0	0
			1	1		
5	H	1	Total	Na	0	0
			1	1		
5	I	1	Total	Na	0	0
			1	1		
5	J	1	Total	Na	0	0
			1	1		
5	K	1	Total	Na	0	0
			1	1		
5	L	1	Total	Na	0	0
			1	1		
5	M	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	1	Total 1	Na 1	0	0
5	O	1	Total 1	Na 1	0	0
5	P	1	Total 1	Na 1	0	0
5	Q	1	Total 1	Na 1	0	0
5	R	1	Total 1	Na 1	0	0
5	S	1	Total 1	Na 1	0	0
5	T	1	Total 1	Na 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total 97	O 97	0	0
6	B	124	Total 124	O 124	0	0
6	C	135	Total 135	O 135	0	0
6	D	124	Total 124	O 124	0	0
6	E	112	Total 112	O 112	0	0
6	F	104	Total 104	O 104	0	0
6	G	110	Total 110	O 110	0	0
6	H	93	Total 93	O 93	0	0
6	I	111	Total 111	O 111	0	0
6	J	94	Total 94	O 94	0	0
6	K	80	Total 80	O 80	0	0
6	L	71	Total 71	O 71	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	52	Total 52	O 52	0	0
6	N	74	Total 74	O 74	0	0
6	O	91	Total 91	O 91	0	0
6	P	70	Total 70	O 70	0	0
6	Q	42	Total 42	O 42	0	0
6	R	43	Total 43	O 43	0	0
6	S	38	Total 38	O 38	0	0
6	T	60	Total 60	O 60	0	0

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.

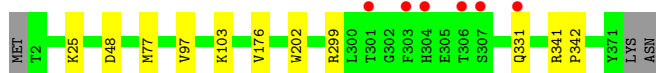
- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



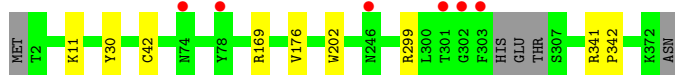
- Molecule 1: Glutamine synthetase



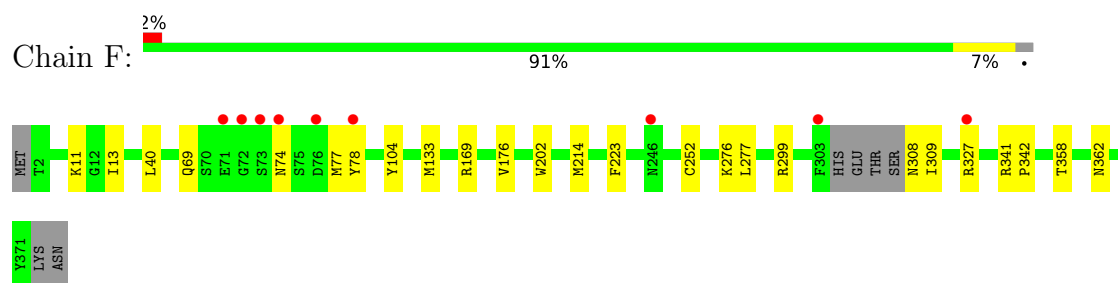
- Molecule 1: Glutamine synthetase



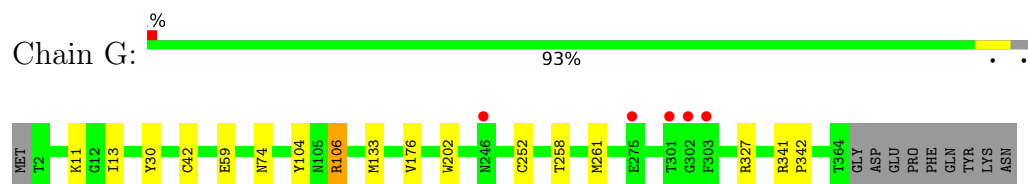
- Molecule 1: Glutamine synthetase



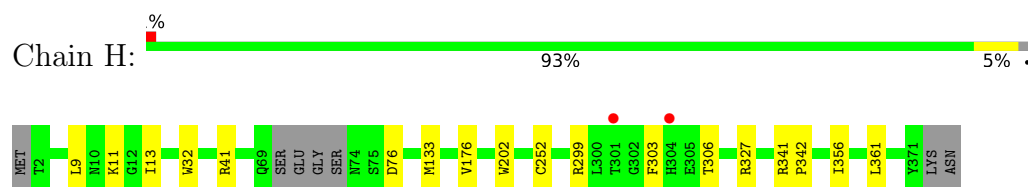
- Molecule 1: Glutamine synthetase



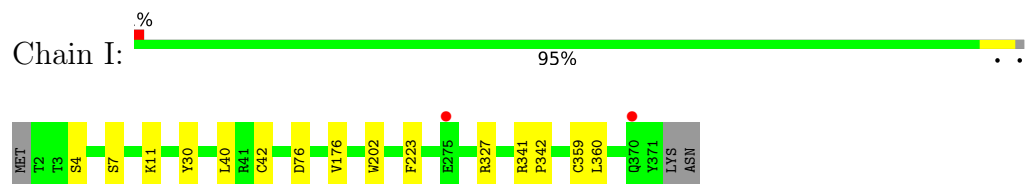
- Molecule 1: Glutamine synthetase



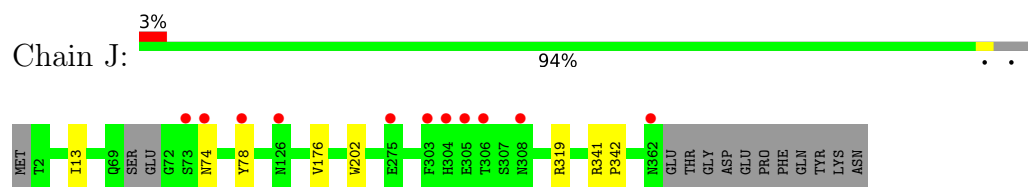
- Molecule 1: Glutamine synthetase



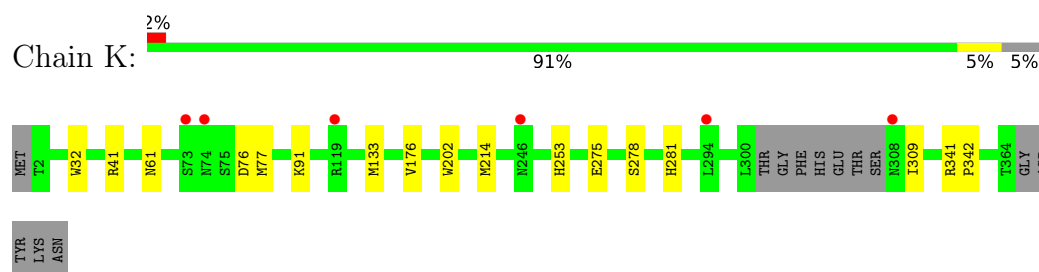
- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



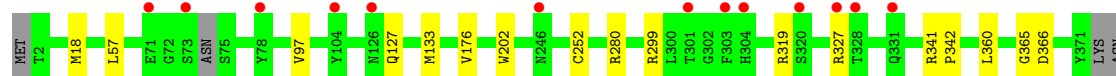
- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



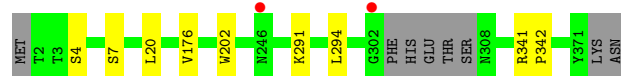
- Molecule 1: Glutamine synthetase



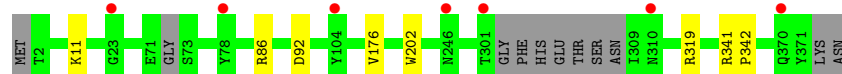
- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



- Molecule 1: Glutamine synthetase



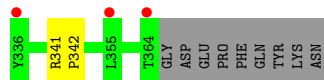
- Molecule 1: Glutamine synthetase





- Molecule 1: Glutamine synthetase

Chain S: 6% 92% 5%



- Molecule 1: Glutamine synthetase

Chain T: 3% 94%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.08Å 213.50Å 199.94Å 90.00° 96.26° 90.00°	Depositor
Resolution (Å)	45.81 – 2.30 45.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.81-2.30) 99.4 (45.81-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_5484: ???)	Depositor
R, R_{free}	0.181 , 0.215 0.185 , 0.217	Depositor DCC
R_{free} test set	16887 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	59088	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: ADP, PO4, MN, NA

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	0.09	0/2923	0.26	0/3963
1	B	0.09	0/2976	0.25	0/4033
1	C	0.10	0/2987	0.25	0/4046
1	D	0.09	0/2982	0.26	0/4040
1	E	0.10	0/2959	0.26	0/4007
1	F	0.09	0/2940	0.25	0/3982
1	G	0.09	0/2911	0.25	0/3943
1	H	0.09	0/2935	0.25	0/3981
1	I	0.09	0/2963	0.25	0/4018
1	J	0.09	0/2865	0.25	0/3881
1	K	0.09	0/2848	0.23	0/3860
1	L	0.08	0/2918	0.24	0/3960
1	M	0.08	0/2888	0.23	0/3922
1	N	0.08	0/2904	0.23	0/3940
1	O	0.08	0/2928	0.24	0/3965
1	P	0.08	0/2880	0.23	0/3906
1	Q	0.08	0/2836	0.23	0/3850
1	R	0.08	0/2840	0.23	0/3860
1	S	0.08	0/2765	0.23	0/3755
1	T	0.08	0/2908	0.23	0/3947
All	All	0.09	0/58156	0.24	0/78859

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	106	ARG	Sidechain

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	2846	0	2686	6	0
1	B	2897	0	2741	11	0
1	C	2908	0	2760	9	0
1	D	2903	0	2757	10	0
1	E	2882	0	2735	7	0
1	F	2864	0	2720	19	0
1	G	2837	0	2705	13	0
1	H	2857	0	2691	14	0
1	I	2884	0	2719	10	0
1	J	2791	0	2659	7	0
1	K	2775	0	2635	11	0
1	L	2842	0	2666	11	0
1	M	2814	0	2627	12	0
1	N	2829	0	2661	6	0
1	O	2853	0	2720	6	0
1	P	2806	0	2639	6	0
1	Q	2762	0	2586	5	0
1	R	2766	0	2573	8	0
1	S	2695	0	2504	9	0
1	T	2831	0	2657	12	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	27	0	12	0	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
2	Q	27	0	12	0	0
2	R	27	0	12	0	0
2	S	27	0	12	0	0
2	T	27	0	12	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	3	0	0	0	0
3	O	3	0	0	0	0
3	P	3	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	5	0	0	0	0
4	L	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	O	5	0	0	0	0
4	P	5	0	0	1	0
4	Q	5	0	0	0	0
4	R	5	0	0	0	0
4	S	5	0	0	0	0
4	T	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	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
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
6	A	97	0	0	0	0
6	B	124	0	0	0	0
6	C	135	0	0	0	0
6	D	124	0	0	1	0
6	E	112	0	0	1	0
6	F	104	0	0	1	0
6	G	110	0	0	0	0
6	H	93	0	0	0	0
6	I	111	0	0	1	0
6	J	94	0	0	0	0
6	K	80	0	0	0	0
6	L	71	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	52	0	0	1	0
6	N	74	0	0	1	0
6	O	91	0	0	0	0
6	P	70	0	0	0	0
6	Q	42	0	0	0	0
6	R	43	0	0	0	0
6	S	38	0	0	0	0
6	T	60	0	0	2	0
All	All	59088	0	53681	170	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 2.

All (170) 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:H:9:LEU:HD12	6:I:532:HOH:O	1.89	0.72
1:F:169:ARG:NH1	6:F:501:HOH:O	2.24	0.70
1:E:169:ARG:NH1	6:E:501:HOH:O	2.24	0.69
1:S:258:THR:O	1:S:260:ALA:N	2.26	0.68
1:M:327:ARG:NH1	6:M:501:HOH:O	2.27	0.67
1:T:69:GLN:HB3	1:T:77:MET:HE2	1.77	0.67
1:L:76:ASP:OD1	1:M:319:ARG:NH1	2.32	0.63
1:H:176:VAL:HG21	1:H:202:TRP:CE3	2.35	0.62
1:D:176:VAL:HG21	1:D:202:TRP:CE3	2.35	0.62
1:F:74:ASN:OD1	1:G:327:ARG:NH2	2.31	0.61
1:F:176:VAL:HG21	1:F:202:TRP:CE3	2.36	0.60
1:M:18:MET:HA	1:M:18:MET:HE2	1.84	0.59
1:A:176:VAL:HG21	1:A:202:TRP:CE3	2.37	0.59
1:R:77:MET:HE3	1:R:103:LYS:HA	1.85	0.59
1:G:133:MET:HE2	1:G:252:CYS:SG	2.43	0.58
1:J:176:VAL:HG21	1:J:202:TRP:CE3	2.39	0.58
1:P:319:ARG:NH1	4:P:405:PO4:O4	2.36	0.58
1:B:299:ARG:NH2	1:B:341:ARG:O	2.37	0.58
1:F:299:ARG:NH2	1:F:341:ARG:O	2.37	0.57
1:P:176:VAL:HG21	1:P:202:TRP:CE3	2.41	0.56
1:M:176:VAL:HG21	1:M:202:TRP:CE3	2.40	0.56
1:F:69:GLN:HB3	1:F:77:MET:HE2	1.88	0.56
1:A:176:VAL:HG21	1:A:202:TRP:CD2	2.40	0.56
1:M:176:VAL:HG21	1:M:202:TRP:CD2	2.41	0.55
1:C:176:VAL:HG21	1:C:202:TRP:CE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ARG:NH2	1:D:341:ARG:O	2.40	0.55
1:A:133:MET:HE2	1:A:252:CYS:SG	2.47	0.55
1:K:76:ASP:OD1	1:L:319:ARG:NH1	2.39	0.55
1:O:176:VAL:HG21	1:O:202:TRP:CE3	2.42	0.55
1:H:303:PHE:O	1:H:306:THR:OG1	2.23	0.54
1:L:176:VAL:HG21	1:L:202:TRP:CE3	2.42	0.54
1:I:176:VAL:HG21	1:I:202:TRP:CE3	2.43	0.54
1:F:176:VAL:HG21	1:F:202:TRP:CD2	2.43	0.54
1:G:59:GLU:OE2	1:G:106:ARG:NH2	2.41	0.54
1:K:91:LYS:HE3	1:O:20:LEU:HD23	1.89	0.54
1:B:30:TYR:HA	1:B:97:VAL:HG13	1.90	0.54
1:K:176:VAL:HG21	1:K:202:TRP:CE3	2.43	0.54
1:O:4:SER:O	1:O:7:SER:OG	2.27	0.53
1:B:176:VAL:HG21	1:B:202:TRP:CE3	2.44	0.52
1:M:280:ARG:NH2	1:M:365:GLY:O	2.40	0.52
1:F:308:ASN:OD1	1:F:309:ILE:N	2.43	0.52
1:C:176:VAL:HG21	1:C:202:TRP:CD2	2.45	0.52
1:S:81:PRO:HB3	1:S:97:VAL:HG21	1.90	0.52
1:D:133:MET:HE2	1:D:252:CYS:SG	2.49	0.52
1:O:291:LYS:HB3	1:O:294:LEU:HD12	1.92	0.52
1:M:133:MET:HE2	1:M:252:CYS:SG	2.50	0.51
1:Q:176:VAL:HG21	1:Q:202:TRP:CE3	2.45	0.51
1:A:13:ILE:HD11	1:B:11:LYS:HE3	1.92	0.51
1:E:299:ARG:NH2	1:E:341:ARG:O	2.43	0.51
1:I:176:VAL:HG21	1:I:202:TRP:CD2	2.47	0.50
1:H:299:ARG:NH2	1:H:341:ARG:O	2.45	0.50
1:P:176:VAL:HG21	1:P:202:TRP:CD2	2.46	0.50
1:K:176:VAL:HG21	1:K:202:TRP:CD2	2.47	0.50
1:L:30:TYR:HA	1:L:97:VAL:HG13	1.92	0.50
1:G:176:VAL:HG21	1:G:202:TRP:CD2	2.47	0.49
1:H:133:MET:HE2	1:H:252:CYS:SG	2.52	0.49
1:E:176:VAL:HG21	1:E:202:TRP:CE3	2.48	0.49
1:B:106:ARG:NH2	1:C:331:GLN:OE1	2.45	0.49
1:L:61:ASN:ND2	6:L:504:HOH:O	2.43	0.49
1:D:176:VAL:HG21	1:D:202:TRP:CD2	2.47	0.49
1:B:123:MET:HE1	1:B:371:TYR:CD2	2.47	0.49
1:D:69:GLN:HB3	1:D:77:MET:HE2	1.95	0.49
1:T:176:VAL:HG21	1:T:202:TRP:CE3	2.48	0.49
1:F:78:TYR:OH	1:G:327:ARG:HG2	2.12	0.49
1:H:76:ASP:OD2	1:I:327:ARG:NE	2.40	0.49
1:L:63:ASP:OD1	1:L:65:SER:OG	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:VAL:HG21	1:H:202:TRP:CD2	2.48	0.48
1:H:356:ILE:HG22	1:H:361:LEU:CD2	2.44	0.48
1:N:341:ARG:N	1:N:342:PRO:CD	2.77	0.48
1:O:341:ARG:N	1:O:342:PRO:CD	2.76	0.48
1:F:133:MET:HE2	1:F:252:CYS:SG	2.54	0.48
1:R:63:ASP:OD1	1:R:65:SER:OG	2.27	0.48
1:S:176:VAL:HG21	1:S:202:TRP:CE3	2.49	0.48
1:G:74:ASN:OD1	1:H:327:ARG:NH2	2.40	0.48
1:S:128:HIS:ND1	1:S:210:GLU:OE2	2.43	0.48
1:C:341:ARG:N	1:C:342:PRO:CD	2.77	0.47
1:R:341:ARG:N	1:R:342:PRO:CD	2.77	0.47
1:L:341:ARG:N	1:L:342:PRO:CD	2.78	0.47
1:T:299:ARG:NH2	1:T:341:ARG:O	2.47	0.47
1:C:25:LYS:NZ	1:C:48:ASP:OD1	2.46	0.47
1:K:275:GLU:O	1:K:278:SER:OG	2.30	0.46
1:Q:341:ARG:N	1:Q:342:PRO:CD	2.78	0.46
1:A:341:ARG:N	1:A:342:PRO:CD	2.79	0.46
1:F:341:ARG:N	1:F:342:PRO:CD	2.79	0.46
1:I:76:ASP:OD1	1:J:319:ARG:NH1	2.44	0.46
1:T:341:ARG:N	1:T:342:PRO:CD	2.78	0.46
1:J:176:VAL:HG21	1:J:202:TRP:CD2	2.50	0.46
1:J:341:ARG:N	1:J:342:PRO:CD	2.79	0.46
1:L:176:VAL:HG21	1:L:202:TRP:CD2	2.50	0.46
1:P:341:ARG:N	1:P:342:PRO:CD	2.78	0.46
1:B:176:VAL:HG21	1:B:202:TRP:CD2	2.50	0.46
1:E:341:ARG:N	1:E:342:PRO:CD	2.78	0.46
1:F:13:ILE:HD11	1:G:11:LYS:HG3	1.97	0.46
1:G:13:ILE:HD11	1:H:11:LYS:HG3	1.96	0.46
1:M:341:ARG:N	1:M:342:PRO:CD	2.79	0.46
1:G:341:ARG:N	1:G:342:PRO:CD	2.78	0.46
1:M:127:GLN:OE1	1:M:360:LEU:HD22	2.16	0.46
1:I:4:SER:O	1:I:7:SER:OG	2.34	0.46
1:L:214:MET:O	1:L:214:MET:HE3	2.15	0.46
1:D:341:ARG:N	1:D:342:PRO:CD	2.79	0.45
1:I:341:ARG:N	1:I:342:PRO:CD	2.79	0.45
1:S:341:ARG:N	1:S:342:PRO:CD	2.79	0.45
1:B:30:TYR:O	1:B:42:CYS:HA	2.17	0.45
1:H:341:ARG:N	1:H:342:PRO:CD	2.80	0.45
1:N:176:VAL:HG21	1:N:202:TRP:CD2	2.51	0.45
1:R:57:LEU:HD11	1:R:84:MET:SD	2.57	0.45
1:G:176:VAL:HG21	1:G:202:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:341:ARG:N	1:K:342:PRO:CD	2.79	0.45
1:D:210:GLU:OE2	6:D:501:HOH:O	2.21	0.45
1:O:176:VAL:HG21	1:O:202:TRP:CD2	2.52	0.44
1:C:77:MET:HE3	1:C:103:LYS:HA	1.99	0.44
1:P:11:LYS:HG3	1:T:13:ILE:HD11	1.99	0.44
1:B:341:ARG:N	1:B:342:PRO:CD	2.80	0.44
1:Q:40:LEU:HD13	1:Q:223:PHE:HB2	1.98	0.44
1:T:168:ASP:O	6:T:501:HOH:O	2.21	0.44
1:I:30:TYR:O	1:I:42:CYS:HA	2.18	0.44
1:G:104:TYR:HB2	1:H:327:ARG:CZ	2.48	0.43
1:K:214:MET:O	1:K:214:MET:HE3	2.18	0.43
1:G:258:THR:HG1	1:G:261:MET:HG3	1.83	0.43
1:B:78:TYR:OH	1:C:331:GLN:NE2	2.52	0.43
1:R:214:MET:HE3	1:R:214:MET:O	2.18	0.43
1:A:26:VAL:HG22	1:A:93:PRO:HG2	2.00	0.43
1:E:176:VAL:HG21	1:E:202:TRP:CD2	2.53	0.43
1:N:176:VAL:HG21	1:N:202:TRP:CE3	2.53	0.43
1:S:176:VAL:HG21	1:S:202:TRP:CD2	2.54	0.43
1:D:13:ILE:HD11	1:E:11:LYS:HE3	2.01	0.42
1:H:13:ILE:HD11	1:I:11:LYS:HE3	2.01	0.42
1:C:299:ARG:NH2	1:C:341:ARG:O	2.52	0.42
1:F:40:LEU:HD13	1:F:223:PHE:HB2	2.02	0.42
1:K:32:TRP:CE2	1:K:41:ARG:HB2	2.54	0.42
1:N:103:LYS:NZ	6:N:501:HOH:O	2.27	0.42
1:R:190:ILE:HA	1:R:206:ILE:HD13	2.02	0.42
1:F:11:LYS:HG3	1:J:13:ILE:HD11	2.02	0.42
1:P:86:ARG:NH2	1:P:92:ASP:OD2	2.46	0.42
1:R:176:VAL:HG21	1:R:202:TRP:CD2	2.54	0.42
1:F:276:LYS:NZ	1:F:362:ASN:OD1	2.37	0.42
1:R:7:SER:HB3	1:R:233:GLY:HA3	2.02	0.42
1:Q:176:VAL:HG21	1:Q:202:TRP:CD2	2.55	0.42
1:S:13:ILE:HD11	1:T:11:LYS:HG3	2.02	0.42
1:C:97:VAL:HG13	1:C:97:VAL:O	2.20	0.41
1:H:32:TRP:CE2	1:H:41:ARG:HB2	2.55	0.41
1:I:40:LEU:HD13	1:I:223:PHE:HB2	2.02	0.41
1:K:281:HIS:NE2	1:K:309:ILE:O	2.39	0.41
1:B:32:TRP:CE2	1:B:41:ARG:HB2	2.55	0.41
1:T:303:PHE:O	1:T:306:THR:OG1	2.36	0.41
1:G:30:TYR:O	1:G:42:CYS:HA	2.21	0.41
1:S:13:ILE:HD11	1:T:11:LYS:HE3	2.02	0.41
1:M:299:ARG:NH2	1:M:341:ARG:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:TYR:O	1:D:42:CYS:HA	2.21	0.41
1:S:274:ILE:CD1	1:S:325:ILE:HD11	2.50	0.41
1:F:214:MET:HE3	1:F:214:MET:O	2.21	0.41
1:F:277:LEU:HD23	1:F:358:THR:HG21	2.02	0.41
1:T:30:TYR:O	1:T:42:CYS:HA	2.21	0.41
1:D:97:VAL:O	1:D:97:VAL:HG13	2.20	0.41
1:F:327:ARG:HB3	1:J:78:TYR:OH	2.21	0.41
1:N:61:ASN:HA	1:N:77:MET:O	2.21	0.41
1:F:78:TYR:CE2	1:F:104:TYR:HA	2.57	0.40
1:L:276:LYS:NZ	1:L:362:ASN:OD1	2.35	0.40
1:Q:30:TYR:O	1:Q:42:CYS:HA	2.21	0.40
1:T:176:VAL:HG21	1:T:202:TRP:CD2	2.57	0.40
1:F:327:ARG:NH2	1:J:74:ASN:OD1	2.54	0.40
1:K:133:MET:HA	1:K:253:HIS:O	2.21	0.40
1:N:252:CYS:O	1:N:253:HIS:C	2.63	0.40
1:I:359:CYS:C	1:I:360:LEU:HD12	2.47	0.40
1:L:133:MET:HA	1:L:253:HIS:O	2.22	0.40
1:E:30:TYR:O	1:E:42:CYS:HA	2.21	0.40
1:K:61:ASN:HA	1:K:77:MET:O	2.22	0.40
1:M:57:LEU:HD13	1:M:97:VAL:HG21	2.03	0.40
1:M:366:ASP:N	1:M:366:ASP:OD1	2.52	0.40
1:T:169:ARG:NH1	6:T:512:HOH:O	2.54	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 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	363/373 (97%)	360 (99%)	3 (1%)	0	100	100
1	B	368/373 (99%)	365 (99%)	3 (1%)	0	100	100
1	C	368/373 (99%)	364 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	368/373 (99%)	363 (99%)	5 (1%)	0	100	100
1	E	364/373 (98%)	360 (99%)	4 (1%)	0	100	100
1	F	362/373 (97%)	356 (98%)	6 (2%)	0	100	100
1	G	361/373 (97%)	357 (99%)	4 (1%)	0	100	100
1	H	362/373 (97%)	357 (99%)	5 (1%)	0	100	100
1	I	368/373 (99%)	365 (99%)	3 (1%)	0	100	100
1	J	355/373 (95%)	352 (99%)	3 (1%)	0	100	100
1	K	352/373 (94%)	347 (99%)	5 (1%)	0	100	100
1	L	364/373 (98%)	359 (99%)	5 (1%)	0	100	100
1	M	365/373 (98%)	362 (99%)	3 (1%)	0	100	100
1	N	363/373 (97%)	358 (99%)	5 (1%)	0	100	100
1	O	361/373 (97%)	359 (99%)	2 (1%)	0	100	100
1	P	356/373 (95%)	353 (99%)	3 (1%)	0	100	100
1	Q	351/373 (94%)	349 (99%)	2 (1%)	0	100	100
1	R	360/373 (96%)	356 (99%)	4 (1%)	0	100	100
1	S	348/373 (93%)	344 (99%)	4 (1%)	0	100	100
1	T	363/373 (97%)	361 (99%)	2 (1%)	0	100	100
All	All	7222/7460 (97%)	7147 (99%)	75 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 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	294/314 (94%)	294 (100%)	0	100	100
1	B	302/314 (96%)	302 (100%)	0	100	100
1	C	305/314 (97%)	305 (100%)	0	100	100
1	D	305/314 (97%)	305 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	302/314 (96%)	302 (100%)	0	100	100
1	F	299/314 (95%)	299 (100%)	0	100	100
1	G	298/314 (95%)	298 (100%)	0	100	100
1	H	297/314 (95%)	297 (100%)	0	100	100
1	I	299/314 (95%)	299 (100%)	0	100	100
1	J	289/314 (92%)	289 (100%)	0	100	100
1	K	290/314 (92%)	290 (100%)	0	100	100
1	L	294/314 (94%)	294 (100%)	0	100	100
1	M	285/314 (91%)	285 (100%)	0	100	100
1	N	292/314 (93%)	292 (100%)	0	100	100
1	O	298/314 (95%)	298 (100%)	0	100	100
1	P	291/314 (93%)	291 (100%)	0	100	100
1	Q	282/314 (90%)	281 (100%)	1 (0%)	84	92
1	R	280/314 (89%)	280 (100%)	0	100	100
1	S	271/314 (86%)	271 (100%)	0	100	100
1	T	290/314 (92%)	290 (100%)	0	100	100
All	All	5863/6280 (93%)	5862 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	69	GLN
1	C	310	ASN
1	D	69	GLN
1	E	8	HIS
1	E	69	GLN
1	F	69	GLN
1	G	61	ASN
1	G	69	GLN
1	G	115	HIS

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Mol	Chain	Res	Type
1	G	310	ASN
1	H	10	ASN
1	H	248	ASN
1	I	69	GLN
1	I	246	ASN
1	J	282	GLN
1	J	362	ASN
1	K	8	HIS
1	K	282	GLN
1	K	308	ASN
1	L	310	ASN
1	M	69	GLN
1	N	8	HIS
1	N	69	GLN
1	O	8	HIS
1	P	69	GLN
1	P	248	ASN
1	Q	310	ASN
1	R	69	GLN
1	R	127	GLN
1	S	8	HIS
1	S	69	GLN
1	T	69	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 121 ligands modelled in this entry, 81 are monoatomic - leaving 40 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$
4	PO4	T	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.45	0
2	ADP	E	401	3	28,29,29	1.39	5 (17%)	43,45,45	1.89	10 (23%)
4	PO4	J	405	5,3	4,4,4	1.57	1 (25%)	6,6,6	0.47	0
2	ADP	L	401	3	28,29,29	1.41	5 (17%)	43,45,45	1.89	10 (23%)
2	ADP	J	401	3	28,29,29	1.39	4 (14%)	43,45,45	1.87	10 (23%)
4	PO4	L	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.46	0
2	ADP	N	401	3	28,29,29	1.39	4 (14%)	43,45,45	1.85	10 (23%)
4	PO4	B	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.53	0
2	ADP	R	401	3	28,29,29	1.39	5 (17%)	43,45,45	1.89	10 (23%)
4	PO4	G	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.47	0
2	ADP	S	401	3	28,29,29	1.40	4 (14%)	43,45,45	1.87	11 (25%)
4	PO4	N	405	5,3	4,4,4	1.61	1 (25%)	6,6,6	0.45	0
4	PO4	H	405	5,3	4,4,4	1.55	1 (25%)	6,6,6	0.49	0
2	ADP	H	401	3	28,29,29	1.40	5 (17%)	43,45,45	1.89	10 (23%)
4	PO4	E	405	5,3	4,4,4	1.58	1 (25%)	6,6,6	0.46	0
2	ADP	G	401	3	28,29,29	1.40	5 (17%)	43,45,45	1.90	10 (23%)
4	PO4	F	405	5,3	4,4,4	1.57	1 (25%)	6,6,6	0.50	0
2	ADP	T	401	3	28,29,29	1.39	4 (14%)	43,45,45	1.87	10 (23%)
2	ADP	F	401	3	28,29,29	1.39	5 (17%)	43,45,45	1.86	10 (23%)
4	PO4	S	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.46	0
4	PO4	I	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.43	0
2	ADP	A	401	3	28,29,29	1.40	5 (17%)	43,45,45	1.86	10 (23%)
2	ADP	I	401	3	28,29,29	1.40	5 (17%)	43,45,45	1.88	10 (23%)
2	ADP	C	401	3	28,29,29	1.40	5 (17%)	43,45,45	1.87	10 (23%)
4	PO4	Q	405	5,3	4,4,4	1.59	1 (25%)	6,6,6	0.46	0
4	PO4	D	405	5,3	4,4,4	1.54	1 (25%)	6,6,6	0.55	0
2	ADP	Q	401	3	28,29,29	1.40	4 (14%)	43,45,45	1.88	10 (23%)
2	ADP	D	401	3	28,29,29	1.37	6 (21%)	43,45,45	1.89	10 (23%)
4	PO4	K	405	5,3	4,4,4	1.57	1 (25%)	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	P	405	5,3	4,4,4	1.56	1 (25%)	6,6,6	0.45	0
2	ADP	K	401	3	28,29,29	1.41	5 (17%)	43,45,45	1.88	10 (23%)
2	ADP	P	401	3	28,29,29	1.39	5 (17%)	43,45,45	1.89	10 (23%)
4	PO4	O	405	5,3	4,4,4	1.57	1 (25%)	6,6,6	0.48	0
4	PO4	R	405	5,3	4,4,4	1.56	1 (25%)	6,6,6	0.48	0
4	PO4	A	405	5,3	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
2	ADP	O	401	3	28,29,29	1.39	4 (14%)	43,45,45	1.90	11 (25%)
4	PO4	M	405	5,3	4,4,4	1.60	1 (25%)	6,6,6	0.51	0
4	PO4	C	405	5,3	4,4,4	1.58	1 (25%)	6,6,6	0.54	0
2	ADP	M	401	3	28,29,29	1.38	4 (14%)	43,45,45	1.89	11 (25%)
2	ADP	B	401	3	28,29,29	1.40	5 (17%)	43,45,45	1.85	10 (23%)

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	401	3	-	4/16/32/32	0/3/3/3
2	ADP	L	401	3	-	4/16/32/32	0/3/3/3
2	ADP	J	401	3	-	4/16/32/32	0/3/3/3
2	ADP	N	401	3	-	5/16/32/32	0/3/3/3
2	ADP	R	401	3	-	3/16/32/32	0/3/3/3
2	ADP	S	401	3	-	3/16/32/32	0/3/3/3
2	ADP	H	401	3	-	3/16/32/32	0/3/3/3
2	ADP	G	401	3	-	3/16/32/32	0/3/3/3
2	ADP	T	401	3	-	4/16/32/32	0/3/3/3
2	ADP	F	401	3	-	4/16/32/32	0/3/3/3
2	ADP	A	401	3	-	5/16/32/32	0/3/3/3
2	ADP	I	401	3	-	5/16/32/32	0/3/3/3
2	ADP	C	401	3	-	4/16/32/32	0/3/3/3
2	ADP	Q	401	3	-	3/16/32/32	0/3/3/3
2	ADP	D	401	3	-	4/16/32/32	0/3/3/3
2	ADP	K	401	3	-	4/16/32/32	0/3/3/3
2	ADP	P	401	3	-	4/16/32/32	0/3/3/3
2	ADP	O	401	3	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	M	401	3	-	3/16/32/32	0/3/3/3
2	ADP	B	401	3	-	4/16/32/32	0/3/3/3

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	401	ADP	C5-C4	4.58	1.47	1.39
2	K	401	ADP	C5-C4	4.53	1.47	1.39
2	R	401	ADP	C5-C4	4.50	1.47	1.39
2	I	401	ADP	C5-C4	4.49	1.47	1.39
2	T	401	ADP	C5-C4	4.49	1.47	1.39
2	L	401	ADP	C5-C4	4.49	1.47	1.39
2	B	401	ADP	C5-C4	4.48	1.47	1.39
2	A	401	ADP	C5-C4	4.48	1.47	1.39
2	J	401	ADP	C5-C4	4.48	1.47	1.39
2	S	401	ADP	C5-C4	4.47	1.47	1.39
2	O	401	ADP	C5-C4	4.47	1.47	1.39
2	H	401	ADP	C5-C4	4.46	1.47	1.39
2	C	401	ADP	C5-C4	4.46	1.47	1.39
2	M	401	ADP	C5-C4	4.45	1.47	1.39
2	N	401	ADP	C5-C4	4.44	1.47	1.39
2	F	401	ADP	C5-C4	4.44	1.47	1.39
2	E	401	ADP	C5-C4	4.42	1.47	1.39
2	P	401	ADP	C5-C4	4.40	1.46	1.39
2	G	401	ADP	C5-C4	4.38	1.46	1.39
2	D	401	ADP	C5-C4	4.34	1.46	1.39
4	N	405	PO4	P-O1	2.81	1.57	1.50
4	I	405	PO4	P-O1	2.80	1.57	1.50
4	G	405	PO4	P-O1	2.80	1.57	1.50
4	B	405	PO4	P-O1	2.79	1.57	1.50
4	M	405	PO4	P-O1	2.79	1.57	1.50
4	T	405	PO4	P-O1	2.78	1.57	1.50
4	S	405	PO4	P-O1	2.78	1.57	1.50
4	L	405	PO4	P-O1	2.78	1.57	1.50
4	Q	405	PO4	P-O1	2.78	1.57	1.50
4	J	405	PO4	P-O1	2.77	1.57	1.50
4	A	405	PO4	P-O1	2.76	1.57	1.50
4	E	405	PO4	P-O1	2.76	1.57	1.50
4	C	405	PO4	P-O1	2.75	1.57	1.50
4	F	405	PO4	P-O1	2.73	1.57	1.50
4	K	405	PO4	P-O1	2.73	1.57	1.50
4	O	405	PO4	P-O1	2.73	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	ADP	C5-C6	2.73	1.48	1.41
4	H	405	PO4	P-O1	2.73	1.57	1.50
2	Q	401	ADP	C5-C6	2.72	1.48	1.41
4	R	405	PO4	P-O1	2.72	1.56	1.50
2	L	401	ADP	C5-C6	2.72	1.48	1.41
2	I	401	ADP	C5-C6	2.71	1.48	1.41
2	P	401	ADP	C5-C6	2.71	1.48	1.41
4	P	405	PO4	P-O1	2.70	1.56	1.50
2	C	401	ADP	C5-C6	2.70	1.48	1.41
2	S	401	ADP	C5-C6	2.70	1.48	1.41
2	H	401	ADP	C5-C6	2.70	1.48	1.41
2	K	401	ADP	C5-C6	2.70	1.48	1.41
2	J	401	ADP	C5-C6	2.69	1.48	1.41
2	E	401	ADP	C5-C6	2.69	1.48	1.41
2	T	401	ADP	C5-C6	2.68	1.48	1.41
2	O	401	ADP	C5-C6	2.67	1.48	1.41
2	R	401	ADP	C5-C6	2.67	1.48	1.41
4	D	405	PO4	P-O1	2.66	1.56	1.50
2	B	401	ADP	C5-C6	2.65	1.48	1.41
2	N	401	ADP	C5-C6	2.65	1.48	1.41
2	F	401	ADP	C5-C6	2.63	1.48	1.41
2	A	401	ADP	C5-C6	2.62	1.48	1.41
2	M	401	ADP	C5-C6	2.59	1.48	1.41
2	H	401	ADP	C8-N7	2.50	1.36	1.31
2	D	401	ADP	C5-C6	2.50	1.48	1.41
2	K	401	ADP	C8-N7	2.48	1.36	1.31
2	I	401	ADP	C8-N7	2.47	1.36	1.31
2	Q	401	ADP	C8-N7	2.47	1.36	1.31
2	N	401	ADP	C8-N7	2.47	1.36	1.31
2	P	401	ADP	C8-N7	2.45	1.36	1.31
2	O	401	ADP	C8-N7	2.45	1.36	1.31
2	J	401	ADP	C8-N7	2.45	1.36	1.31
2	D	401	ADP	C8-N7	2.45	1.36	1.31
2	E	401	ADP	C8-N7	2.43	1.36	1.31
2	L	401	ADP	C8-N7	2.42	1.36	1.31
2	G	401	ADP	C8-N7	2.42	1.36	1.31
2	T	401	ADP	C8-N7	2.41	1.36	1.31
2	M	401	ADP	C8-N7	2.40	1.36	1.31
2	S	401	ADP	C8-N7	2.40	1.36	1.31
2	F	401	ADP	C8-N7	2.40	1.36	1.31
2	R	401	ADP	C8-N7	2.40	1.36	1.31
2	C	401	ADP	C8-N7	2.38	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	ADP	PA-O3A	2.38	1.62	1.59
2	A	401	ADP	C8-N7	2.37	1.36	1.31
2	B	401	ADP	C8-N7	2.33	1.36	1.31
2	K	401	ADP	C5-N7	-2.28	1.34	1.39
2	N	401	ADP	C5-N7	-2.28	1.34	1.39
2	F	401	ADP	C5-N7	-2.27	1.34	1.39
2	L	401	ADP	C5-N7	-2.26	1.35	1.39
2	C	401	ADP	C5-N7	-2.26	1.35	1.39
2	Q	401	ADP	C5-N7	-2.24	1.35	1.39
2	M	401	ADP	C5-N7	-2.24	1.35	1.39
2	O	401	ADP	C5-N7	-2.24	1.35	1.39
2	T	401	ADP	C5-N7	-2.23	1.35	1.39
2	A	401	ADP	C5-N7	-2.22	1.35	1.39
2	B	401	ADP	C5-N7	-2.22	1.35	1.39
2	J	401	ADP	C5-N7	-2.22	1.35	1.39
2	S	401	ADP	C5-N7	-2.21	1.35	1.39
2	G	401	ADP	C5-N7	-2.20	1.35	1.39
2	R	401	ADP	C5-N7	-2.20	1.35	1.39
2	P	401	ADP	C5-N7	-2.19	1.35	1.39
2	I	401	ADP	C5-N7	-2.18	1.35	1.39
2	H	401	ADP	C5-N7	-2.17	1.35	1.39
2	D	401	ADP	C5-N7	-2.16	1.35	1.39
2	K	401	ADP	PA-O3A	2.15	1.61	1.59
2	A	401	ADP	PA-O3A	2.14	1.61	1.59
2	C	401	ADP	PA-O3A	2.13	1.61	1.59
2	B	401	ADP	PA-O3A	2.13	1.61	1.59
2	D	401	ADP	PA-O3A	2.12	1.61	1.59
2	E	401	ADP	C5-N7	-2.12	1.35	1.39
2	L	401	ADP	PA-O3A	2.10	1.61	1.59
2	E	401	ADP	PA-O3A	2.08	1.61	1.59
2	H	401	ADP	PA-O3A	2.06	1.61	1.59
2	F	401	ADP	C4-N9	-2.04	1.33	1.37
2	P	401	ADP	PA-O3A	2.03	1.61	1.59
2	R	401	ADP	PA-O3A	2.03	1.61	1.59
2	D	401	ADP	C4-N9	-2.02	1.33	1.37
2	I	401	ADP	PA-O3A	2.01	1.61	1.59

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	ADP	C5-C4-N3	-5.76	118.78	126.72
2	Q	401	ADP	C5-C4-N3	-5.72	118.84	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	401	ADP	C5-C4-N3	-5.70	118.86	126.72
2	T	401	ADP	C5-C4-N3	-5.68	118.89	126.72
2	H	401	ADP	C5-C4-N3	-5.64	118.94	126.72
2	I	401	ADP	C5-C4-N3	-5.64	118.95	126.72
2	J	401	ADP	C5-C4-N3	-5.61	118.99	126.72
2	C	401	ADP	C5-C4-N3	-5.61	118.99	126.72
2	S	401	ADP	C5-C4-N3	-5.60	119.00	126.72
2	M	401	ADP	C5-C4-N3	-5.60	119.01	126.72
2	N	401	ADP	C5-C4-N3	-5.58	119.03	126.72
2	G	401	ADP	C5-C4-N3	-5.56	119.06	126.72
2	R	401	ADP	C5-C4-N3	-5.53	119.11	126.72
2	L	401	ADP	C5-C4-N3	-5.49	119.15	126.72
2	A	401	ADP	C5-C4-N3	-5.47	119.19	126.72
2	P	401	ADP	C5-C4-N3	-5.45	119.22	126.72
2	F	401	ADP	C5-C4-N3	-5.44	119.22	126.72
2	B	401	ADP	C5-C4-N3	-5.43	119.24	126.72
2	D	401	ADP	C5-C4-N3	-5.42	119.26	126.72
2	E	401	ADP	C5-C4-N3	-5.31	119.40	126.72
2	Q	401	ADP	N3-C4-N9	4.52	134.85	127.17
2	T	401	ADP	N3-C4-N9	4.48	134.78	127.17
2	O	401	ADP	N3-C4-N9	4.47	134.77	127.17
2	M	401	ADP	N3-C4-N9	4.46	134.76	127.17
2	K	401	ADP	N3-C4-N9	4.45	134.73	127.17
2	D	401	ADP	N3-C4-N9	4.44	134.71	127.17
2	C	401	ADP	N3-C4-N9	4.43	134.69	127.17
2	S	401	ADP	N3-C4-N9	4.40	134.65	127.17
2	A	401	ADP	N3-C4-N9	4.40	134.65	127.17
2	R	401	ADP	N3-C4-N9	4.39	134.64	127.17
2	H	401	ADP	N3-C4-N9	4.39	134.63	127.17
2	B	401	ADP	N3-C4-N9	4.38	134.62	127.17
2	I	401	ADP	N3-C4-N9	4.37	134.60	127.17
2	N	401	ADP	N3-C4-N9	4.35	134.57	127.17
2	F	401	ADP	N3-C4-N9	4.34	134.55	127.17
2	L	401	ADP	N3-C4-N9	4.34	134.55	127.17
2	G	401	ADP	N3-C4-N9	4.31	134.49	127.17
2	E	401	ADP	N3-C4-N9	4.30	134.49	127.17
2	J	401	ADP	N3-C4-N9	4.30	134.48	127.17
2	P	401	ADP	N3-C4-N9	4.28	134.45	127.17
2	D	401	ADP	N3-C2-N1	-3.98	122.55	128.58
2	L	401	ADP	N3-C2-N1	-3.91	122.66	128.58
2	O	401	ADP	C2-N3-C4	3.90	121.35	111.83
2	K	401	ADP	C2-N3-C4	3.88	121.31	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	401	ADP	C2-N3-C4	3.88	121.30	111.83
2	Q	401	ADP	C2-N3-C4	3.87	121.28	111.83
2	D	401	ADP	C2-N3-C4	3.86	121.26	111.83
2	R	401	ADP	C2-N3-C4	3.86	121.26	111.83
2	E	401	ADP	N3-C2-N1	-3.86	122.74	128.58
2	M	401	ADP	C2-N3-C4	3.86	121.25	111.83
2	R	401	ADP	N3-C2-N1	-3.85	122.75	128.58
2	H	401	ADP	C2-N3-C4	3.85	121.24	111.83
2	L	401	ADP	C2-N3-C4	3.85	121.24	111.83
2	J	401	ADP	C2-N3-C4	3.85	121.23	111.83
2	F	401	ADP	N3-C2-N1	-3.85	122.76	128.58
2	I	401	ADP	C2-N3-C4	3.85	121.22	111.83
2	M	401	ADP	N3-C2-N1	-3.83	122.78	128.58
2	G	401	ADP	C2-N3-C4	3.83	121.19	111.83
2	C	401	ADP	C2-N3-C4	3.83	121.18	111.83
2	O	401	ADP	N3-C2-N1	-3.81	122.81	128.58
2	N	401	ADP	C2-N3-C4	3.81	121.14	111.83
2	T	401	ADP	N3-C2-N1	-3.81	122.81	128.58
2	S	401	ADP	C2-N3-C4	3.81	121.13	111.83
2	F	401	ADP	C2-N3-C4	3.79	121.10	111.83
2	P	401	ADP	N3-C2-N1	-3.78	122.85	128.58
2	N	401	ADP	N3-C2-N1	-3.78	122.86	128.58
2	E	401	ADP	C2-N3-C4	3.78	121.06	111.83
2	J	401	ADP	N3-C2-N1	-3.78	122.86	128.58
2	P	401	ADP	C2-N3-C4	3.78	121.05	111.83
2	C	401	ADP	N3-C2-N1	-3.76	122.88	128.58
2	G	401	ADP	N3-C2-N1	-3.76	122.88	128.58
2	I	401	ADP	N3-C2-N1	-3.76	122.89	128.58
2	S	401	ADP	N3-C2-N1	-3.76	122.90	128.58
2	A	401	ADP	N3-C2-N1	-3.75	122.90	128.58
2	H	401	ADP	N3-C2-N1	-3.74	122.91	128.58
2	Q	401	ADP	N3-C2-N1	-3.74	122.92	128.58
2	A	401	ADP	C2-N3-C4	3.73	120.94	111.83
2	G	401	ADP	C4-C5-N7	-3.73	106.32	110.58
2	K	401	ADP	N3-C2-N1	-3.71	122.96	128.58
2	B	401	ADP	C2-N3-C4	3.69	120.84	111.83
2	B	401	ADP	N3-C2-N1	-3.68	123.01	128.58
2	H	401	ADP	C4-C5-N7	-3.67	106.39	110.58
2	K	401	ADP	C4-C5-N7	-3.67	106.39	110.58
2	J	401	ADP	C4-C5-N7	-3.66	106.39	110.58
2	P	401	ADP	C4-C5-N7	-3.64	106.42	110.58
2	C	401	ADP	C4-C5-N7	-3.64	106.42	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	ADP	C4-C5-N7	-3.64	106.42	110.58
2	O	401	ADP	C4-C5-N7	-3.62	106.44	110.58
2	L	401	ADP	C4-C5-N7	-3.62	106.44	110.58
2	Q	401	ADP	C4-C5-N7	-3.62	106.44	110.58
2	S	401	ADP	C4-C5-N7	-3.59	106.48	110.58
2	R	401	ADP	C4-C5-N7	-3.57	106.50	110.58
2	T	401	ADP	C4-C5-N7	-3.57	106.50	110.58
2	B	401	ADP	C4-C5-N7	-3.55	106.52	110.58
2	N	401	ADP	C4-C5-N7	-3.51	106.57	110.58
2	F	401	ADP	C4-C5-N7	-3.50	106.58	110.58
2	E	401	ADP	C4-C5-N7	-3.49	106.59	110.58
2	A	401	ADP	C4-C5-N7	-3.48	106.61	110.58
2	M	401	ADP	C4-C5-N7	-3.44	106.65	110.58
2	D	401	ADP	C4-N9-C8	3.42	109.33	105.74
2	E	401	ADP	C4-N9-C8	3.39	109.30	105.74
2	D	401	ADP	C4-C5-N7	-3.32	106.78	110.58
2	B	401	ADP	C4-N9-C8	3.25	109.15	105.74
2	P	401	ADP	C4-N9-C8	3.21	109.11	105.74
2	F	401	ADP	C4-N9-C8	3.17	109.07	105.74
2	R	401	ADP	C4-N9-C8	3.14	109.04	105.74
2	L	401	ADP	C4-N9-C8	3.13	109.02	105.74
2	A	401	ADP	C4-N9-C8	3.12	109.01	105.74
2	C	401	ADP	C4-N9-C8	3.08	108.97	105.74
2	Q	401	ADP	C4-N9-C8	3.06	108.95	105.74
2	G	401	ADP	C4-N9-C8	3.05	108.94	105.74
2	H	401	ADP	C4-N9-C8	3.03	108.92	105.74
2	M	401	ADP	C4-N9-C8	3.02	108.91	105.74
2	O	401	ADP	C4-N9-C8	2.98	108.87	105.74
2	S	401	ADP	C4-N9-C8	2.98	108.87	105.74
2	T	401	ADP	C4-N9-C8	2.93	108.81	105.74
2	N	401	ADP	C4-N9-C8	2.90	108.79	105.74
2	I	401	ADP	C4-N9-C8	2.89	108.78	105.74
2	G	401	ADP	C5-N7-C8	2.88	107.98	103.45
2	P	401	ADP	C5-N7-C8	2.86	107.95	103.45
2	H	401	ADP	C5-N7-C8	2.86	107.95	103.45
2	C	401	ADP	C5-N7-C8	2.86	107.94	103.45
2	O	401	ADP	C5-N7-C8	2.84	107.92	103.45
2	J	401	ADP	C4-N9-C8	2.84	108.72	105.74
2	K	401	ADP	C4-N9-C8	2.84	108.72	105.74
2	L	401	ADP	C5-N7-C8	2.83	107.89	103.45
2	Q	401	ADP	C5-N7-C8	2.82	107.88	103.45
2	I	401	ADP	C5-N7-C8	2.80	107.85	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	ADP	C5-N7-C8	2.80	107.85	103.45
2	K	401	ADP	C5-N7-C8	2.80	107.85	103.45
2	B	401	ADP	C5-N7-C8	2.80	107.84	103.45
2	R	401	ADP	C5-N7-C8	2.79	107.83	103.45
2	E	401	ADP	C5-N7-C8	2.78	107.82	103.45
2	S	401	ADP	C5-N7-C8	2.76	107.78	103.45
2	T	401	ADP	C5-N7-C8	2.76	107.78	103.45
2	F	401	ADP	C5-N7-C8	2.75	107.77	103.45
2	A	401	ADP	C5-N7-C8	2.74	107.75	103.45
2	M	401	ADP	C5-N7-C8	2.73	107.75	103.45
2	N	401	ADP	C5-N7-C8	2.72	107.72	103.45
2	D	401	ADP	C5-N7-C8	2.68	107.66	103.45
2	E	401	ADP	N9-C8-N7	-2.65	110.18	113.94
2	D	401	ADP	N9-C8-N7	-2.64	110.20	113.94
2	P	401	ADP	N9-C8-N7	-2.64	110.20	113.94
2	G	401	ADP	N9-C8-N7	-2.56	110.30	113.94
2	H	401	ADP	N9-C8-N7	-2.54	110.33	113.94
2	L	401	ADP	N9-C8-N7	-2.53	110.34	113.94
2	B	401	ADP	N9-C8-N7	-2.53	110.35	113.94
2	F	401	ADP	N9-C8-N7	-2.52	110.36	113.94
2	C	401	ADP	N9-C8-N7	-2.52	110.36	113.94
2	R	401	ADP	N9-C8-N7	-2.51	110.38	113.94
2	O	401	ADP	N9-C8-N7	-2.49	110.41	113.94
2	Q	401	ADP	N9-C8-N7	-2.48	110.42	113.94
2	G	401	ADP	C6-C5-N7	2.48	136.87	132.09
2	L	401	ADP	C6-C5-N7	2.47	136.85	132.09
2	P	401	ADP	C6-C5-N7	2.45	136.82	132.09
2	E	401	ADP	C6-C5-N7	2.45	136.81	132.09
2	M	401	ADP	N9-C8-N7	-2.45	110.46	113.94
2	A	401	ADP	N9-C8-N7	-2.45	110.46	113.94
2	R	401	ADP	C6-C5-N7	2.43	136.77	132.09
2	J	401	ADP	C6-C5-N7	2.42	136.75	132.09
2	I	401	ADP	N9-C8-N7	-2.41	110.51	113.94
2	J	401	ADP	N9-C8-N7	-2.41	110.51	113.94
2	S	401	ADP	N9-C8-N7	-2.41	110.52	113.94
2	N	401	ADP	N9-C8-N7	-2.40	110.53	113.94
2	H	401	ADP	C6-C5-N7	2.40	136.71	132.09
2	D	401	ADP	C6-C5-N7	2.37	136.67	132.09
2	K	401	ADP	N9-C8-N7	-2.37	110.57	113.94
2	T	401	ADP	N9-C8-N7	-2.37	110.57	113.94
2	F	401	ADP	C6-C5-N7	2.37	136.66	132.09
2	C	401	ADP	C6-C5-N7	2.37	136.65	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	ADP	C6-C5-N7	2.34	136.60	132.09
2	O	401	ADP	C6-C5-N7	2.33	136.59	132.09
2	K	401	ADP	C6-C5-N7	2.33	136.57	132.09
2	Q	401	ADP	C6-C5-N7	2.31	136.54	132.09
2	B	401	ADP	C6-C5-N7	2.30	136.53	132.09
2	S	401	ADP	C6-C5-N7	2.30	136.51	132.09
2	T	401	ADP	C6-C5-N7	2.28	136.49	132.09
2	E	401	ADP	C2-N1-C6	2.27	122.45	118.73
2	M	401	ADP	C6-C5-N7	2.25	136.43	132.09
2	N	401	ADP	C6-C5-N7	2.24	136.41	132.09
2	L	401	ADP	C2-N1-C6	2.23	122.39	118.73
2	A	401	ADP	C6-C5-N7	2.22	136.38	132.09
2	P	401	ADP	C2-N1-C6	2.17	122.30	118.73
2	A	401	ADP	C2-N1-C6	2.17	122.29	118.73
2	F	401	ADP	C2-N1-C6	2.15	122.26	118.73
2	N	401	ADP	C2-N1-C6	2.14	122.25	118.73
2	B	401	ADP	C2-N1-C6	2.13	122.24	118.73
2	R	401	ADP	C2-N1-C6	2.13	122.23	118.73
2	J	401	ADP	C2-N1-C6	2.13	122.23	118.73
2	S	401	ADP	C2-N1-C6	2.12	122.22	118.73
2	M	401	ADP	O4'-C1'-N9	2.11	112.15	108.09
2	C	401	ADP	C2-N1-C6	2.10	122.18	118.73
2	G	401	ADP	C2-N1-C6	2.09	122.17	118.73
2	T	401	ADP	C2-N1-C6	2.09	122.17	118.73
2	O	401	ADP	O4'-C1'-N9	2.09	112.10	108.09
2	Q	401	ADP	C2-N1-C6	2.08	122.15	118.73
2	O	401	ADP	C2-N1-C6	2.08	122.14	118.73
2	D	401	ADP	C2-N1-C6	2.07	122.14	118.73
2	I	401	ADP	C2-N1-C6	2.07	122.14	118.73
2	M	401	ADP	C2-N1-C6	2.06	122.12	118.73
2	H	401	ADP	C2-N1-C6	2.04	122.08	118.73
2	K	401	ADP	C2-N1-C6	2.03	122.07	118.73
2	S	401	ADP	O4'-C1'-N9	2.03	111.99	108.09

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	PA-O3A-PB-O2B
2	D	401	ADP	PA-O3A-PB-O2B
2	J	401	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	K	401	ADP	PA-O3A-PB-O2B
2	L	401	ADP	PA-O3A-PB-O2B
2	P	401	ADP	PA-O3A-PB-O2B
2	Q	401	ADP	PA-O3A-PB-O2B
2	S	401	ADP	PA-O3A-PB-O2B
2	T	401	ADP	PA-O3A-PB-O2B
2	A	401	ADP	O4'-C4'-C5'-O5'
2	B	401	ADP	O4'-C4'-C5'-O5'
2	F	401	ADP	O4'-C4'-C5'-O5'
2	H	401	ADP	O4'-C4'-C5'-O5'
2	J	401	ADP	O4'-C4'-C5'-O5'
2	L	401	ADP	O4'-C4'-C5'-O5'
2	N	401	ADP	O4'-C4'-C5'-O5'
2	Q	401	ADP	O4'-C4'-C5'-O5'
2	R	401	ADP	O4'-C4'-C5'-O5'
2	S	401	ADP	O4'-C4'-C5'-O5'
2	A	401	ADP	C3'-C4'-C5'-O5'
2	B	401	ADP	C3'-C4'-C5'-O5'
2	C	401	ADP	O4'-C4'-C5'-O5'
2	C	401	ADP	C3'-C4'-C5'-O5'
2	F	401	ADP	C3'-C4'-C5'-O5'
2	H	401	ADP	C3'-C4'-C5'-O5'
2	J	401	ADP	C3'-C4'-C5'-O5'
2	L	401	ADP	C3'-C4'-C5'-O5'
2	N	401	ADP	C3'-C4'-C5'-O5'
2	Q	401	ADP	C3'-C4'-C5'-O5'
2	R	401	ADP	C3'-C4'-C5'-O5'
2	S	401	ADP	C3'-C4'-C5'-O5'
2	D	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	C3'-C4'-C5'-O5'
2	E	401	ADP	O4'-C4'-C5'-O5'
2	E	401	ADP	C3'-C4'-C5'-O5'
2	G	401	ADP	O4'-C4'-C5'-O5'
2	K	401	ADP	O4'-C4'-C5'-O5'
2	M	401	ADP	O4'-C4'-C5'-O5'
2	M	401	ADP	C3'-C4'-C5'-O5'
2	O	401	ADP	O4'-C4'-C5'-O5'
2	P	401	ADP	O4'-C4'-C5'-O5'
2	P	401	ADP	C3'-C4'-C5'-O5'
2	T	401	ADP	O4'-C4'-C5'-O5'
2	G	401	ADP	C3'-C4'-C5'-O5'
2	K	401	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	O	401	ADP	C3'-C4'-C5'-O5'
2	T	401	ADP	C3'-C4'-C5'-O5'
2	I	401	ADP	O4'-C4'-C5'-O5'
2	I	401	ADP	C3'-C4'-C5'-O5'
2	I	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	PA-O3A-PB-O2B
2	G	401	ADP	PA-O3A-PB-O2B
2	O	401	ADP	PA-O3A-PB-O2B
2	R	401	ADP	PB-O3A-PA-O2A
2	F	401	ADP	PB-O3A-PA-O1A
2	E	401	ADP	PA-O3A-PB-O2B
2	F	401	ADP	PA-O3A-PB-O2B
2	I	401	ADP	PA-O3A-PB-O2B
2	I	401	ADP	PA-O3A-PB-O3B
2	N	401	ADP	PA-O3A-PB-O2B
2	A	401	ADP	PB-O3A-PA-O2A
2	B	401	ADP	PB-O3A-PA-O1A
2	D	401	ADP	PB-O3A-PA-O1A
2	E	401	ADP	PB-O3A-PA-O2A
2	H	401	ADP	PB-O3A-PA-O2A
2	K	401	ADP	PB-O3A-PA-O1A
2	M	401	ADP	PB-O3A-PA-O1A
2	N	401	ADP	PB-O3A-PA-O1A
2	N	401	ADP	PB-O3A-PA-O2A
2	J	401	ADP	C2'-C1'-N9-C8
2	A	401	ADP	PB-O3A-PA-O1A
2	C	401	ADP	PB-O3A-PA-O1A
2	L	401	ADP	PB-O3A-PA-O1A
2	P	401	ADP	PB-O3A-PA-O1A
2	T	401	ADP	PB-O3A-PA-O1A

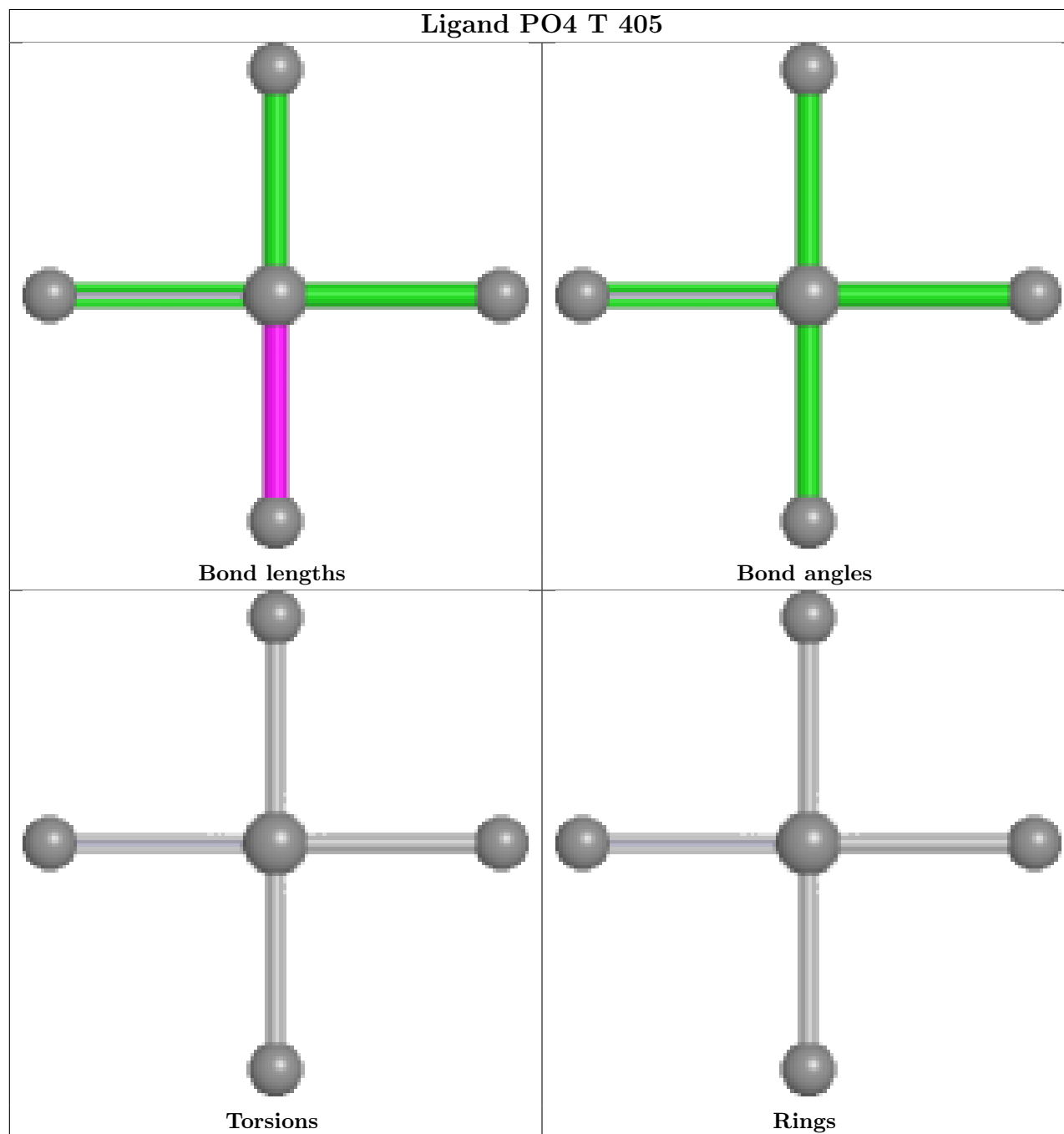
There are no ring outliers.

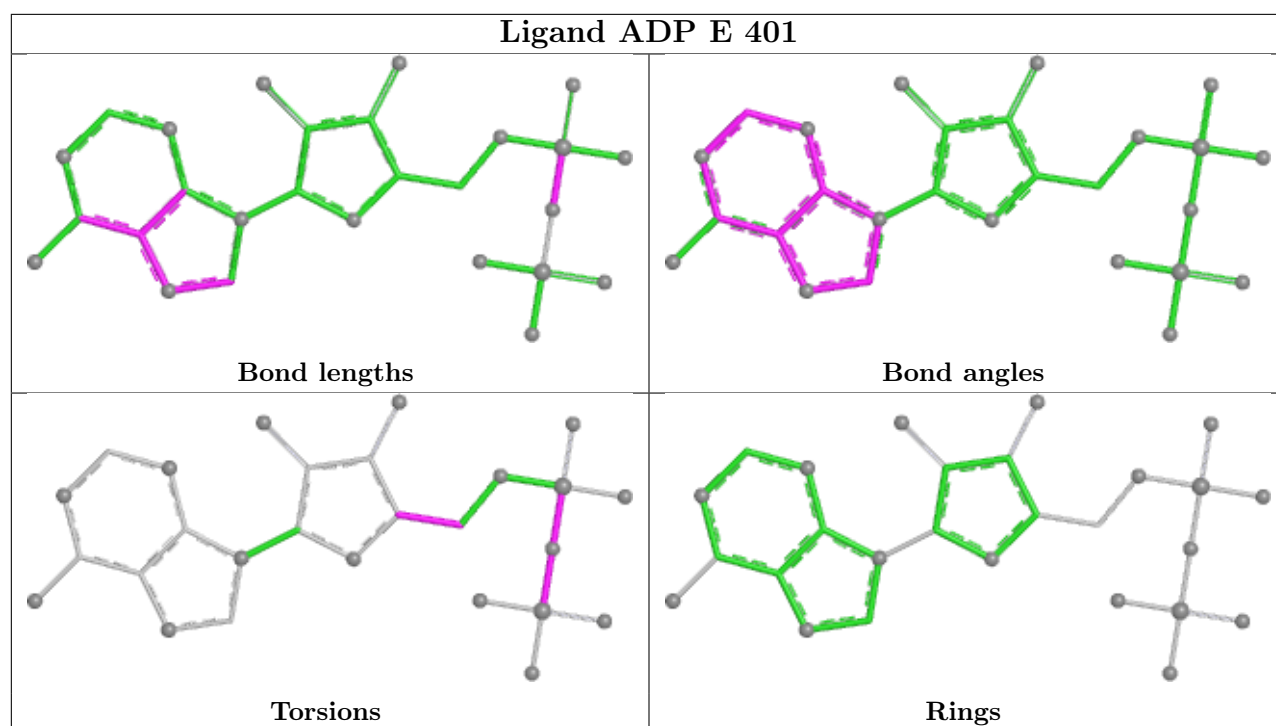
1 monomer is involved in 1 short contact:

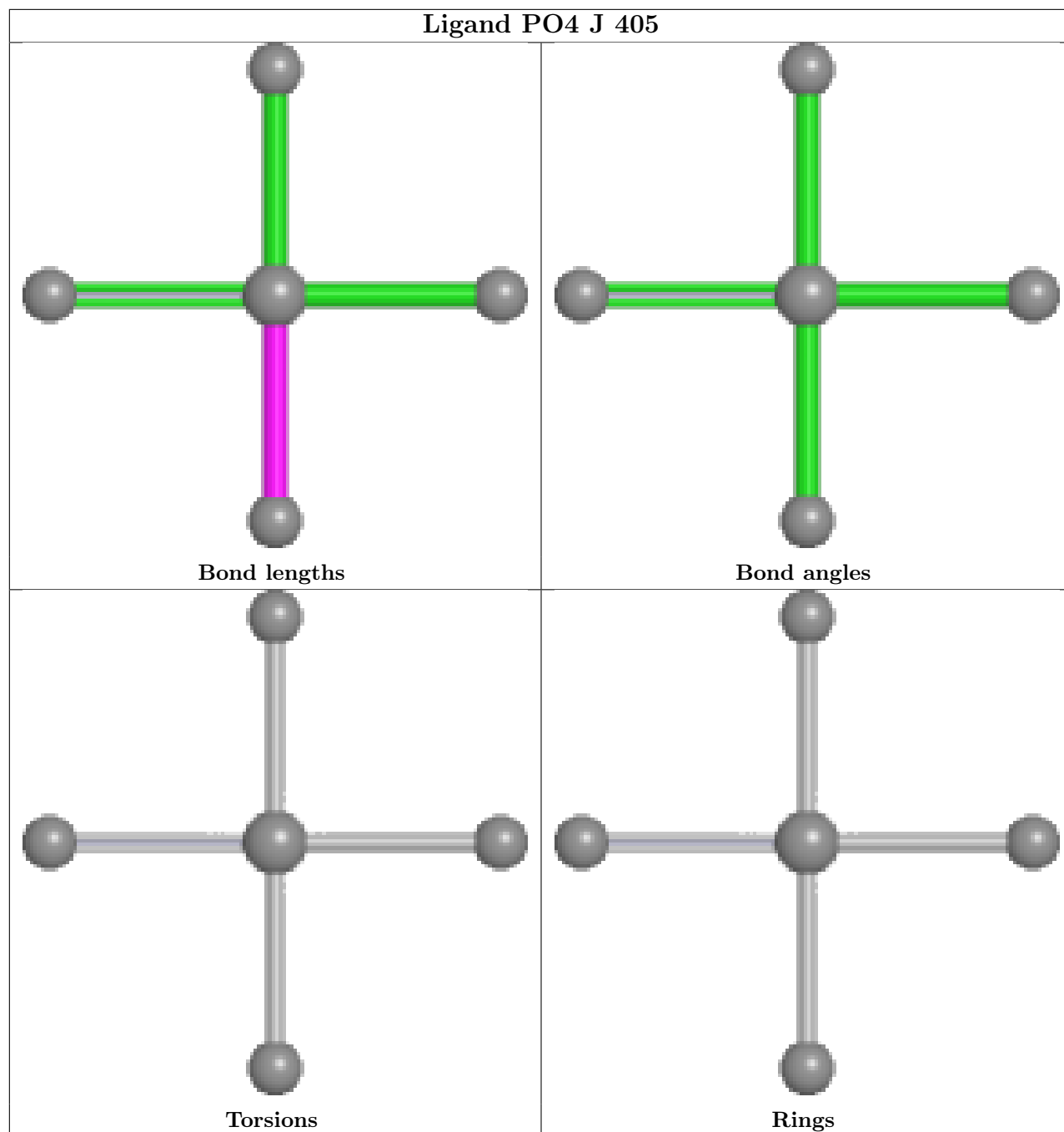
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	405	PO4	1	0

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.

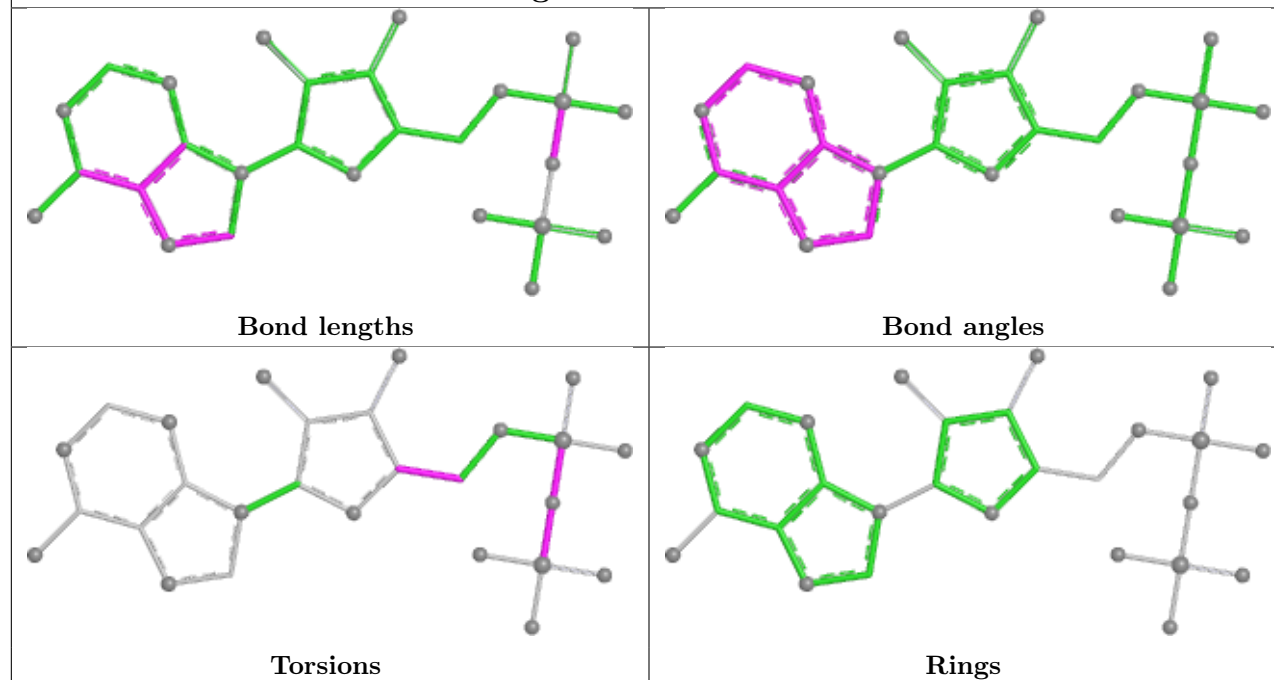
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



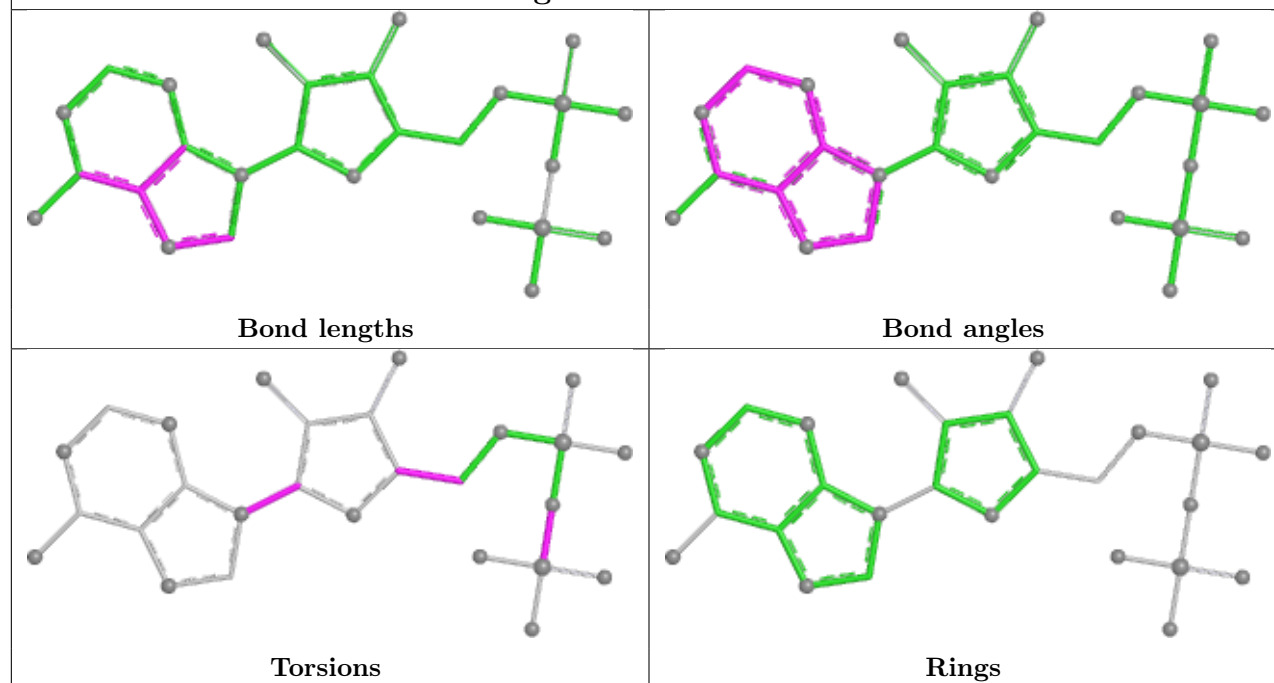


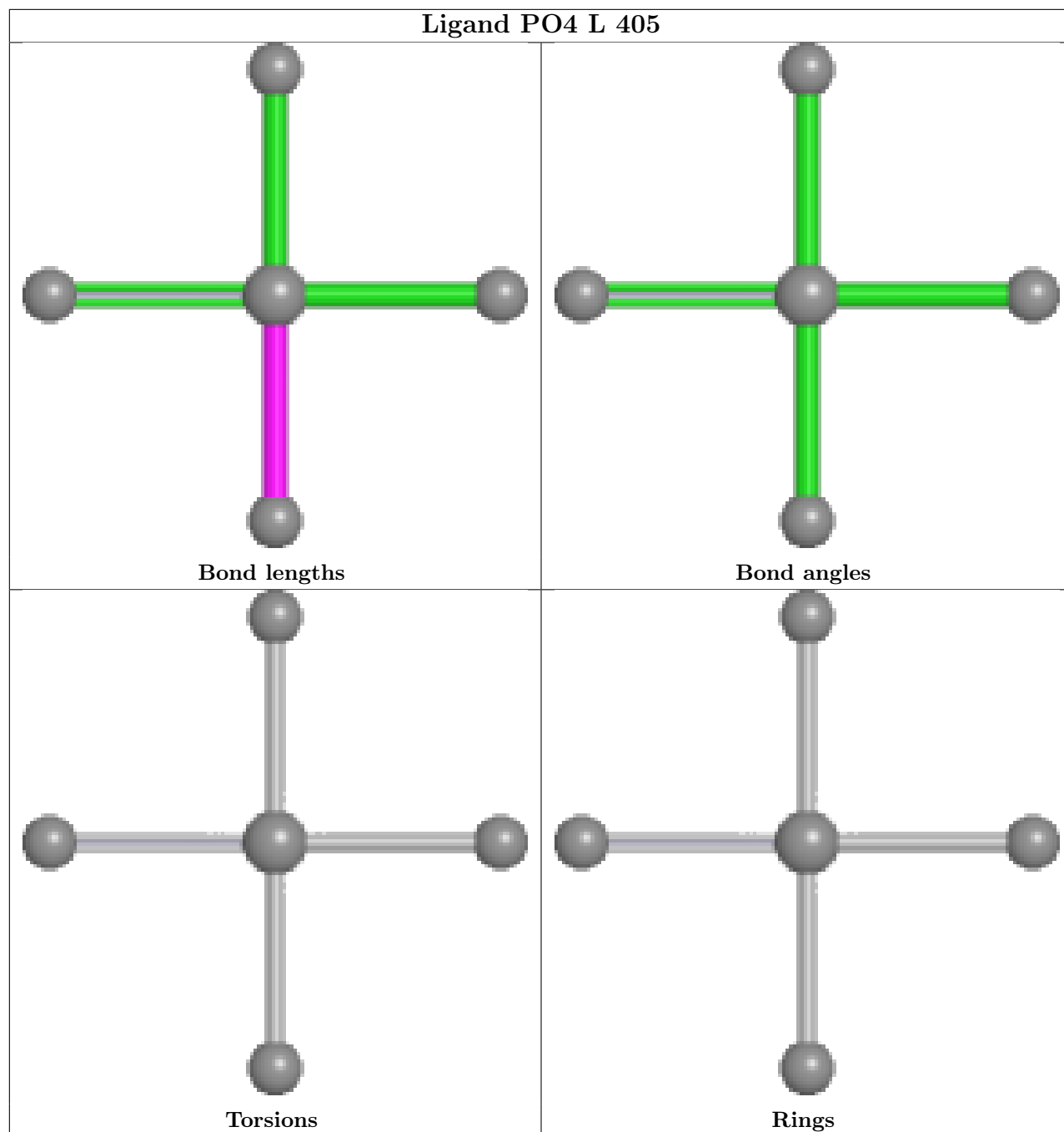


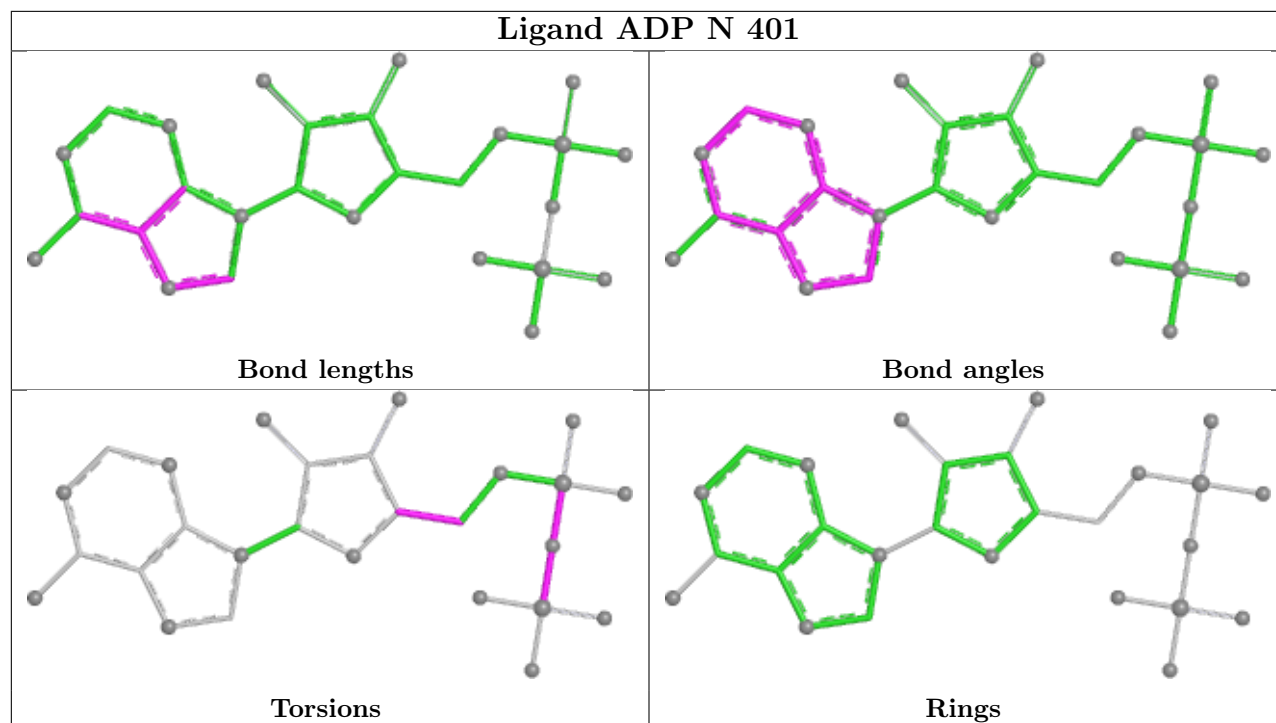
Ligand ADP L 401

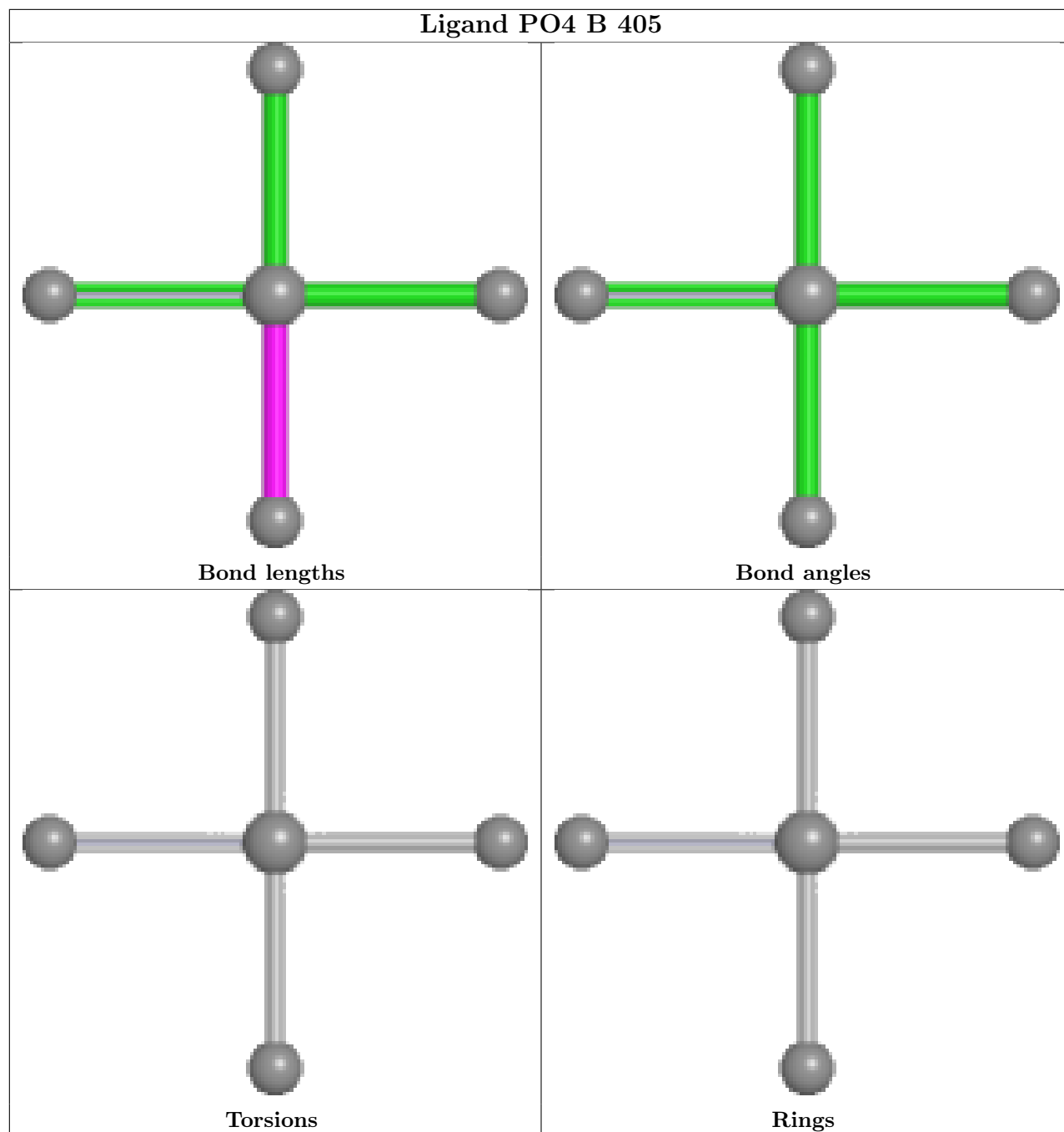


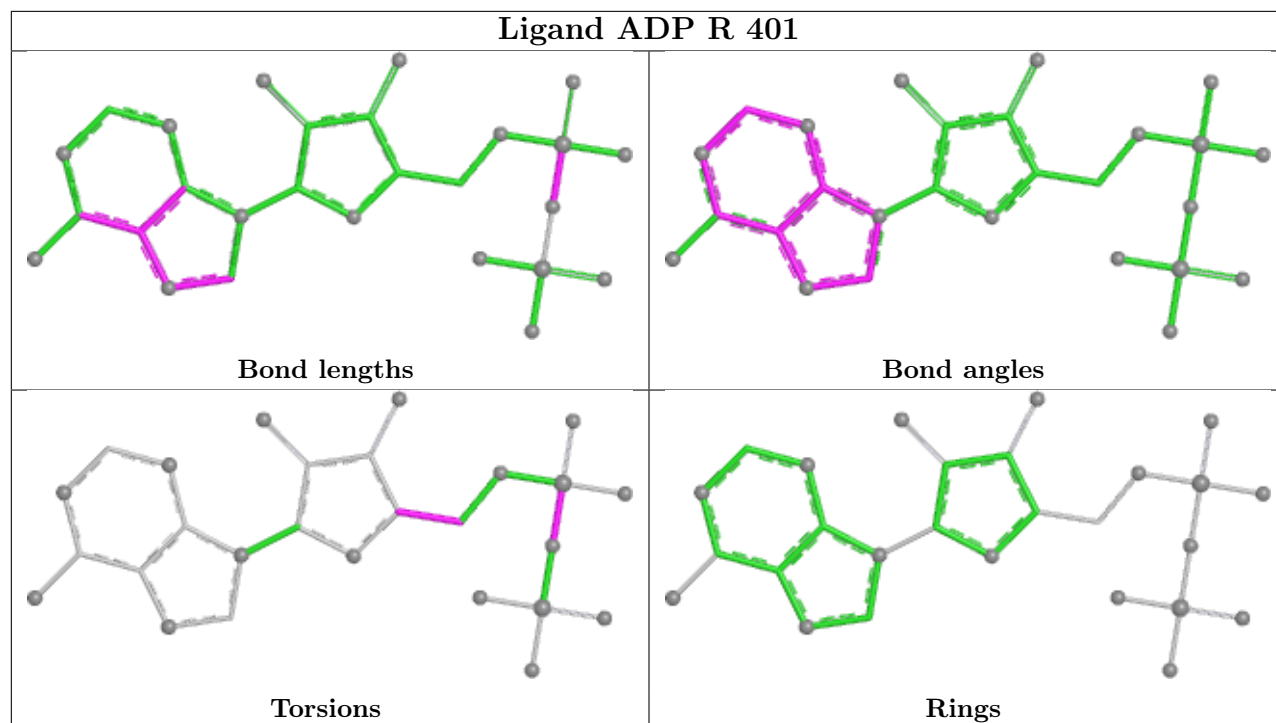
Ligand ADP J 401

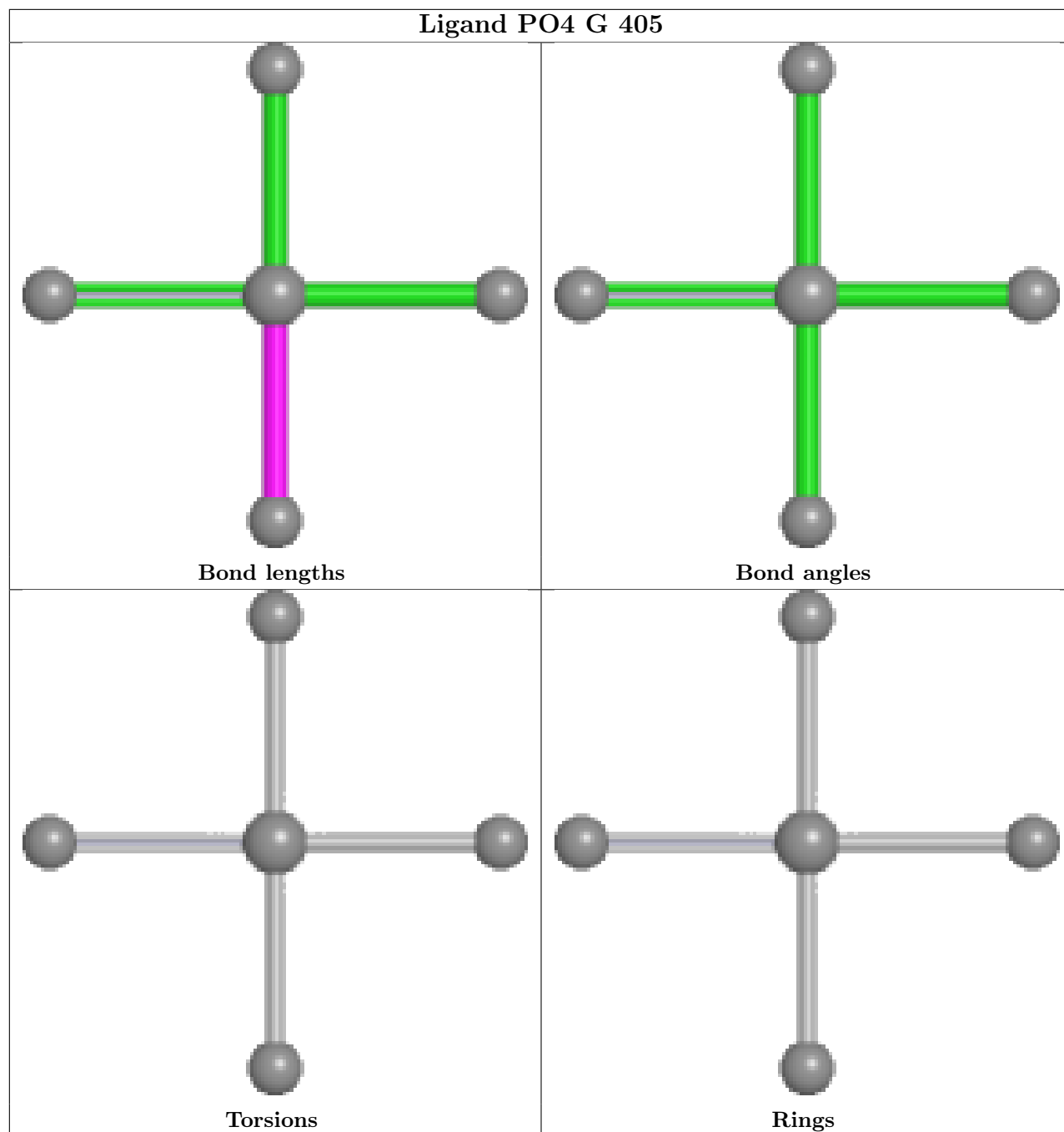


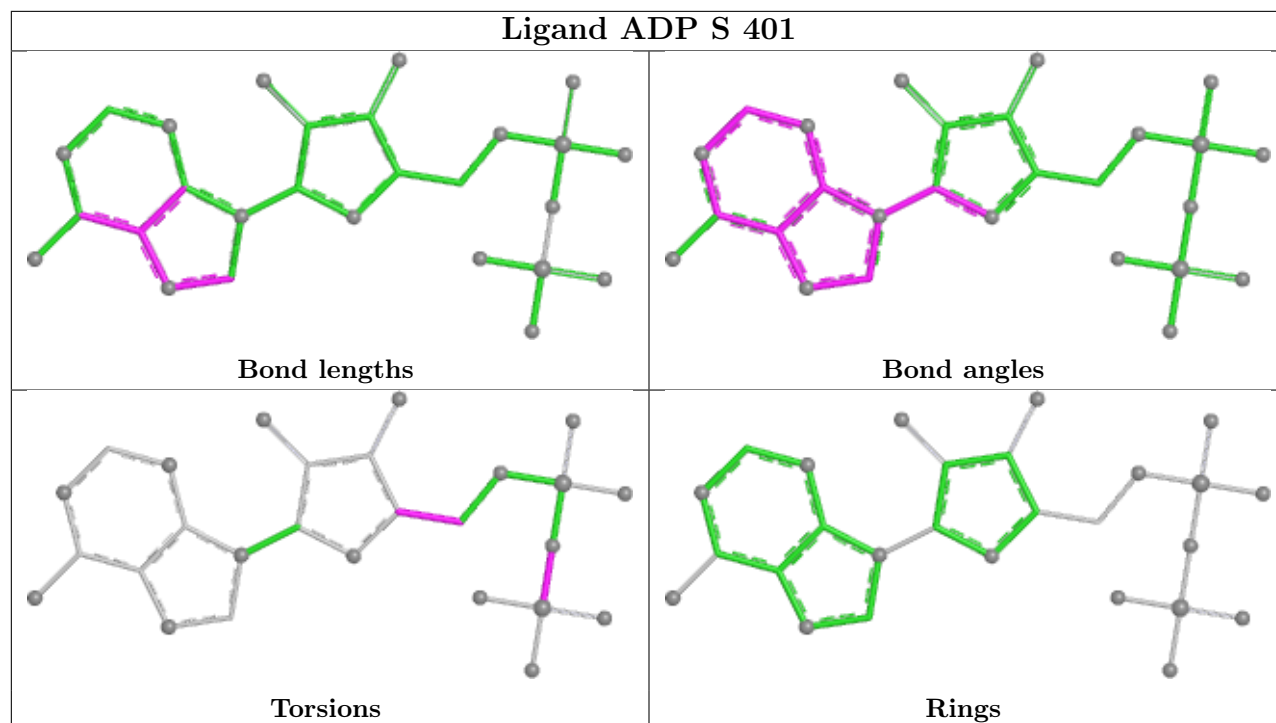


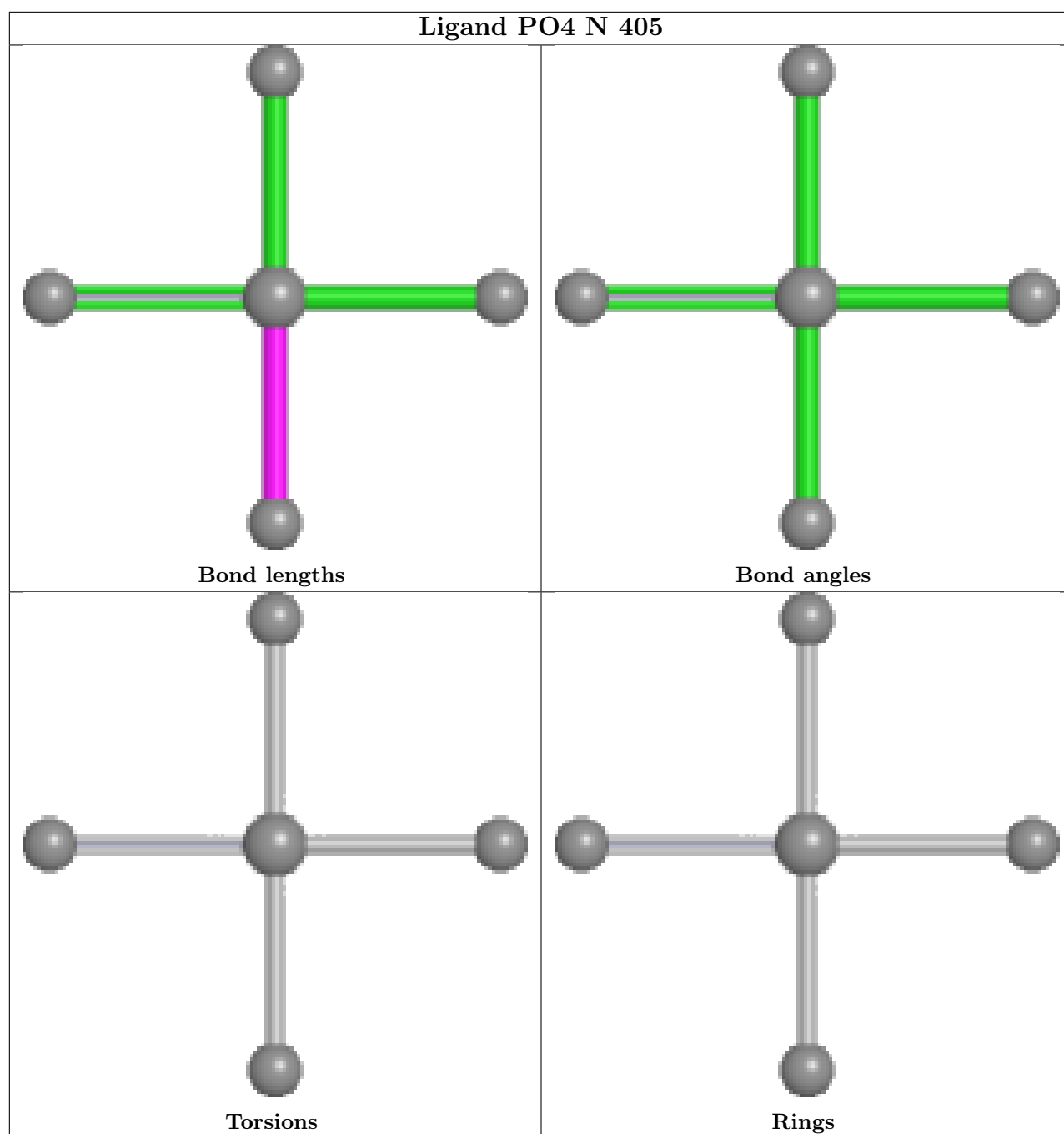


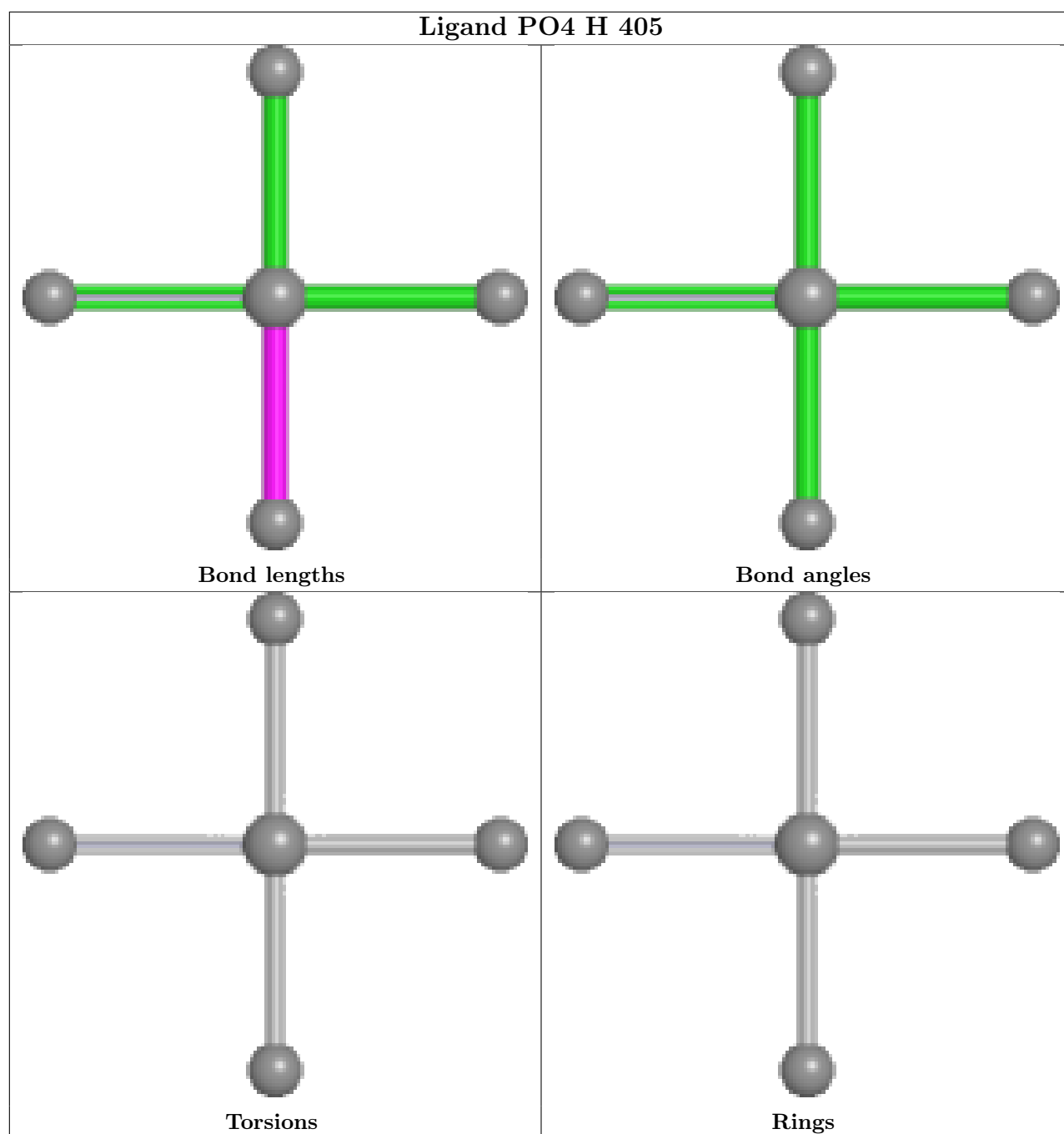


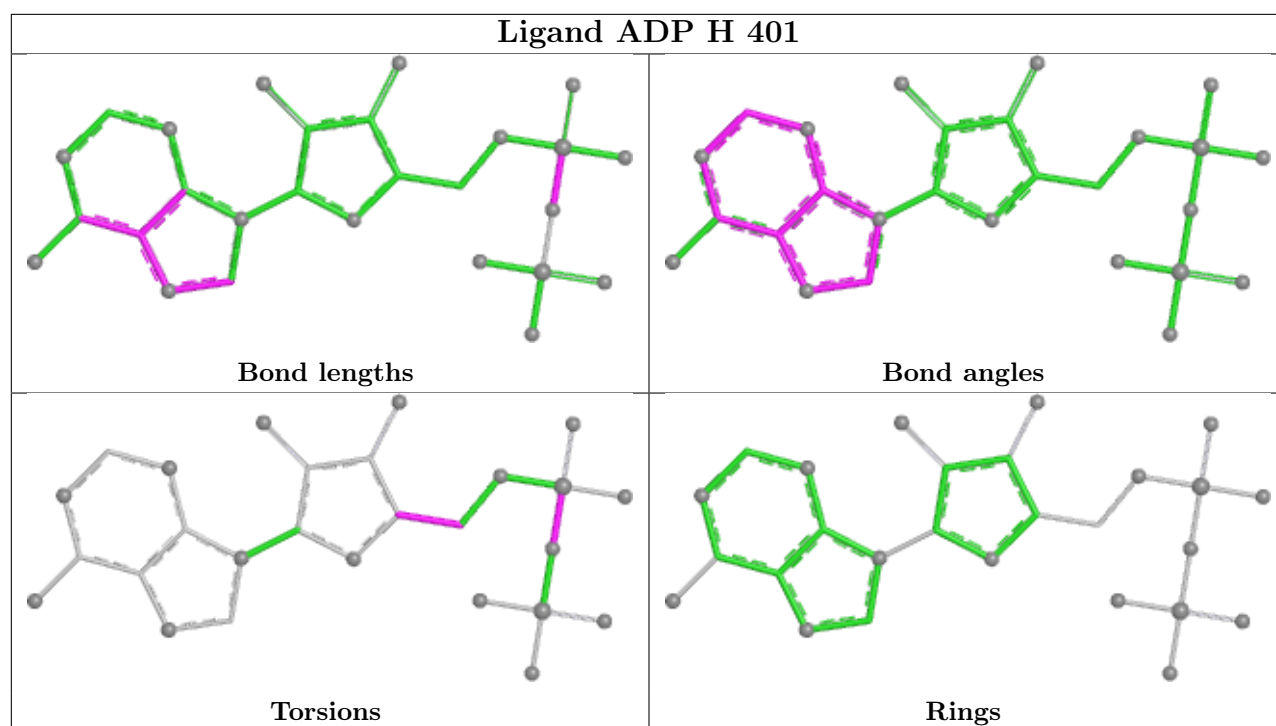


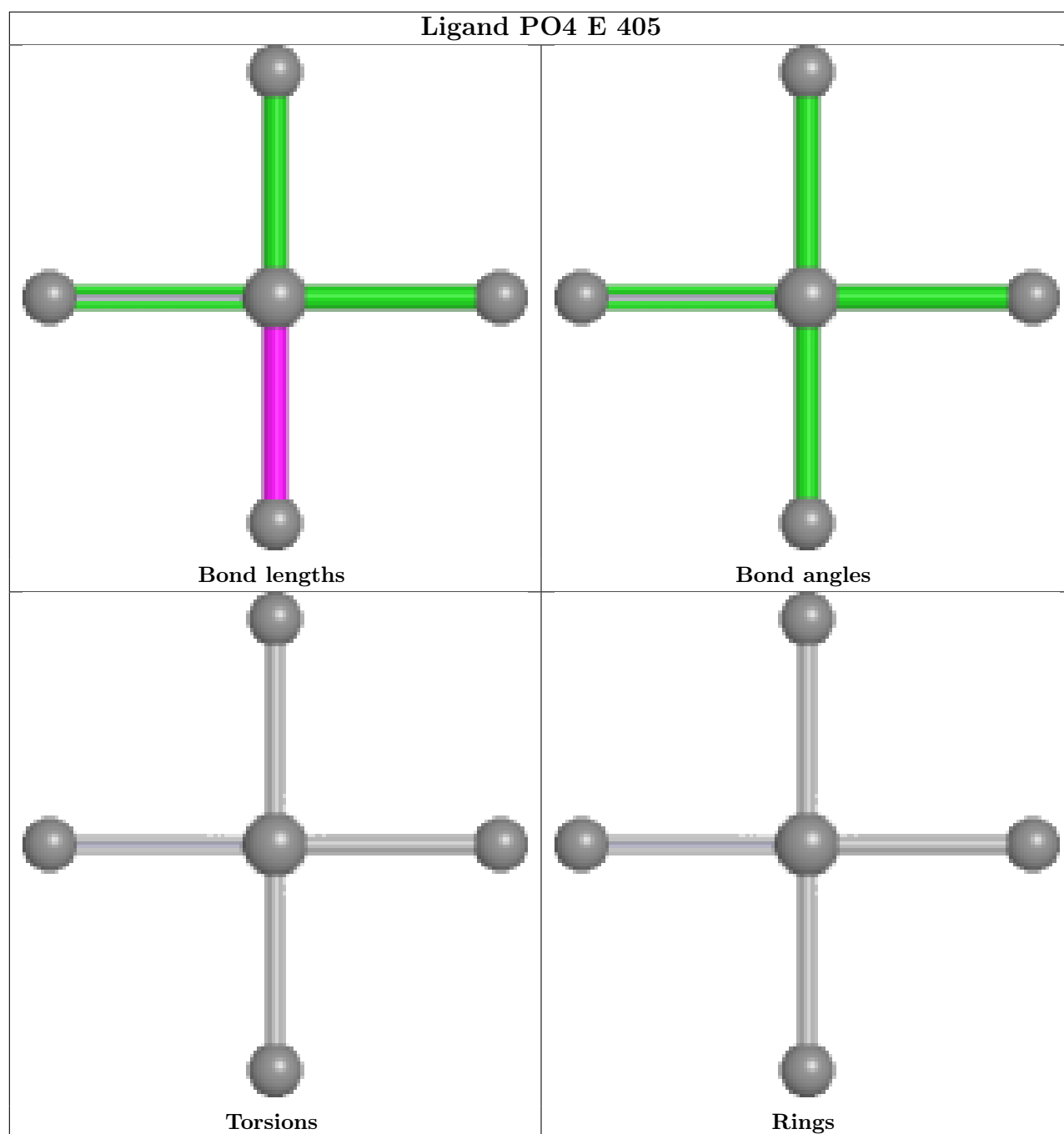


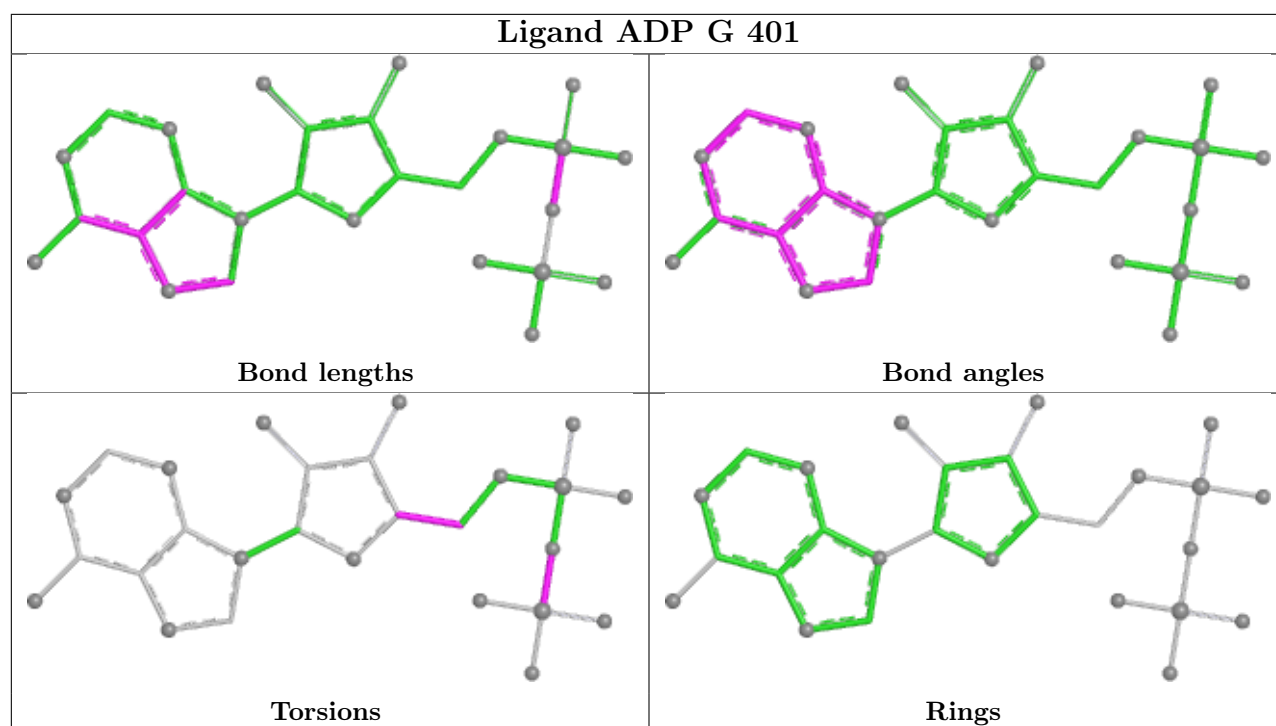


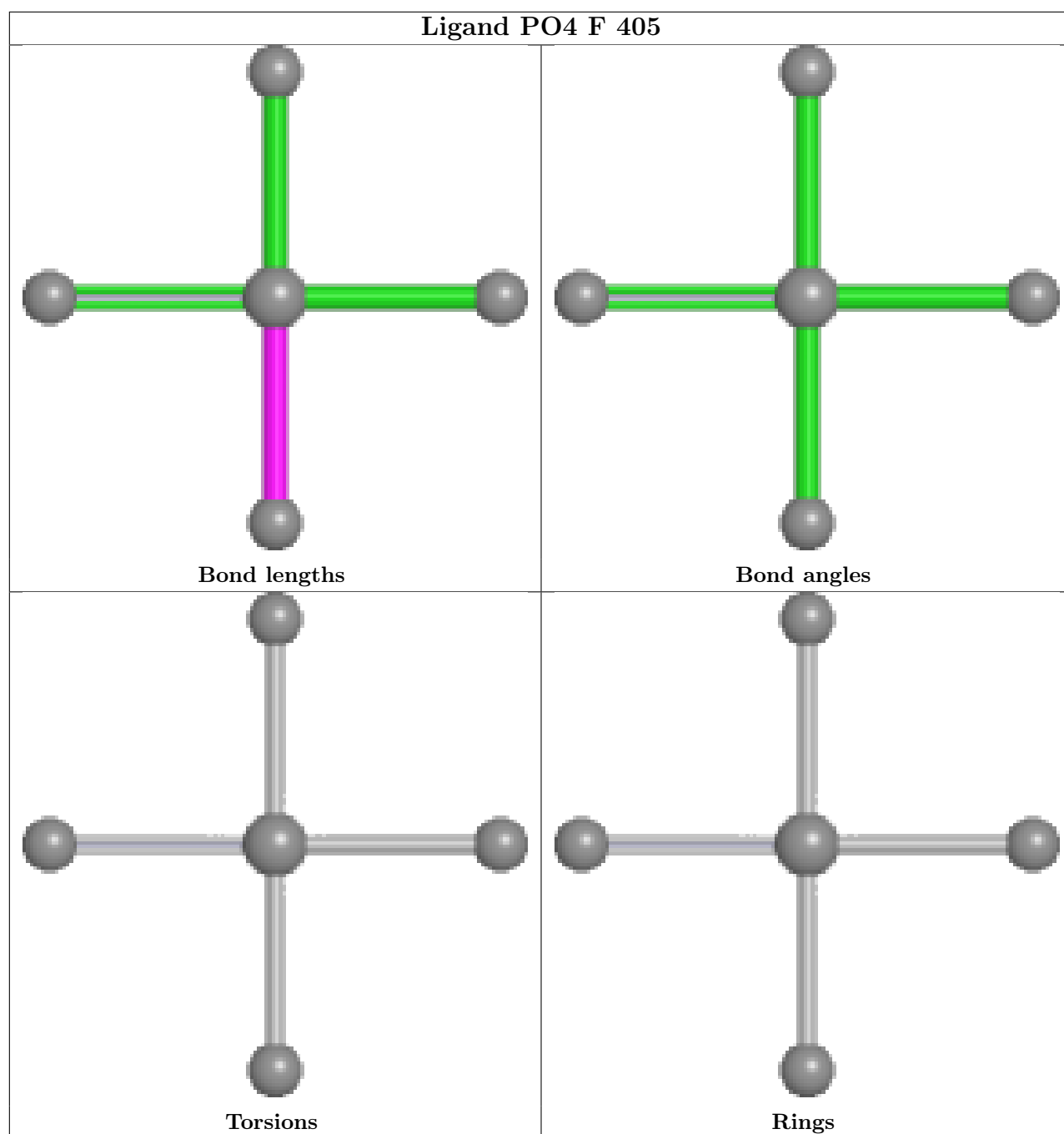


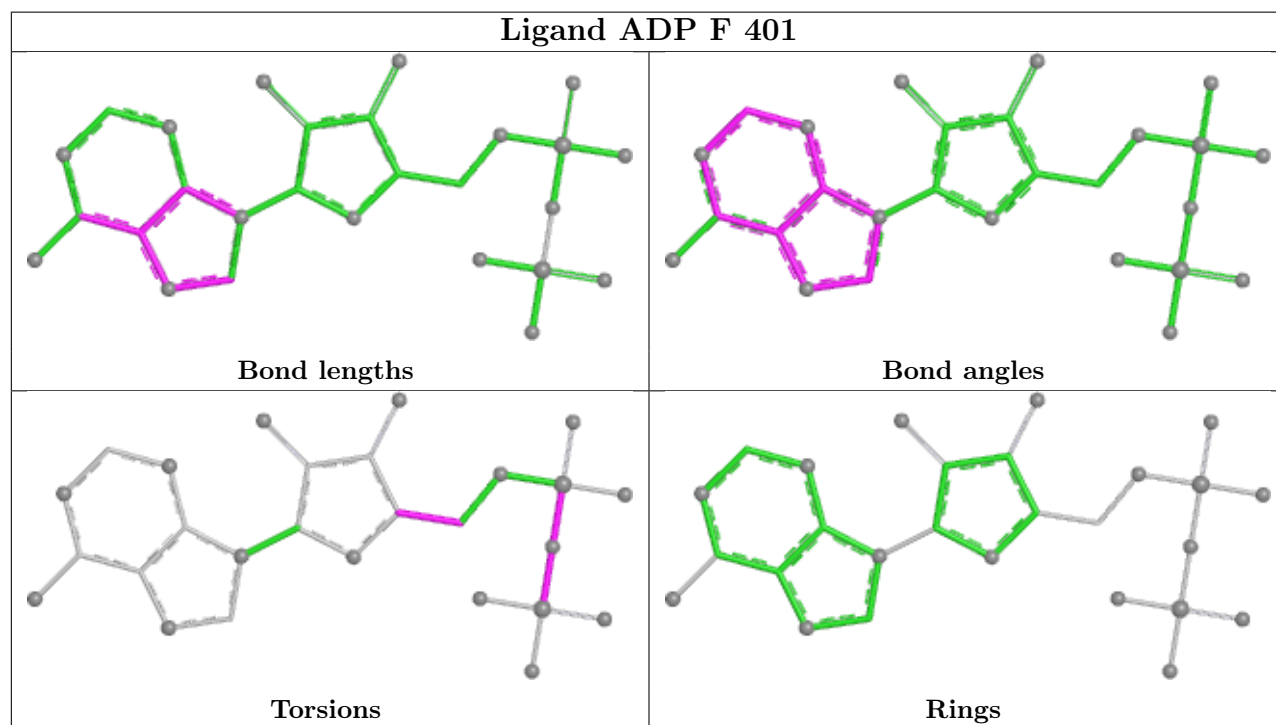
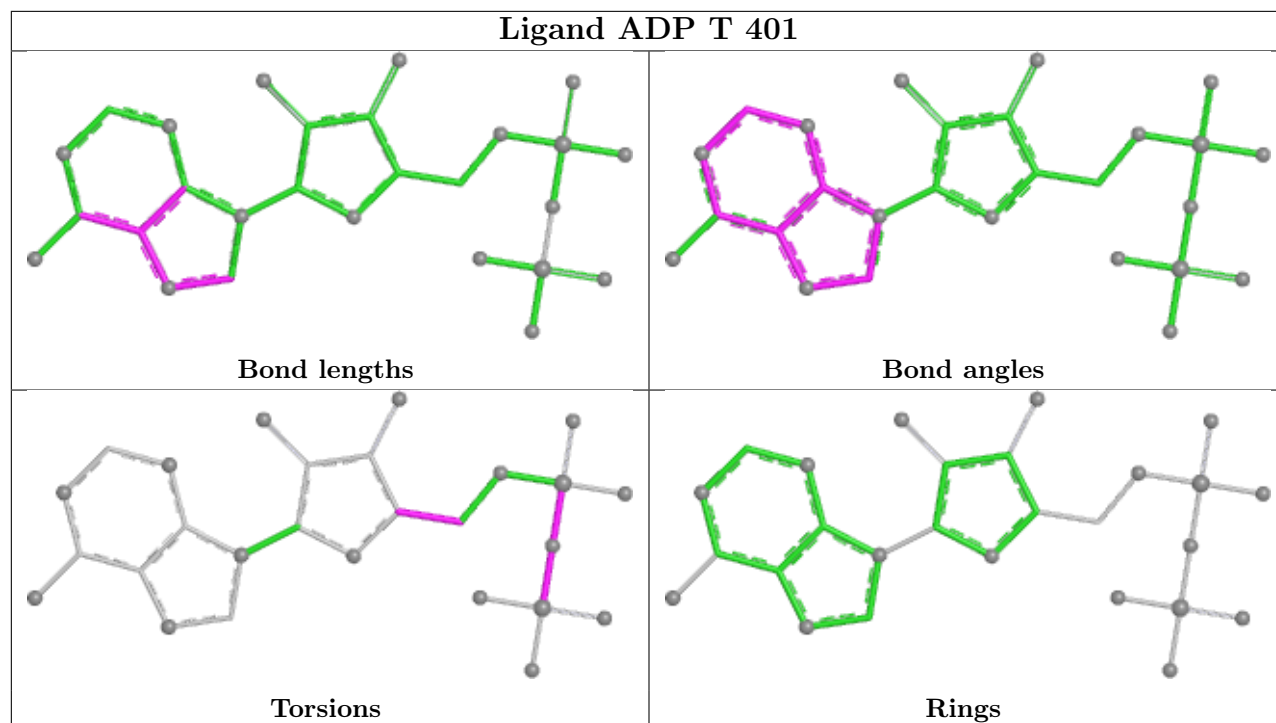


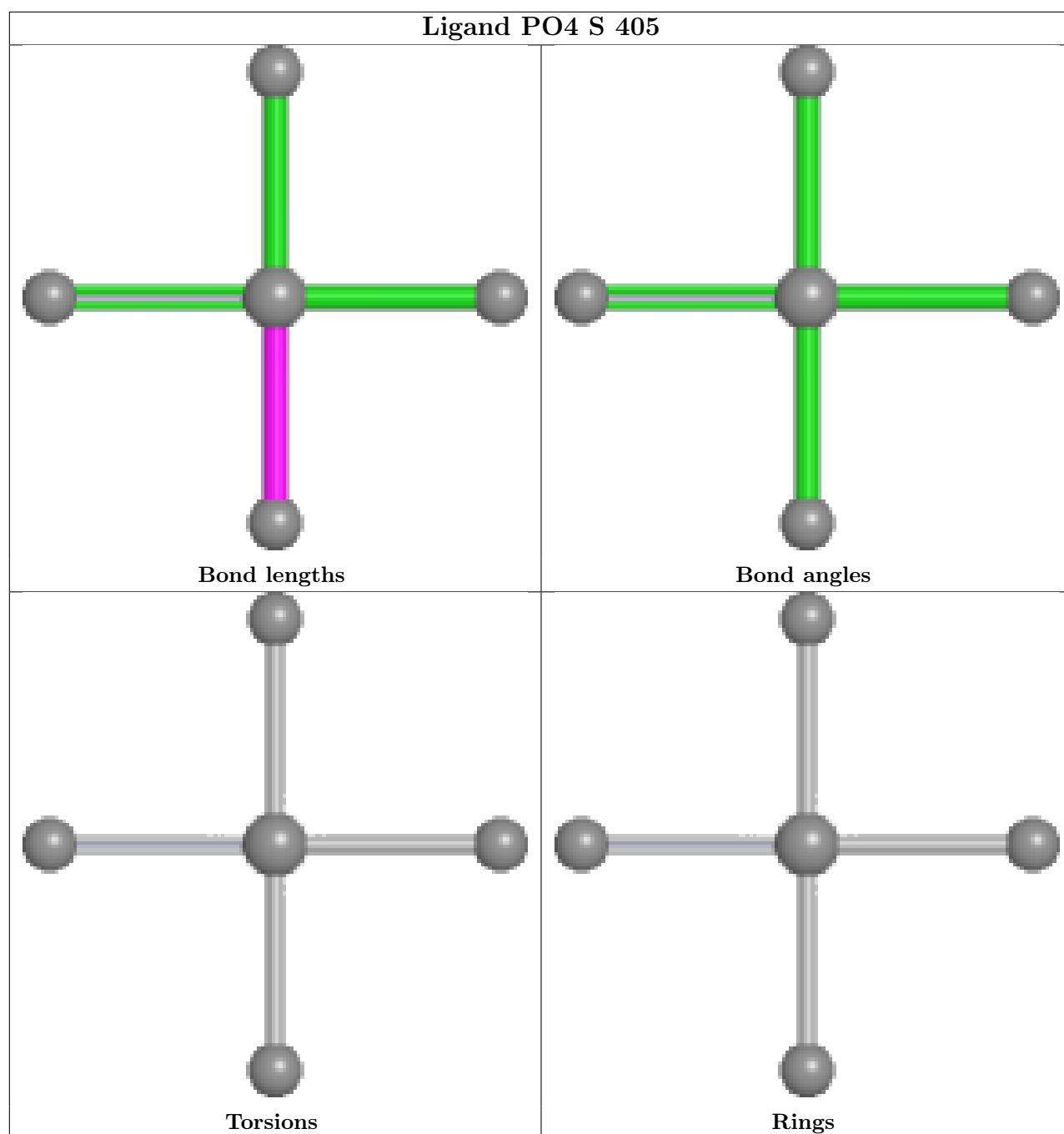


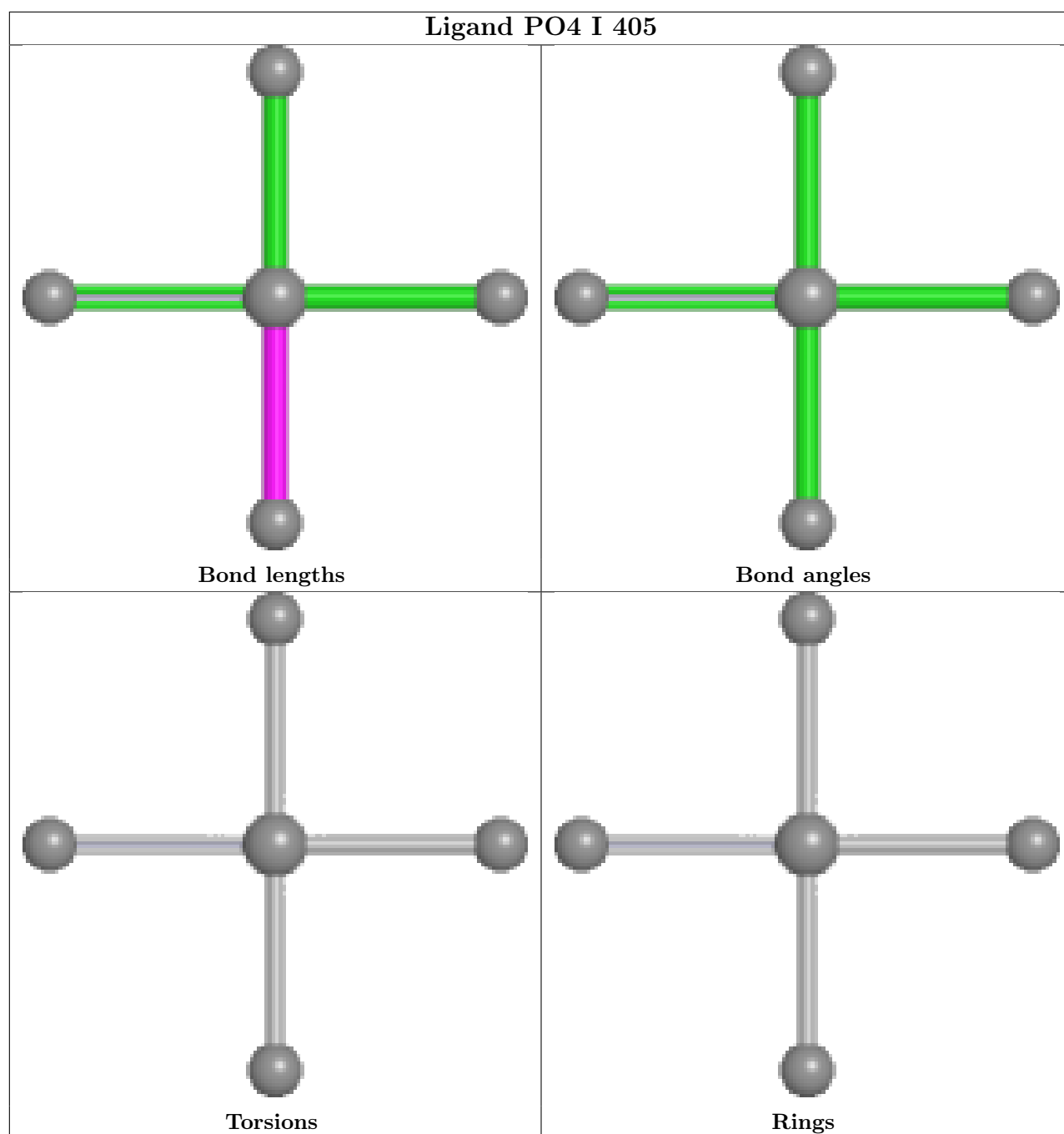


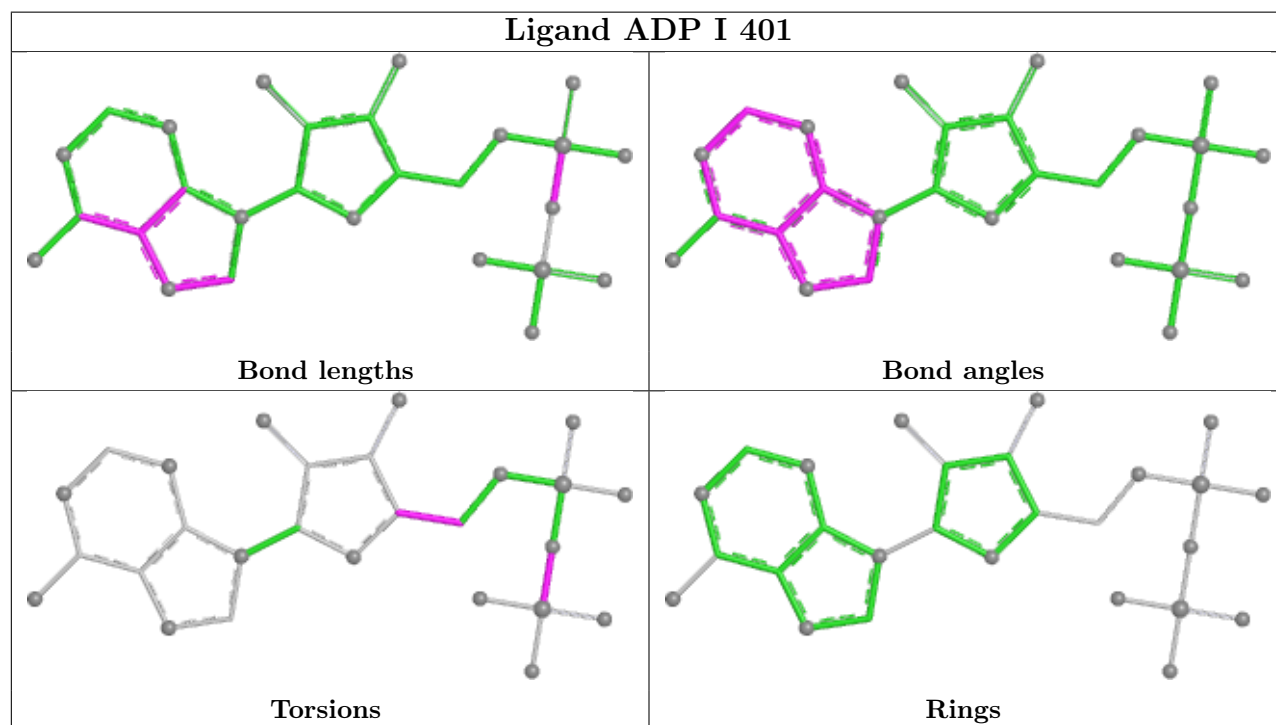
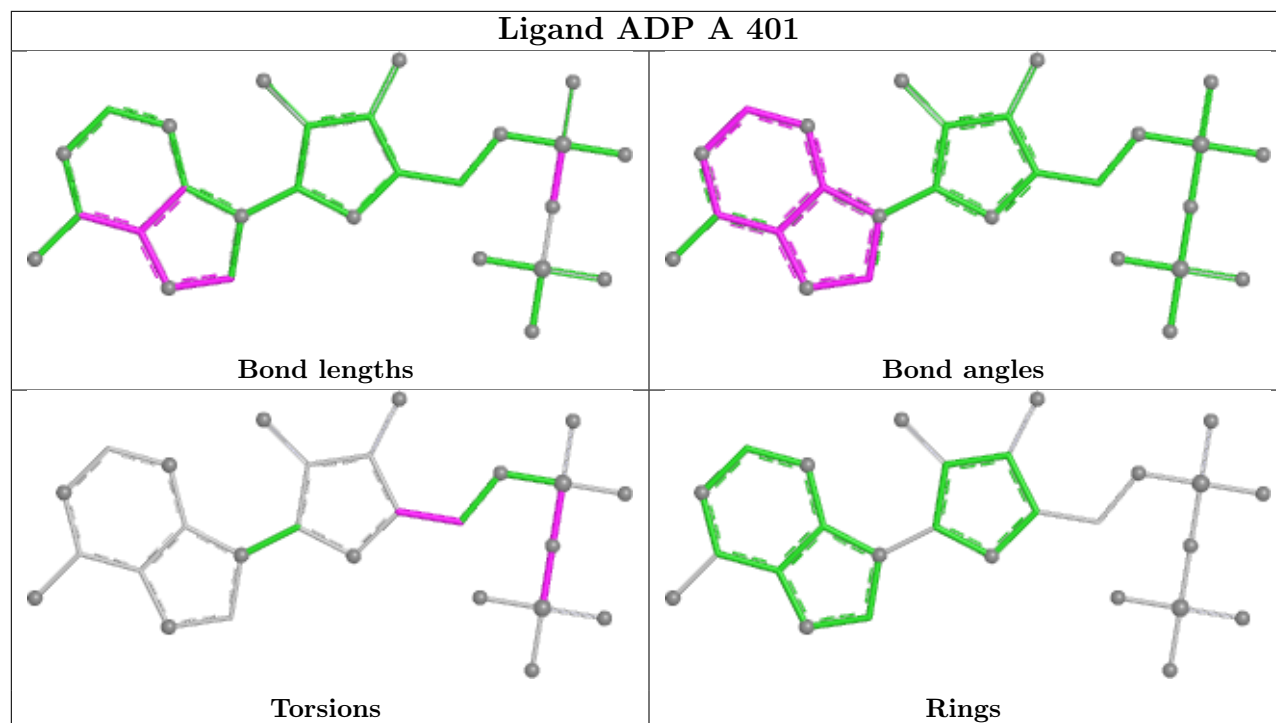


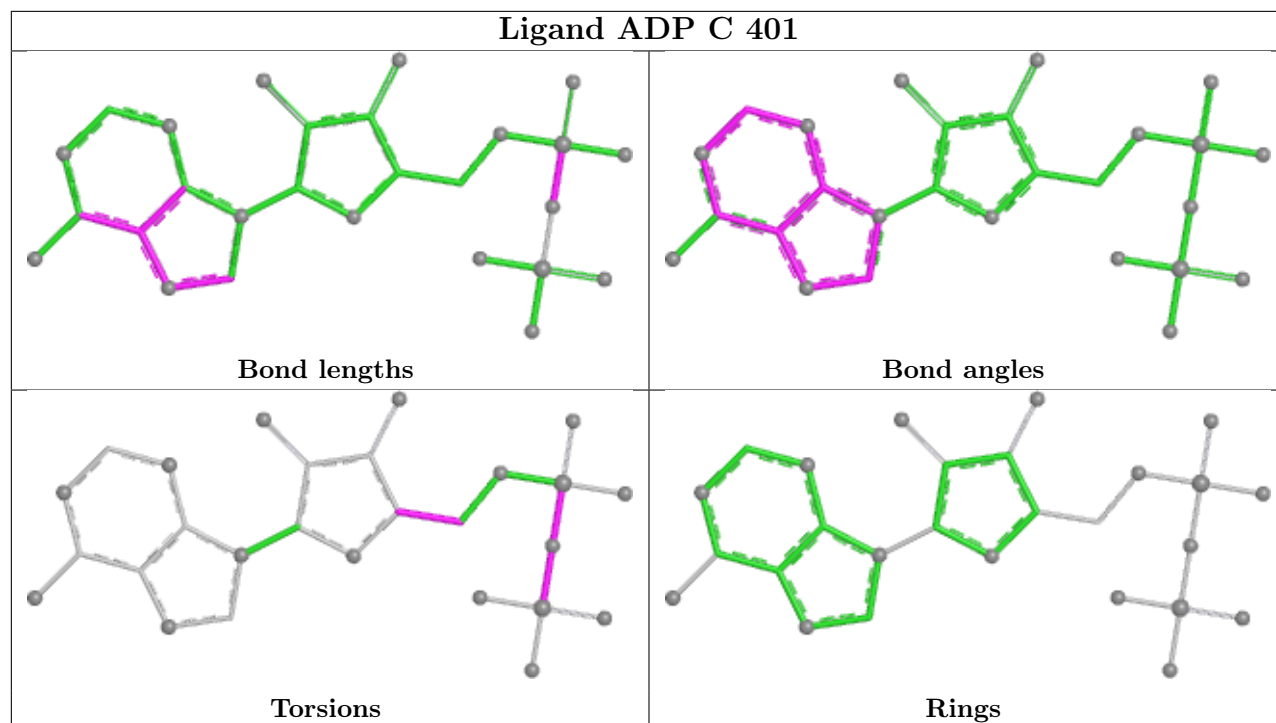


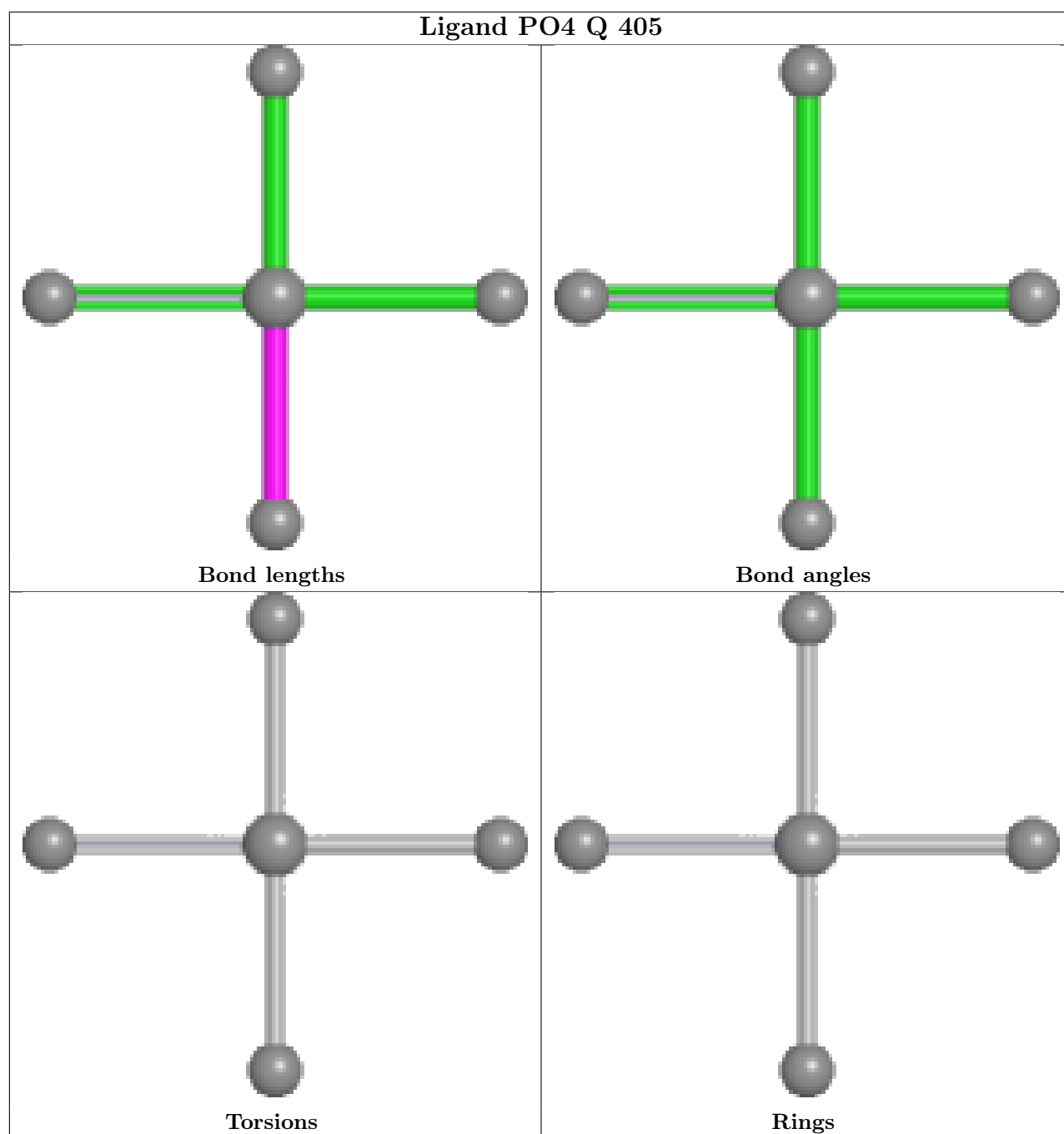


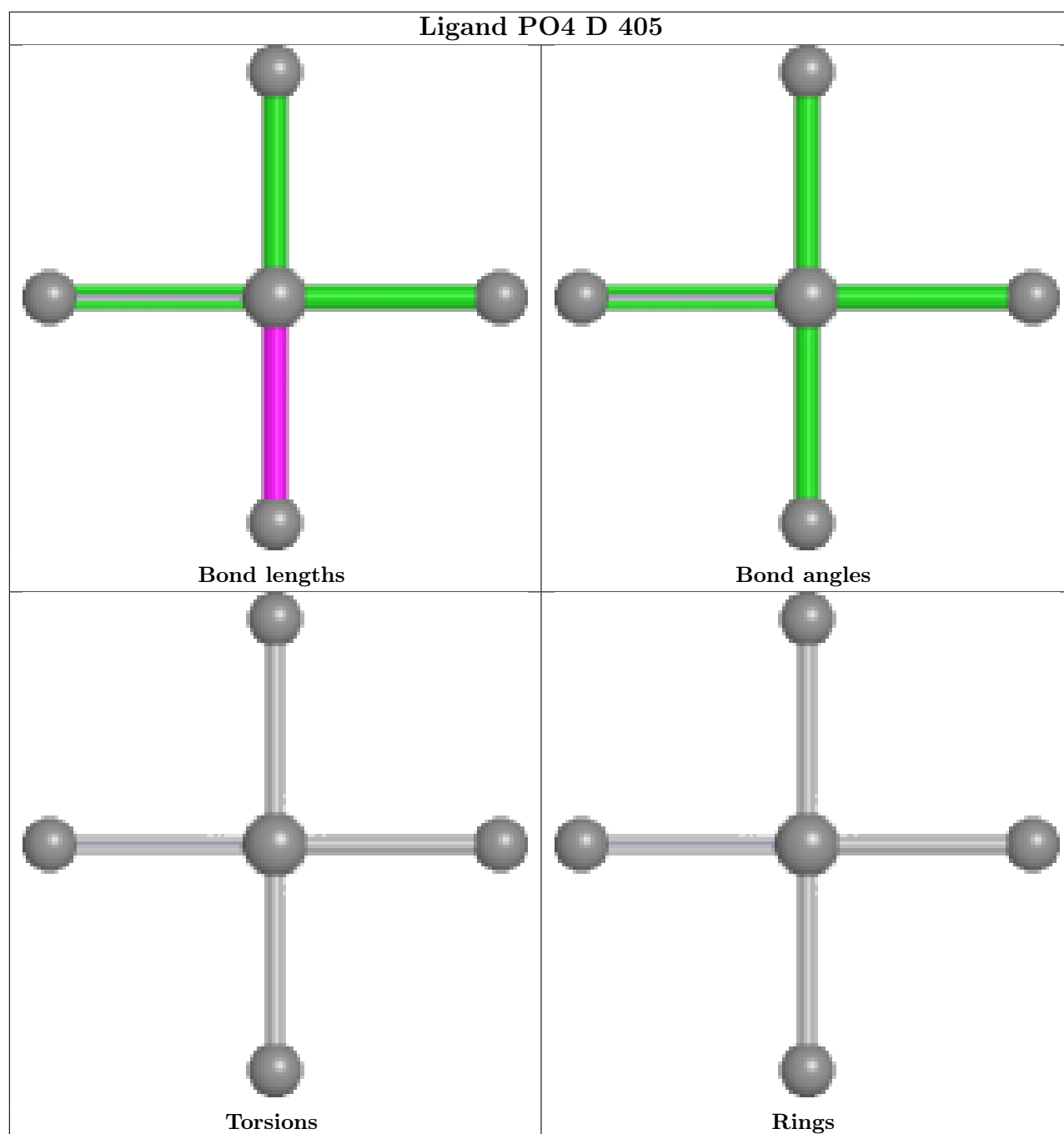


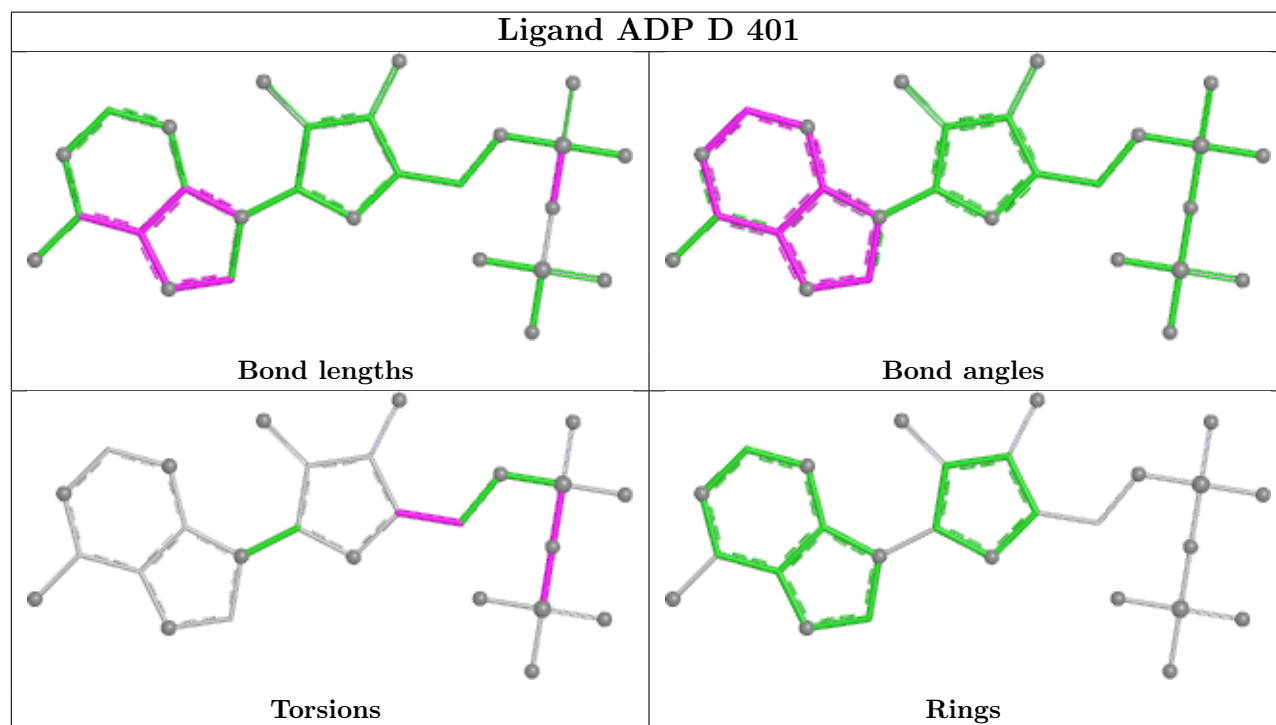
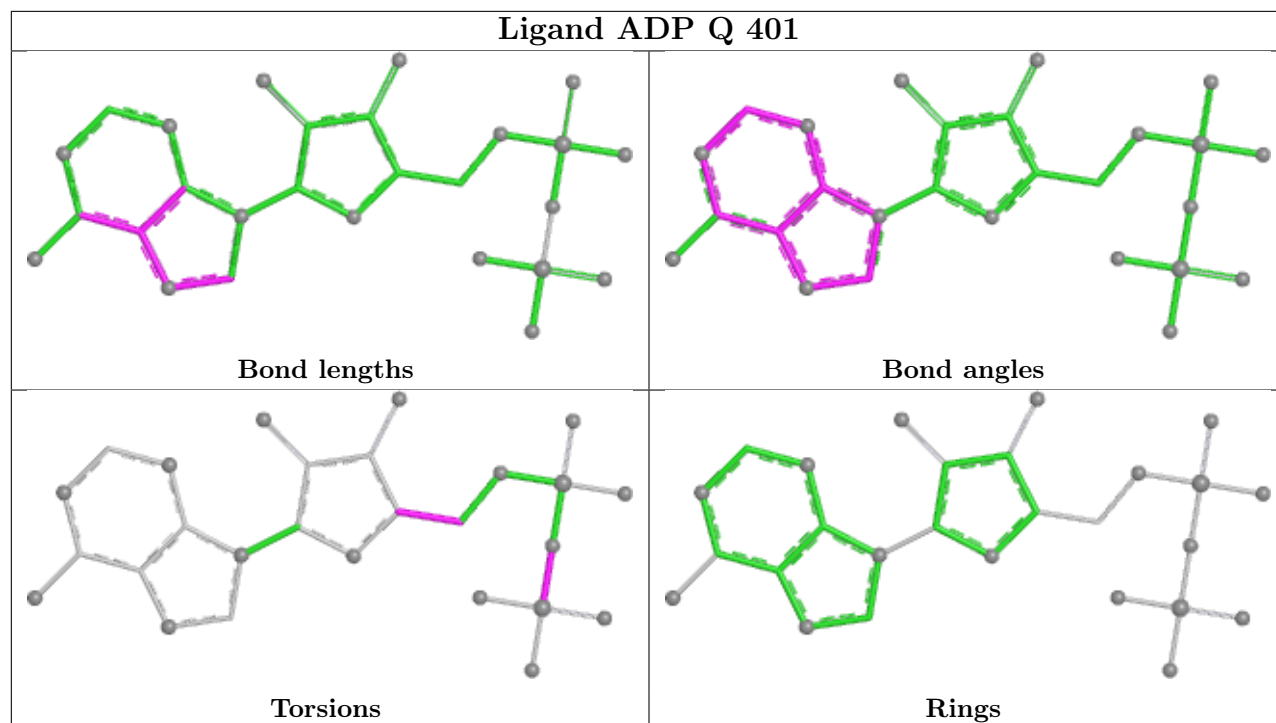


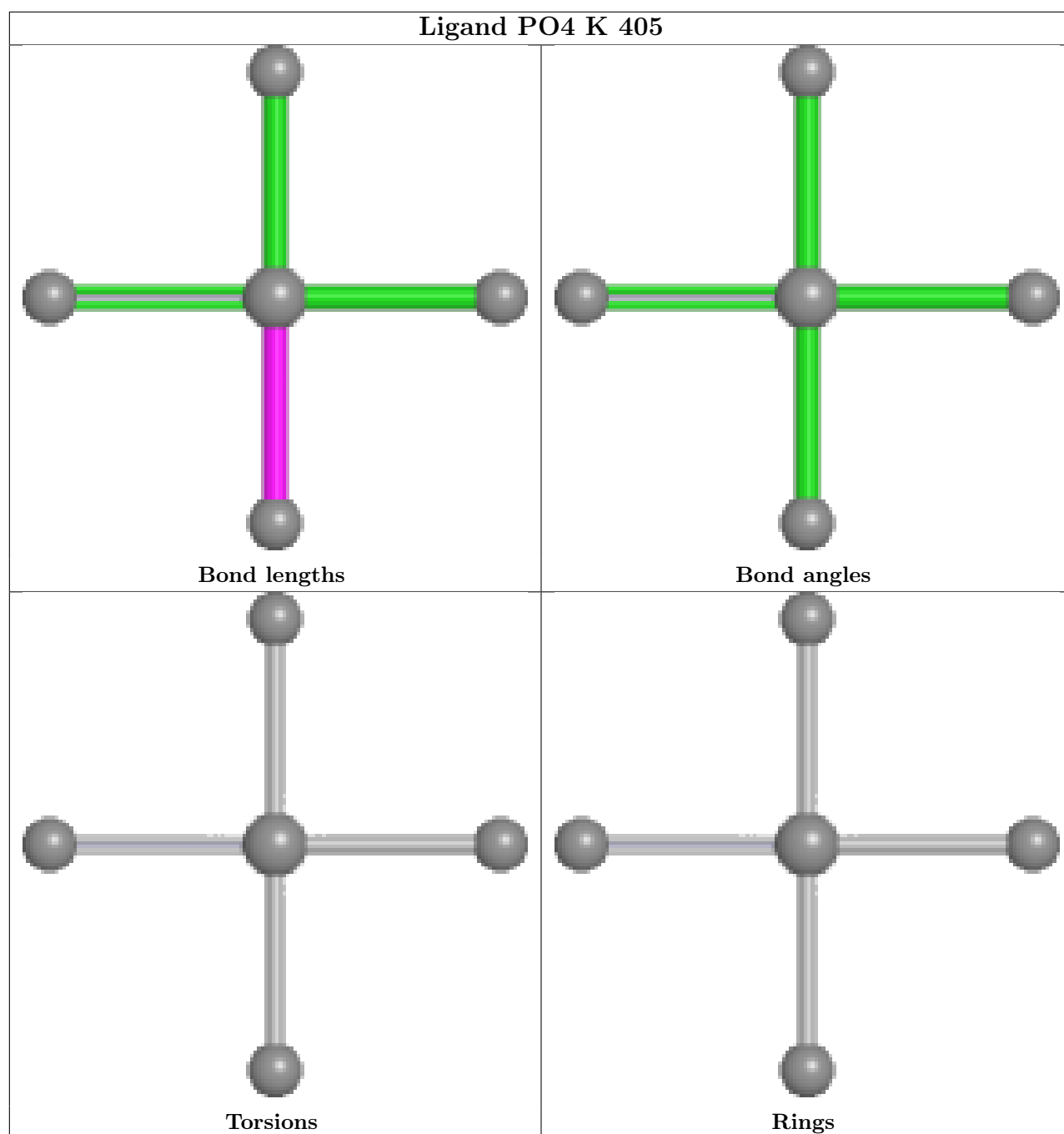


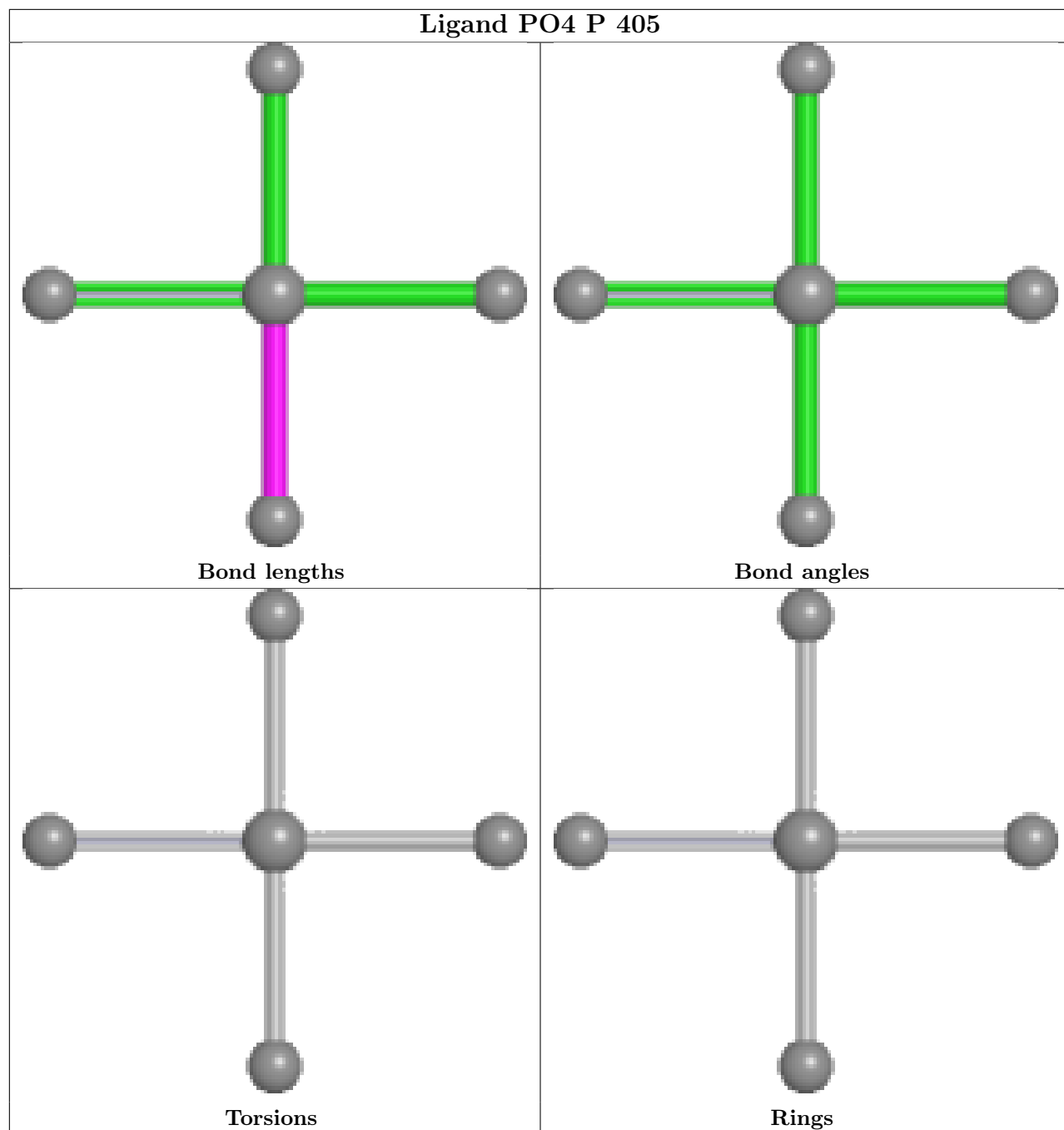


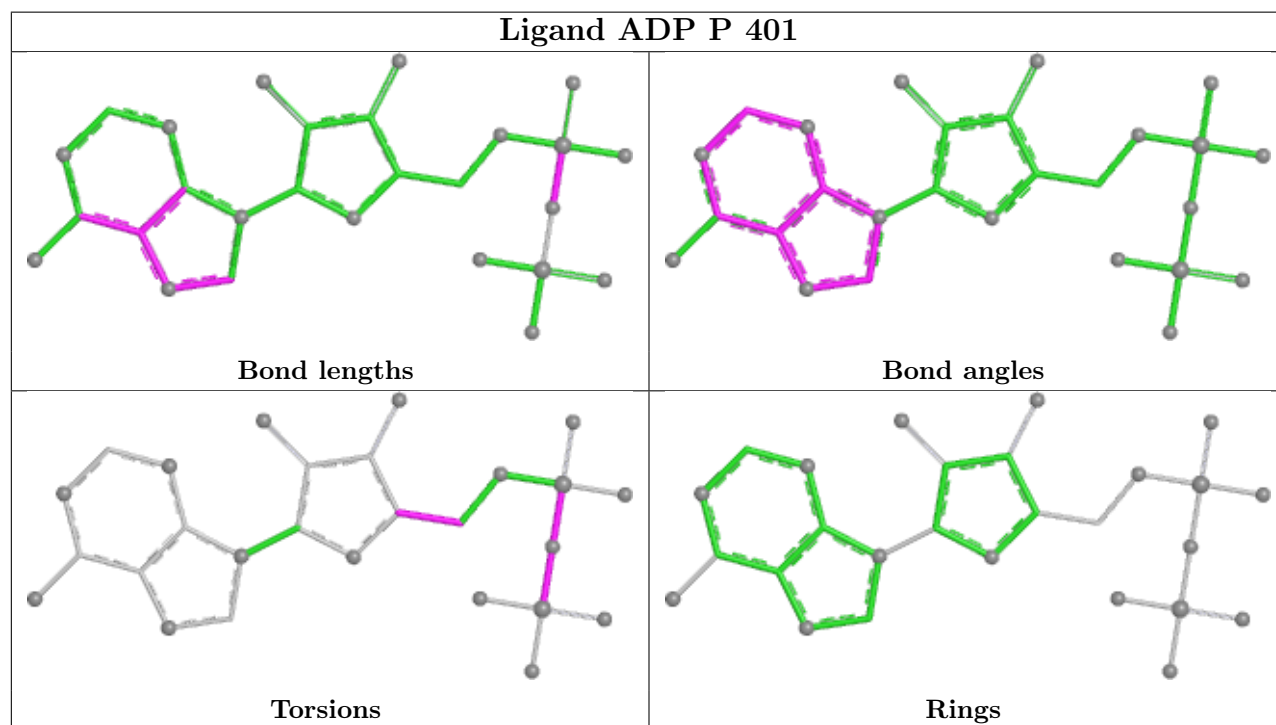
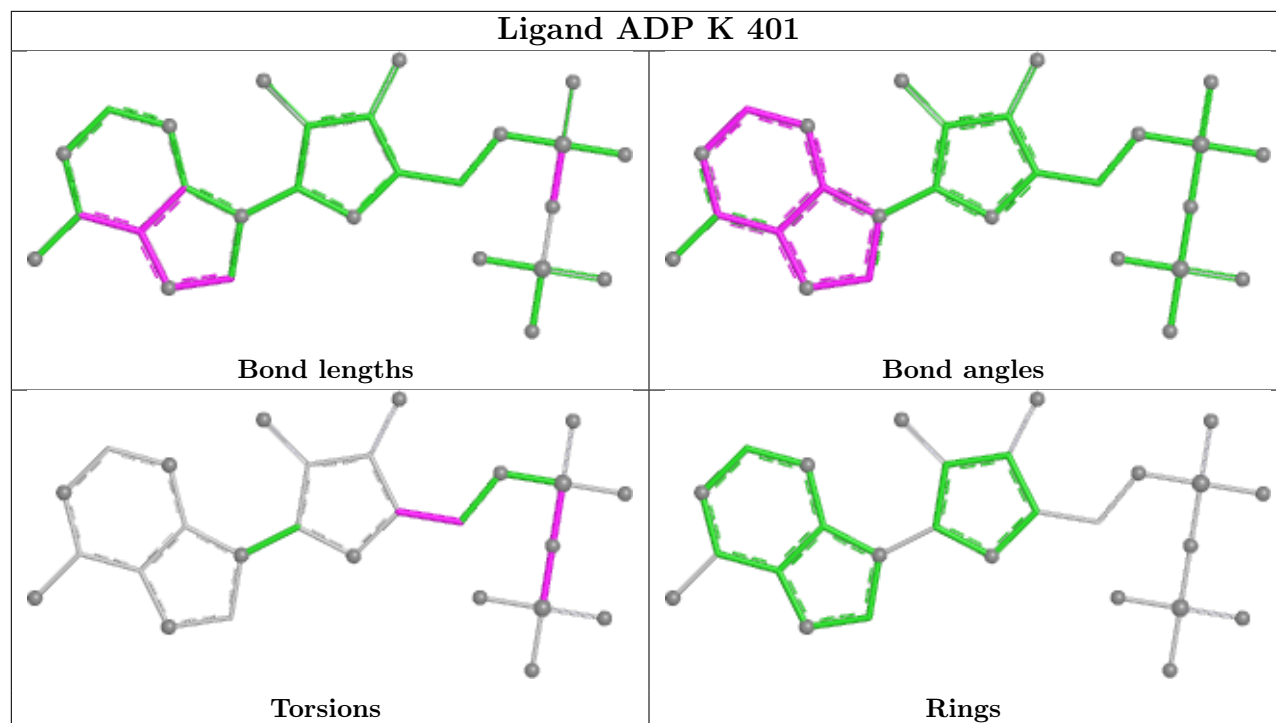


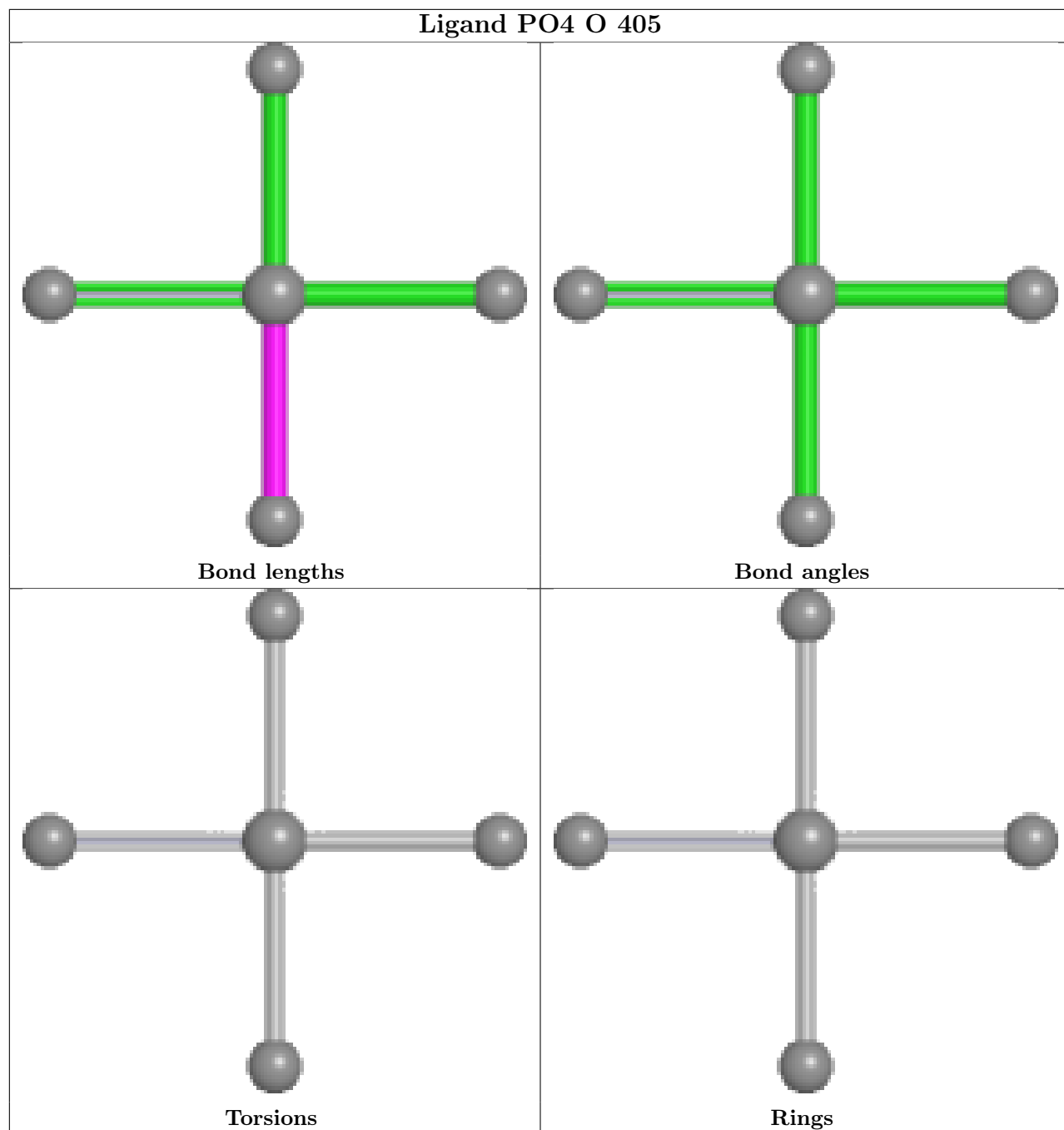


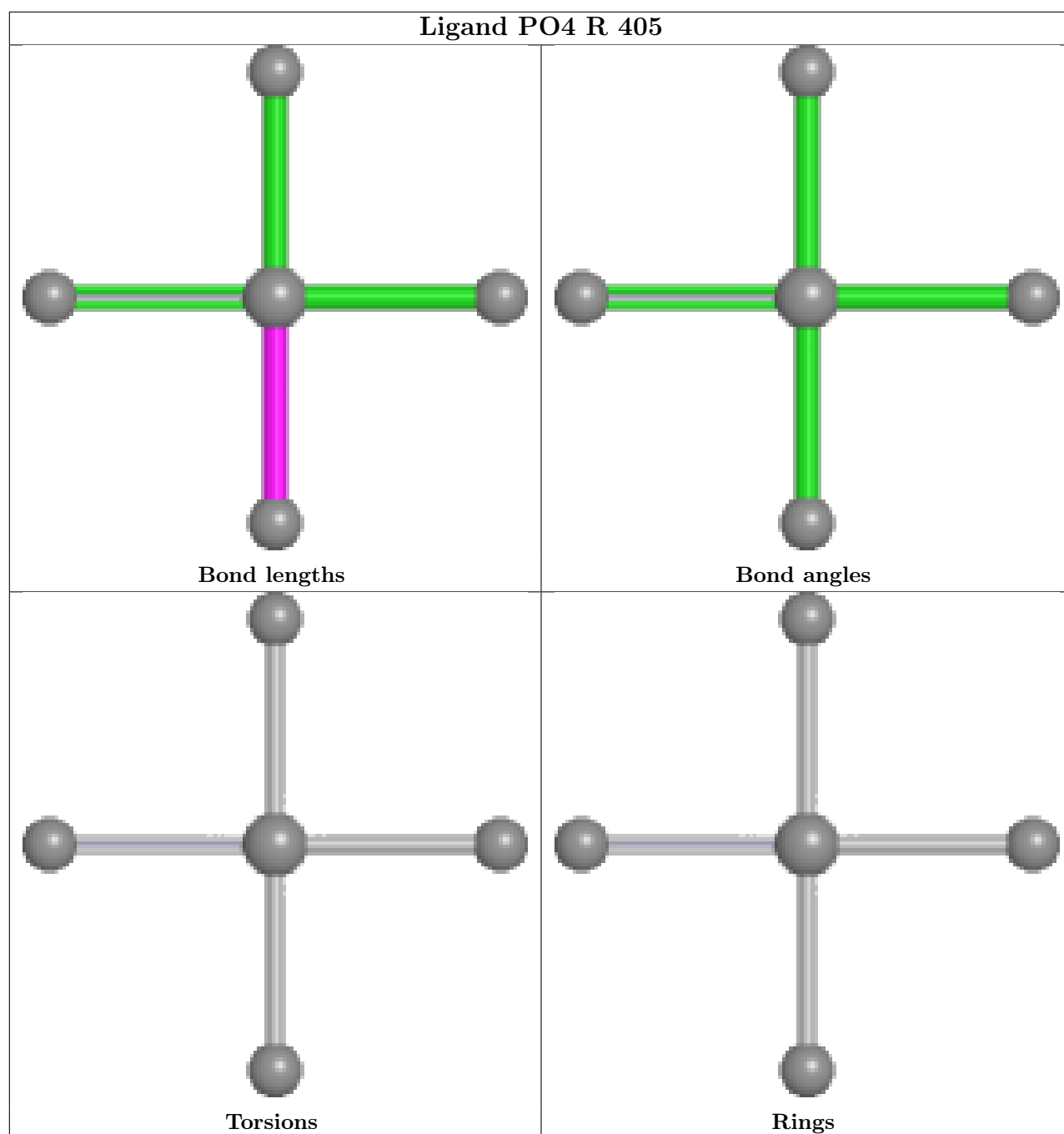


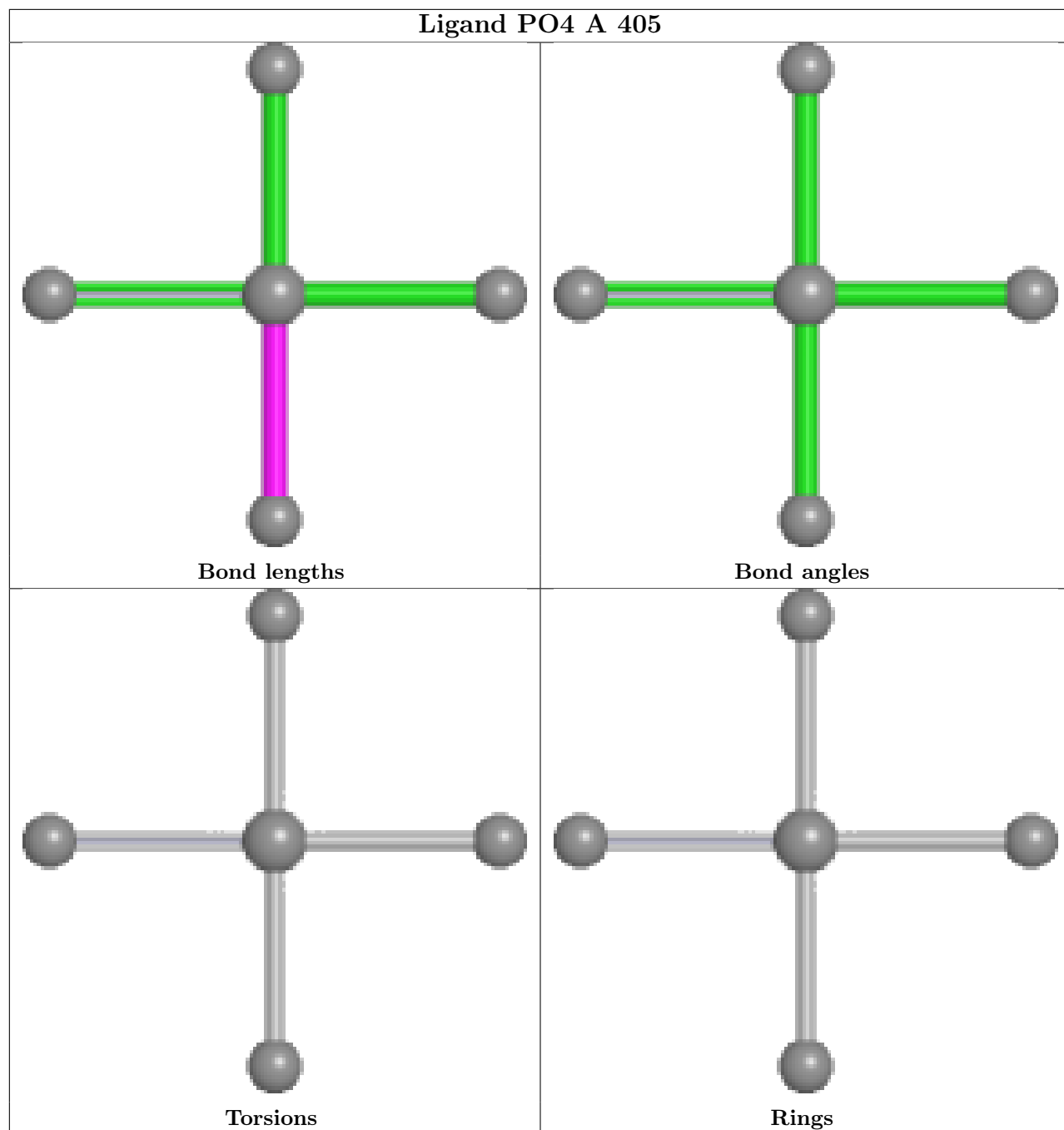


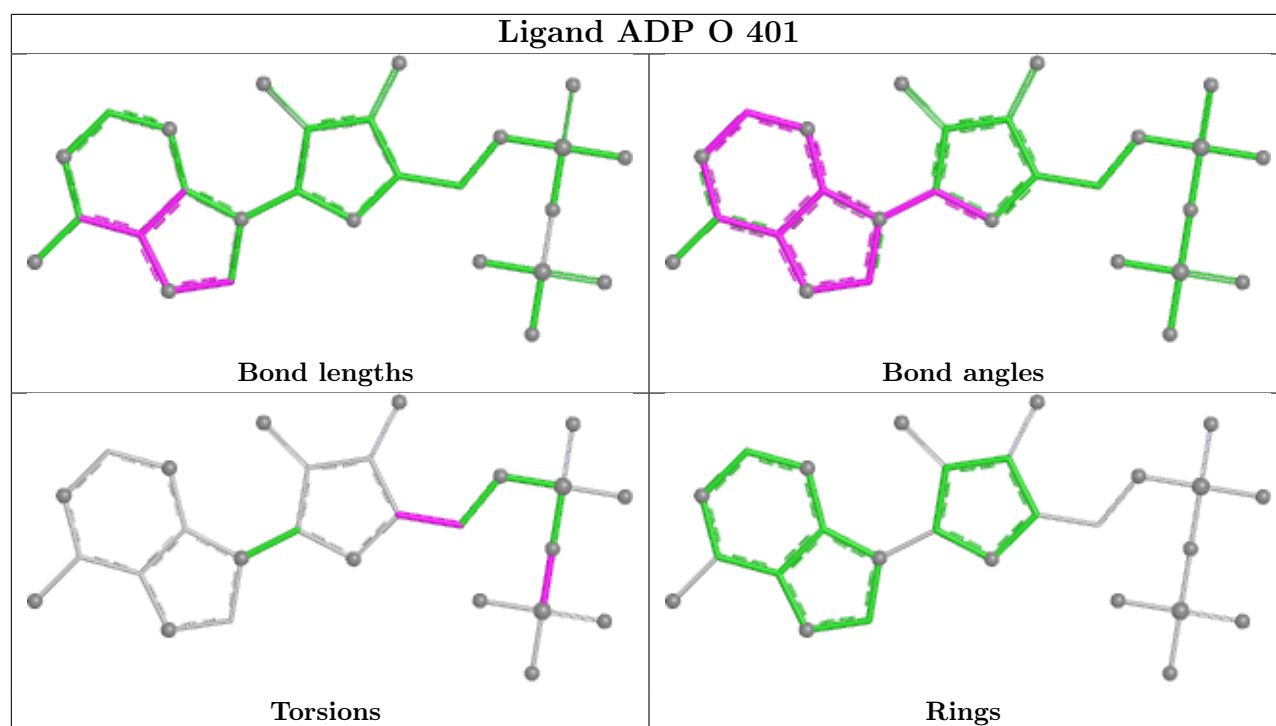


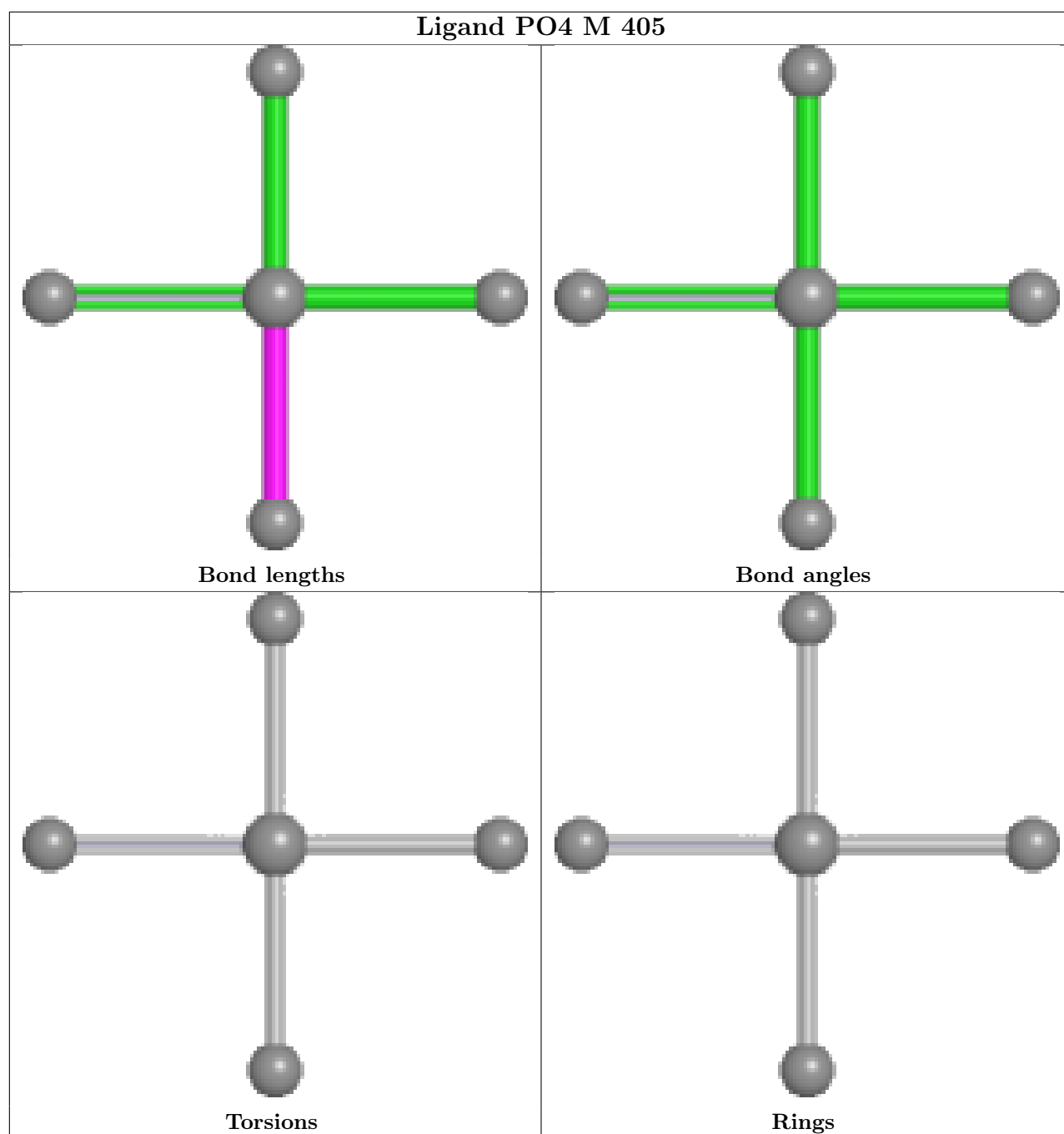


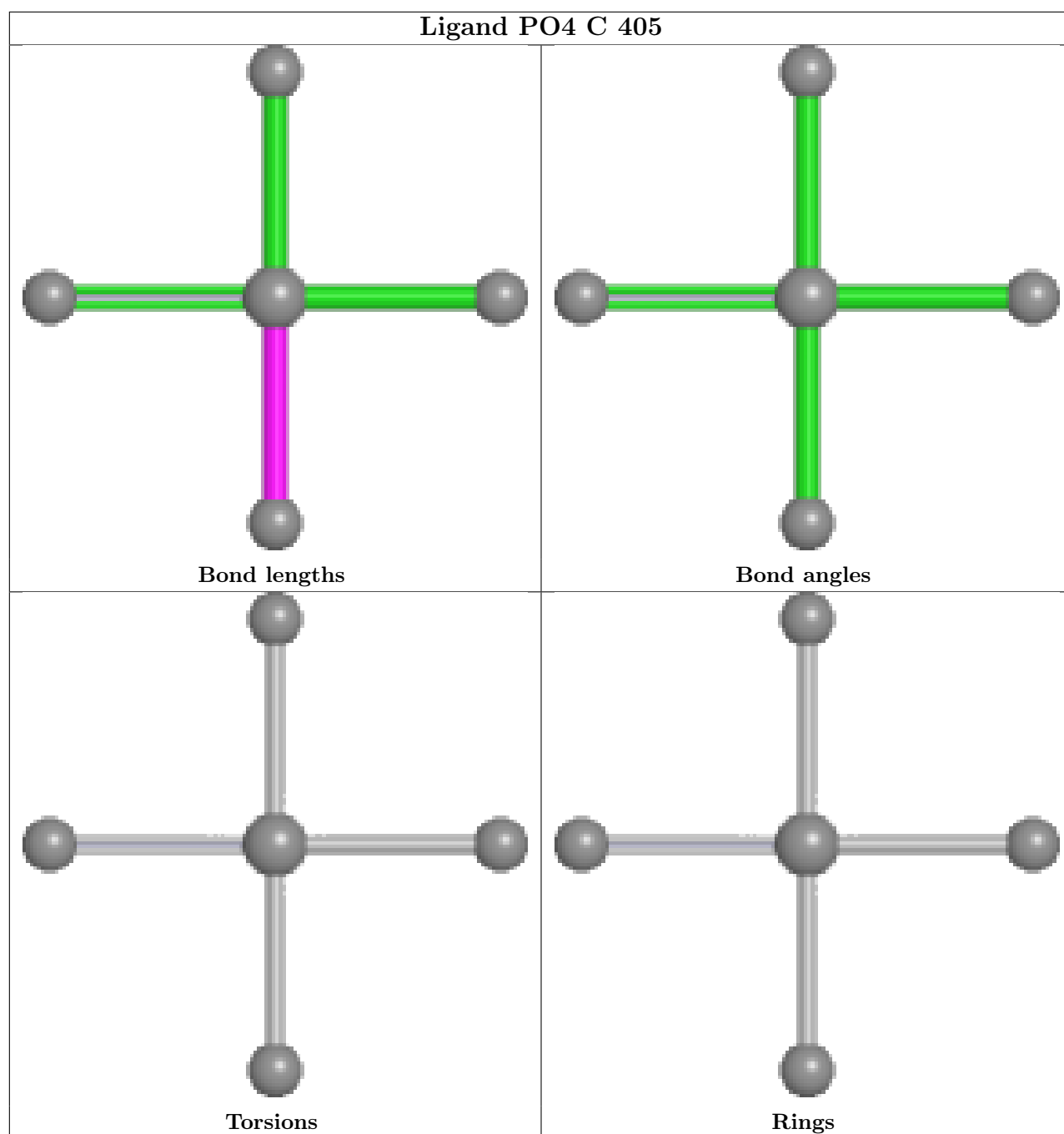


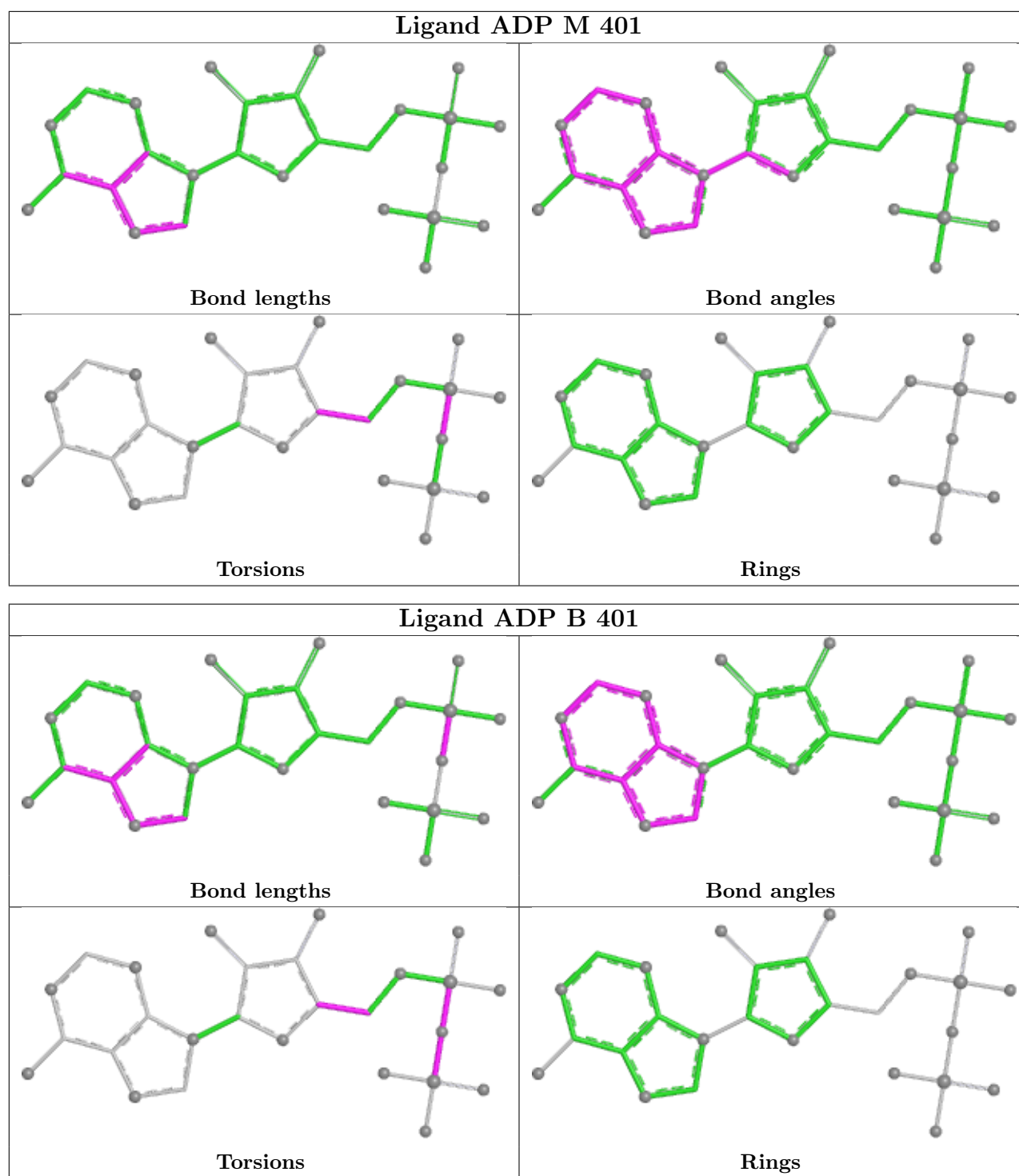












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	367/373 (98%)	-0.13	9 (2%) 58 60	21, 30, 58, 74	0
1	B	370/373 (99%)	-0.16	3 (0%) 82 83	21, 29, 51, 72	0
1	C	370/373 (99%)	-0.19	6 (1%) 70 72	21, 30, 47, 76	0
1	D	370/373 (99%)	-0.15	5 (1%) 73 75	21, 31, 53, 74	0
1	E	368/373 (98%)	-0.19	6 (1%) 70 72	21, 28, 53, 89	0
1	F	366/373 (98%)	0.03	9 (2%) 58 60	22, 33, 63, 85	0
1	G	363/373 (97%)	-0.18	5 (1%) 73 75	20, 30, 52, 73	0
1	H	366/373 (98%)	-0.04	2 (0%) 87 87	21, 35, 56, 74	0
1	I	370/373 (99%)	-0.09	2 (0%) 87 87	23, 34, 53, 63	0
1	J	359/373 (96%)	0.01	11 (3%) 51 53	23, 34, 58, 86	0
1	K	356/373 (95%)	0.04	6 (1%) 69 70	26, 38, 56, 85	0
1	L	368/373 (98%)	0.17	6 (1%) 70 72	27, 42, 65, 94	0
1	M	369/373 (98%)	0.38	13 (3%) 47 49	28, 44, 73, 94	0
1	N	367/373 (98%)	0.21	10 (2%) 56 58	27, 41, 66, 93	0
1	O	365/373 (97%)	0.08	2 (0%) 87 87	28, 38, 59, 79	0
1	P	362/373 (97%)	0.20	7 (1%) 66 68	28, 42, 60, 79	0
1	Q	359/373 (96%)	0.40	12 (3%) 49 51	31, 47, 73, 102	0
1	R	364/373 (97%)	0.44	13 (3%) 46 48	32, 48, 72, 91	0
1	S	356/373 (95%)	0.55	22 (6%) 26 28	30, 54, 80, 93	0
1	T	367/373 (98%)	0.27	12 (3%) 49 51	28, 43, 68, 91	0
All	All	7302/7460 (97%)	0.08	161 (2%) 62 64	20, 38, 66, 102	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	303	PHE	5.3
1	O	302	GLY	4.9
1	E	78	TYR	4.4
1	L	73	SER	4.4
1	Q	78	TYR	4.3
1	S	303	PHE	4.2
1	N	246	ASN	4.1
1	E	303	PHE	4.1
1	A	303	PHE	3.9
1	G	303	PHE	3.9
1	F	73	SER	3.8
1	T	304	HIS	3.8
1	E	74	ASN	3.8
1	T	306	THR	3.8
1	Q	246	ASN	3.8
1	P	78	TYR	3.7
1	R	246	ASN	3.7
1	S	265	ASN	3.7
1	F	303	PHE	3.6
1	S	301	THR	3.6
1	A	246	ASN	3.5
1	F	76	ASP	3.4
1	N	306	THR	3.4
1	R	307	SER	3.4
1	T	303	PHE	3.3
1	R	126	ASN	3.3
1	Q	301	THR	3.3
1	T	246	ASN	3.2
1	R	74	ASN	3.2
1	P	301	THR	3.2
1	K	246	ASN	3.2
1	N	302	GLY	3.1
1	M	126	ASN	3.1
1	Q	369	PHE	3.1
1	N	78	TYR	3.1
1	C	306	THR	3.1
1	J	73	SER	3.1
1	A	78	TYR	3.1
1	N	365	GLY	3.1
1	M	328	THR	3.0
1	B	246	ASN	3.0
1	D	303	PHE	3.0
1	K	73	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	104	TYR	3.0
1	F	74	ASN	3.0
1	Q	364	THR	2.9
1	M	304	HIS	2.9
1	P	246	ASN	2.9
1	T	78	TYR	2.9
1	L	303	PHE	2.9
1	S	364	THR	2.9
1	A	301	THR	2.8
1	Q	104	TYR	2.8
1	C	303	PHE	2.8
1	S	309	ILE	2.7
1	S	260	ALA	2.7
1	J	304	HIS	2.7
1	D	72	GLY	2.7
1	E	302	GLY	2.7
1	Q	75	SER	2.7
1	B	303	PHE	2.7
1	S	246	ASN	2.7
1	D	78	TYR	2.6
1	J	78	TYR	2.6
1	O	246	ASN	2.6
1	P	310	ASN	2.6
1	J	306	THR	2.6
1	S	82	ALA	2.6
1	J	303	PHE	2.6
1	L	371	TYR	2.6
1	N	307	SER	2.6
1	T	70	SER	2.6
1	S	71	GLU	2.6
1	Q	335	GLY	2.6
1	S	302	GLY	2.6
1	S	264	GLU	2.6
1	N	301	THR	2.6
1	M	331	GLN	2.5
1	Q	370	GLN	2.5
1	S	283	TYR	2.5
1	Q	307	SER	2.5
1	E	246	ASN	2.5
1	R	71	GLU	2.4
1	D	71	GLU	2.4
1	I	275	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	371	TYR	2.4
1	S	75	SER	2.4
1	M	104	TYR	2.4
1	R	104	TYR	2.4
1	T	331	GLN	2.4
1	F	71	GLU	2.4
1	F	246	ASN	2.4
1	R	72	GLY	2.4
1	R	59	GLU	2.4
1	T	265	ASN	2.3
1	T	75	SER	2.3
1	T	126	ASN	2.3
1	S	78	TYR	2.3
1	G	301	THR	2.3
1	C	307	SER	2.3
1	G	275	GLU	2.3
1	S	355	LEU	2.3
1	M	78	TYR	2.3
1	K	119	ARG	2.3
1	C	304	HIS	2.3
1	L	369	PHE	2.3
1	M	246	ASN	2.3
1	A	371	TYR	2.3
1	F	78	TYR	2.3
1	S	269	TYR	2.3
1	G	246	ASN	2.2
1	R	76	ASP	2.2
1	C	301	THR	2.2
1	A	72	GLY	2.2
1	C	331	GLN	2.2
1	E	301	THR	2.2
1	S	126	ASN	2.2
1	F	72	GLY	2.2
1	H	301	THR	2.2
1	S	258	THR	2.2
1	J	126	ASN	2.2
1	J	308	ASN	2.2
1	K	308	ASN	2.2
1	N	126	ASN	2.2
1	T	369	PHE	2.2
1	I	370	GLN	2.2
1	P	370	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	73	SER	2.2
1	M	327	ARG	2.1
1	J	74	ASN	2.1
1	J	362	ASN	2.1
1	A	71	GLU	2.1
1	J	305	GLU	2.1
1	G	302	GLY	2.1
1	T	328	THR	2.1
1	R	269	TYR	2.1
1	S	336	TYR	2.1
1	L	126	ASN	2.1
1	R	316	VAL	2.1
1	F	327	ARG	2.1
1	M	301	THR	2.1
1	K	294	LEU	2.1
1	D	76	ASP	2.1
1	M	71	GLU	2.1
1	A	74	ASN	2.1
1	H	304	HIS	2.1
1	Q	361	LEU	2.1
1	K	74	ASN	2.1
1	B	306	THR	2.0
1	M	320	SER	2.0
1	N	328	THR	2.0
1	J	275	GLU	2.0
1	L	74	ASN	2.0
1	R	368	PRO	2.0
1	P	23	GLY	2.0
1	S	268	LYS	2.0
1	A	73	SER	2.0
1	N	73	SER	2.0
1	R	213	SER	2.0
1	S	68	LEU	2.0
1	S	294	LEU	2.0

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

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(\AA^2)	Q<0.9
5	NA	Q	406	1/1	0.78	0.13	52,52,52,52	0
5	NA	B	406	1/1	0.87	0.12	36,36,36,36	0
5	NA	M	406	1/1	0.88	0.22	54,54,54,54	0
5	NA	J	406	1/1	0.88	0.18	40,40,40,40	0
5	NA	N	406	1/1	0.89	0.16	47,47,47,47	0
5	NA	C	407	1/1	0.89	0.07	35,35,35,35	0
5	NA	T	406	1/1	0.90	0.15	45,45,45,45	0
5	NA	R	406	1/1	0.91	0.18	48,48,48,48	0
5	NA	S	406	1/1	0.92	0.09	45,45,45,45	0
2	ADP	R	401	27/27	0.93	0.10	35,48,53,64	0
5	NA	E	406	1/1	0.94	0.13	37,37,37,37	0
2	ADP	S	401	27/27	0.95	0.09	41,55,64,67	0
2	ADP	T	401	27/27	0.95	0.09	30,47,55,60	0
5	NA	K	406	1/1	0.95	0.07	41,41,41,41	0
5	NA	L	406	1/1	0.95	0.09	39,39,39,39	0
5	NA	D	406	1/1	0.95	0.06	26,26,26,26	0
2	ADP	N	401	27/27	0.96	0.08	27,43,50,54	0
2	ADP	P	401	27/27	0.96	0.08	25,39,46,49	0
2	ADP	Q	401	27/27	0.96	0.08	37,48,54,62	0
5	NA	F	406	1/1	0.96	0.17	42,42,42,42	0
5	NA	I	406	1/1	0.96	0.07	37,37,37,37	0
2	ADP	A	401	27/27	0.96	0.08	20,29,36,39	0
2	ADP	I	401	27/27	0.96	0.07	24,33,38,39	0
2	ADP	J	401	27/27	0.96	0.07	27,33,37,39	0
4	PO4	M	405	5/5	0.96	0.06	29,36,36,41	0
4	PO4	N	405	5/5	0.96	0.06	32,34,37,40	0
5	NA	O	406	1/1	0.96	0.09	35,35,35,35	0
4	PO4	S	405	5/5	0.96	0.07	38,47,56,57	0
4	PO4	T	405	5/5	0.96	0.07	33,39,45,51	0
5	NA	A	406	1/1	0.96	0.05	31,31,31,31	0
2	ADP	M	401	27/27	0.96	0.09	31,45,55,60	0
2	ADP	D	401	27/27	0.97	0.07	21,27,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	Q	405	5/5	0.97	0.06	32,42,44,50	0
4	PO4	R	405	5/5	0.97	0.06	40,41,43,43	0
2	ADP	E	401	27/27	0.97	0.06	21,25,32,36	0
2	ADP	O	401	27/27	0.97	0.07	28,39,45,46	0
2	ADP	G	401	27/27	0.97	0.06	20,27,30,32	0
2	ADP	H	401	27/27	0.97	0.07	24,36,41,43	0
5	NA	P	406	1/1	0.97	0.05	41,41,41,41	0
2	ADP	B	401	27/27	0.97	0.06	19,28,32,39	0
2	ADP	C	401	27/27	0.97	0.07	22,27,32,35	0
2	ADP	K	401	27/27	0.97	0.07	22,33,40,41	0
2	ADP	L	401	27/27	0.97	0.07	27,39,45,47	0
2	ADP	F	401	27/27	0.98	0.06	20,33,37,38	0
3	MN	S	404	1/1	0.98	0.03	44,44,44,44	0
5	NA	C	406	1/1	0.98	0.06	25,25,25,25	0
4	PO4	O	405	5/5	0.98	0.05	28,30,34,36	0
4	PO4	P	405	5/5	0.98	0.05	24,37,42,42	0
4	PO4	F	405	5/5	0.98	0.05	26,28,28,29	0
4	PO4	J	405	5/5	0.98	0.05	29,29,30,34	0
5	NA	H	406	1/1	0.98	0.04	28,28,28,28	0
4	PO4	K	405	5/5	0.98	0.07	23,29,31,38	0
4	PO4	L	405	5/5	0.98	0.05	26,30,33,38	0
3	MN	F	402	1/1	0.99	0.03	28,28,28,28	0
3	MN	F	403	1/1	0.99	0.04	25,25,25,25	0
3	MN	I	403	1/1	0.99	0.02	30,30,30,30	0
3	MN	J	403	1/1	0.99	0.02	30,30,30,30	0
3	MN	J	404	1/1	0.99	0.02	27,27,27,27	0
3	MN	K	402	1/1	0.99	0.02	28,28,28,28	0
3	MN	K	403	1/1	0.99	0.02	34,34,34,34	0
3	MN	L	402	1/1	0.99	0.02	31,31,31,31	0
3	MN	M	402	1/1	0.99	0.02	35,35,35,35	0
3	MN	N	403	1/1	0.99	0.03	40,40,40,40	0
3	MN	O	402	1/1	0.99	0.02	32,32,32,32	0
3	MN	O	403	1/1	0.99	0.02	31,31,31,31	0
3	MN	Q	402	1/1	0.99	0.03	36,36,36,36	0
3	MN	Q	404	1/1	0.99	0.02	42,42,42,42	0
3	MN	R	402	1/1	0.99	0.02	42,42,42,42	0
3	MN	R	404	1/1	0.99	0.03	37,37,37,37	0
3	MN	S	402	1/1	0.99	0.03	40,40,40,40	0
3	MN	S	403	1/1	0.99	0.03	45,45,45,45	0
5	NA	G	406	1/1	0.99	0.09	33,33,33,33	0
3	MN	A	402	1/1	0.99	0.01	24,24,24,24	0
3	MN	T	402	1/1	0.99	0.03	38,38,38,38	0

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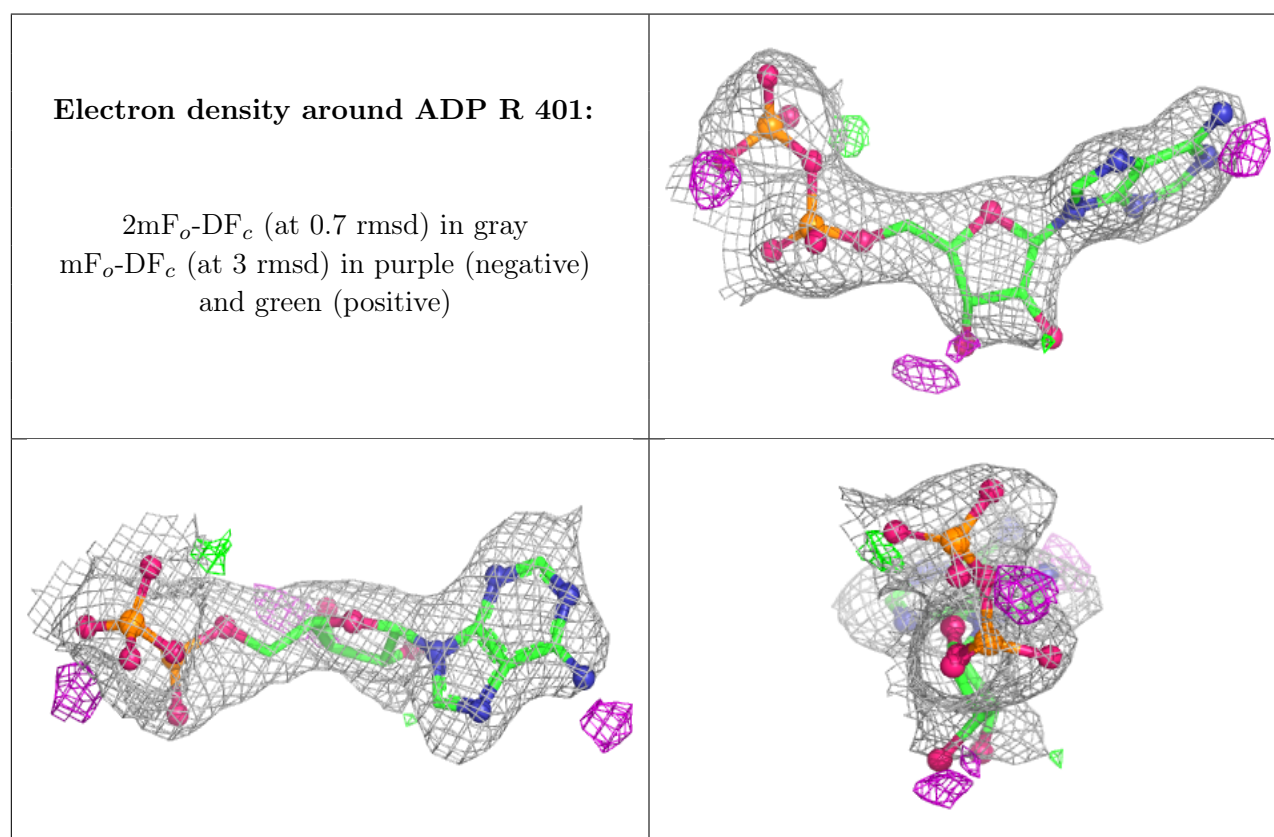
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MN	T	403	1/1	0.99	0.04	40,40,40,40	0
3	MN	T	404	1/1	0.99	0.02	38,38,38,38	0
4	PO4	A	405	5/5	0.99	0.04	24,26,28,28	0
4	PO4	B	405	5/5	0.99	0.04	24,25,27,33	0
4	PO4	C	405	5/5	0.99	0.04	25,26,26,28	0
4	PO4	D	405	5/5	0.99	0.04	22,24,27,30	0
4	PO4	E	405	5/5	0.99	0.05	22,23,31,32	0
3	MN	E	403	1/1	0.99	0.02	25,25,25,25	0
4	PO4	G	405	5/5	0.99	0.03	22,24,26,28	0
4	PO4	H	405	5/5	0.99	0.05	25,27,28,30	0
4	PO4	I	405	5/5	0.99	0.04	28,28,32,38	0
3	MN	C	402	1/1	1.00	0.01	23,23,23,23	0
3	MN	C	403	1/1	1.00	0.03	25,25,25,25	0
3	MN	C	404	1/1	1.00	0.02	23,23,23,23	0
3	MN	K	404	1/1	1.00	0.01	29,29,29,29	0
3	MN	D	402	1/1	1.00	0.01	24,24,24,24	0
3	MN	L	403	1/1	1.00	0.03	34,34,34,34	0
3	MN	L	404	1/1	1.00	0.02	29,29,29,29	0
3	MN	D	403	1/1	1.00	0.02	28,28,28,28	0
3	MN	M	403	1/1	1.00	0.03	37,37,37,37	0
3	MN	M	404	1/1	1.00	0.03	31,31,31,31	0
3	MN	N	402	1/1	1.00	0.01	37,37,37,37	0
3	MN	D	404	1/1	1.00	0.02	22,22,22,22	0
3	MN	N	404	1/1	1.00	0.02	31,31,31,31	0
3	MN	E	402	1/1	1.00	0.01	26,26,26,26	0
3	MN	A	403	1/1	1.00	0.02	27,27,27,27	0
3	MN	O	404	1/1	1.00	0.02	32,32,32,32	0
3	MN	P	402	1/1	1.00	0.01	37,37,37,37	0
3	MN	P	403	1/1	1.00	0.03	37,37,37,37	0
3	MN	P	404	1/1	1.00	0.02	34,34,34,34	0
3	MN	E	404	1/1	1.00	0.02	23,23,23,23	0
3	MN	Q	403	1/1	1.00	0.03	43,43,43,43	0
3	MN	A	404	1/1	1.00	0.01	21,21,21,21	0
3	MN	B	402	1/1	1.00	0.02	24,24,24,24	0
3	MN	R	403	1/1	1.00	0.02	39,39,39,39	0
3	MN	F	404	1/1	1.00	0.02	26,26,26,26	0
3	MN	G	402	1/1	1.00	0.01	23,23,23,23	0
3	MN	G	403	1/1	1.00	0.03	28,28,28,28	0
3	MN	G	404	1/1	1.00	0.01	23,23,23,23	0
3	MN	H	402	1/1	1.00	0.01	28,28,28,28	0
3	MN	H	403	1/1	1.00	0.04	29,29,29,29	0
3	MN	H	404	1/1	1.00	0.02	26,26,26,26	0

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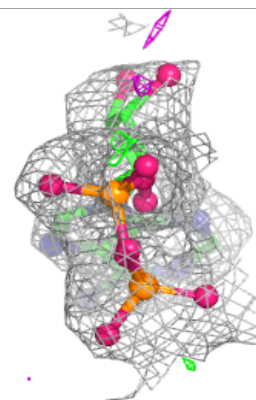
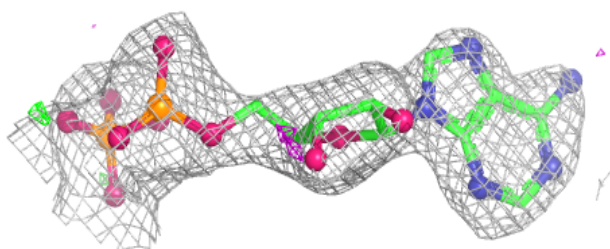
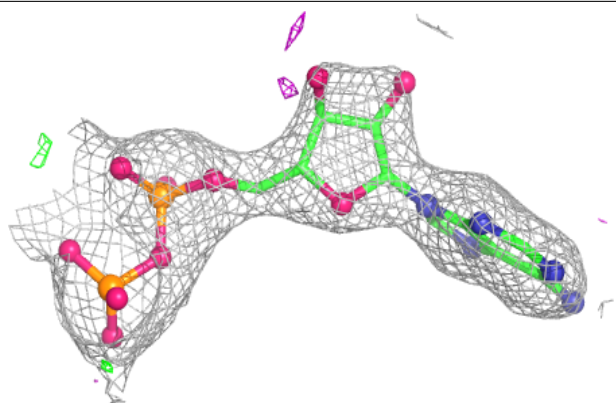
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MN	I	402	1/1	1.00	0.01	27,27,27,27	0
3	MN	B	403	1/1	1.00	0.03	23,23,23,23	0
3	MN	I	404	1/1	1.00	0.01	28,28,28,28	0
3	MN	J	402	1/1	1.00	0.01	28,28,28,28	0
3	MN	B	404	1/1	1.00	0.01	23,23,23,23	0

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.

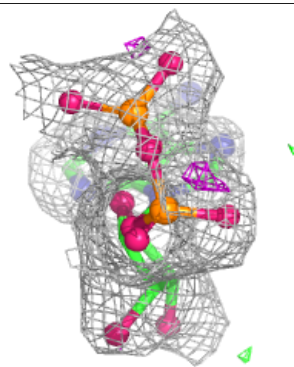
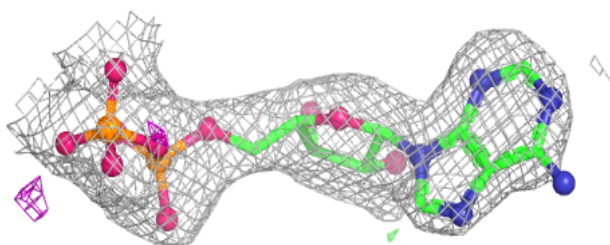
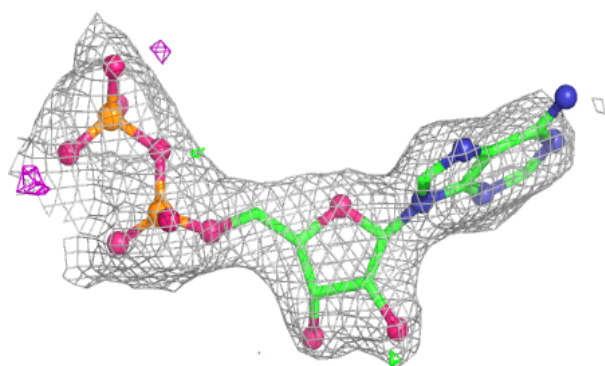


Electron density around ADP S 401:

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

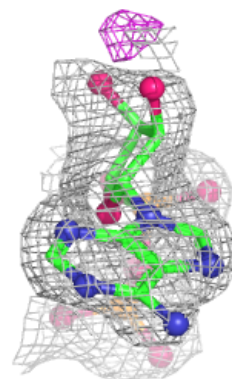
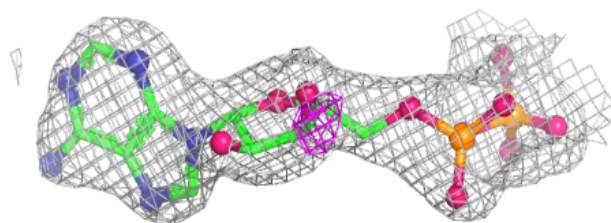
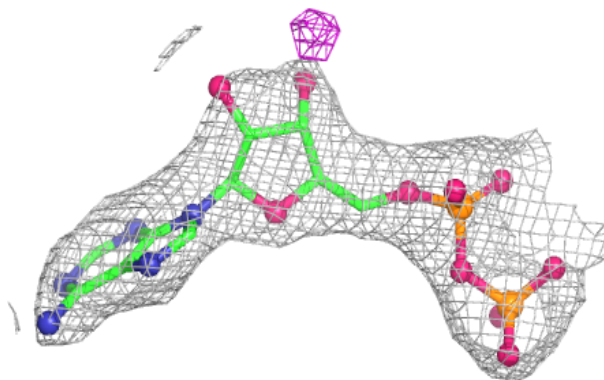
**Electron density around ADP T 401:**

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

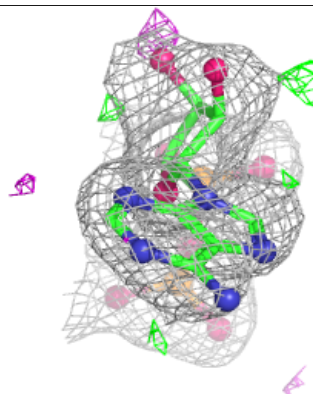
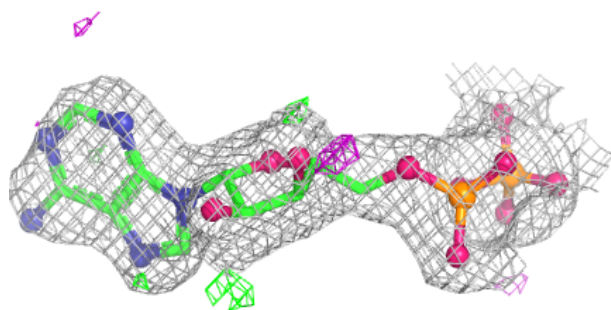
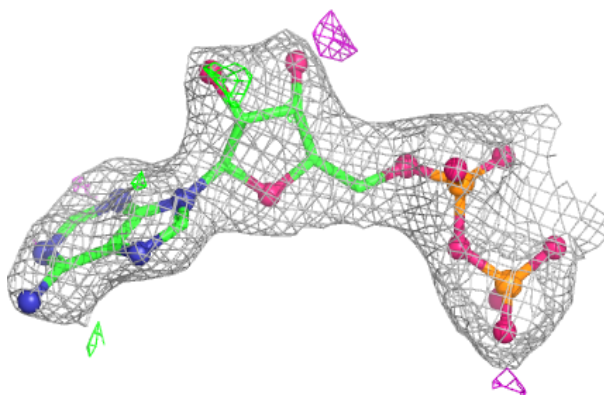


Electron density around ADP N 401:

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

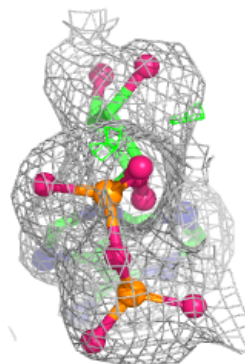
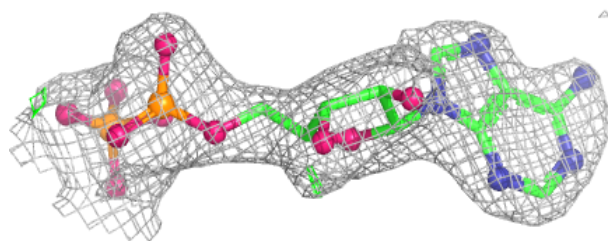
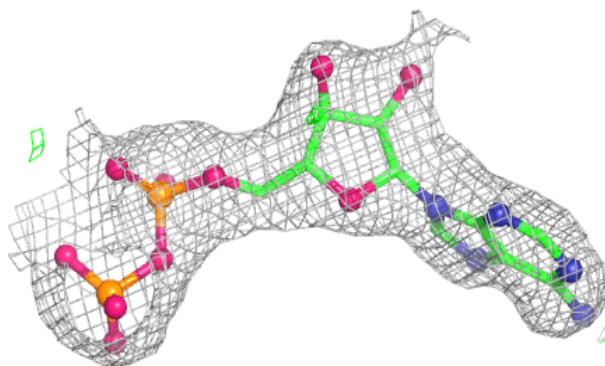
**Electron density around ADP P 401:**

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

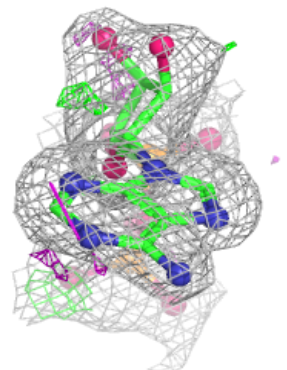
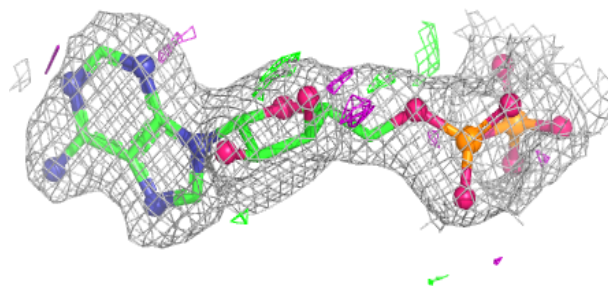
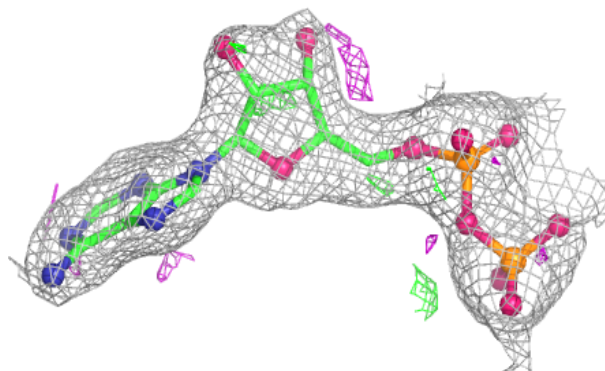


Electron density around ADP Q 401:

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

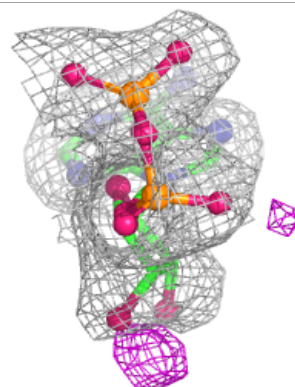
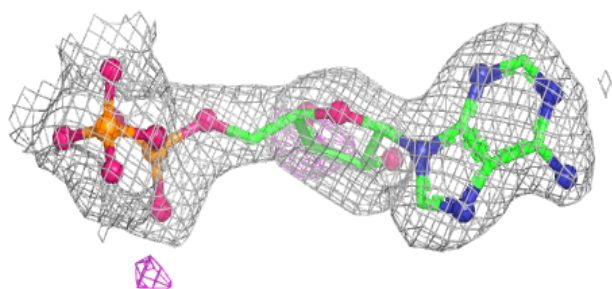
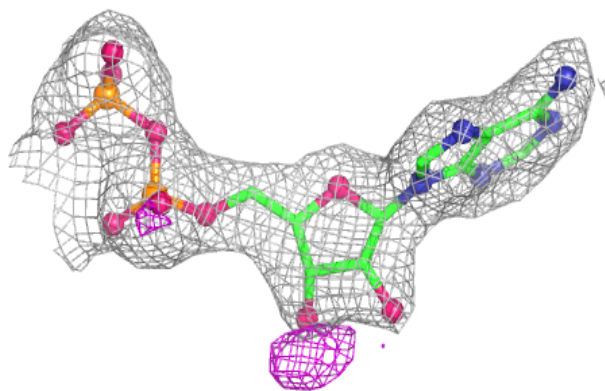
**Electron density around ADP A 401:**

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

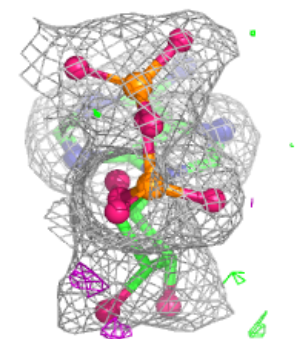
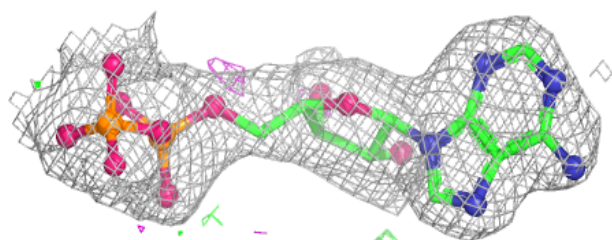
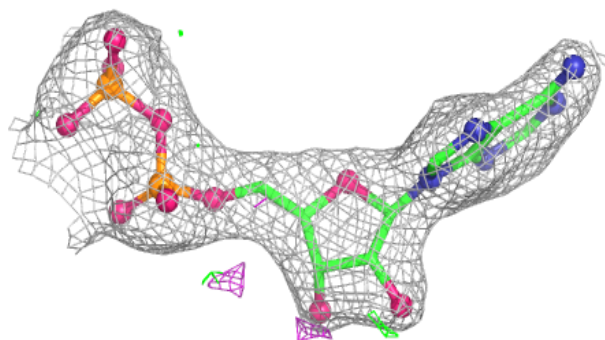


Electron density around ADP I 401:

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

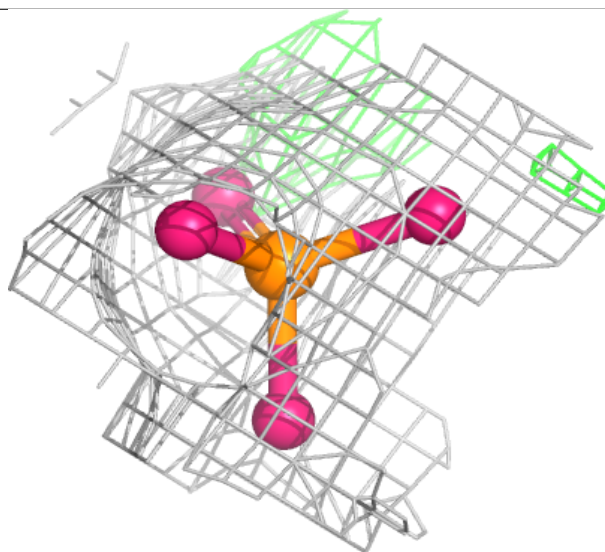
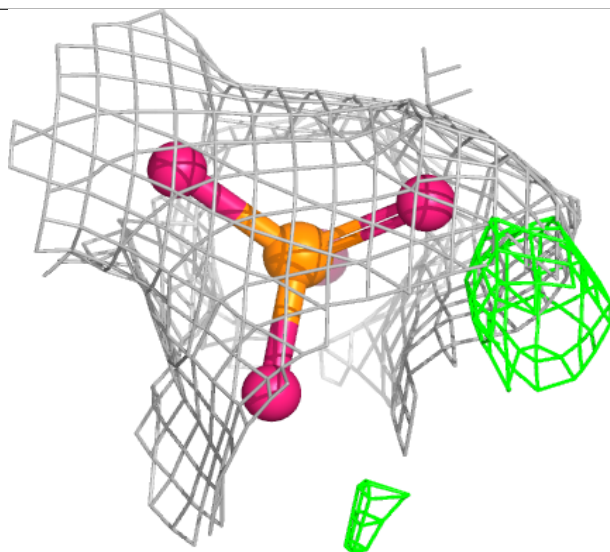
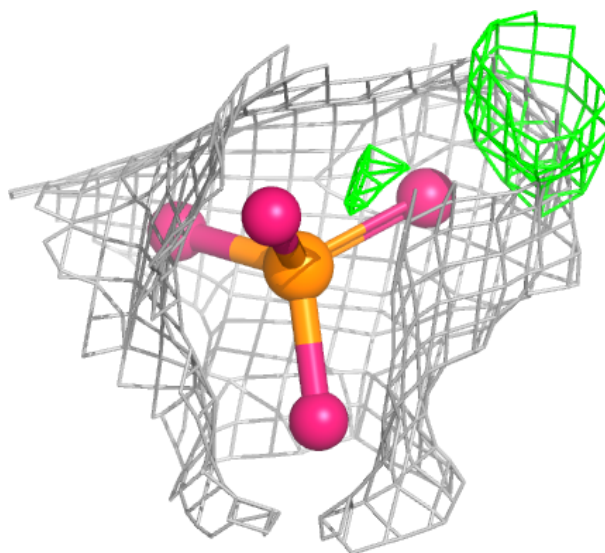
**Electron density around ADP J 401:**

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



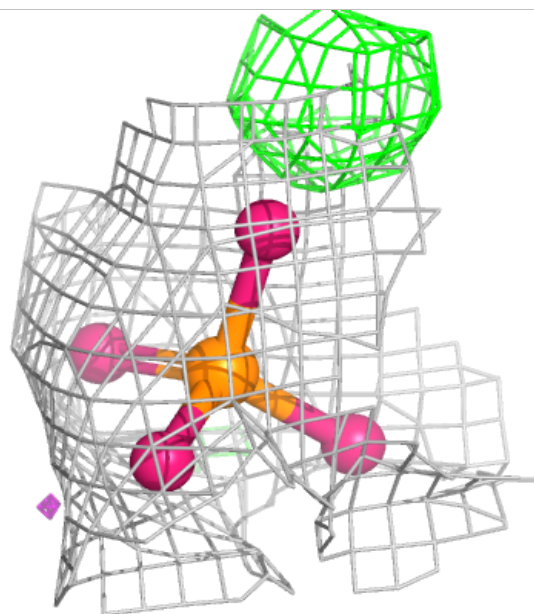
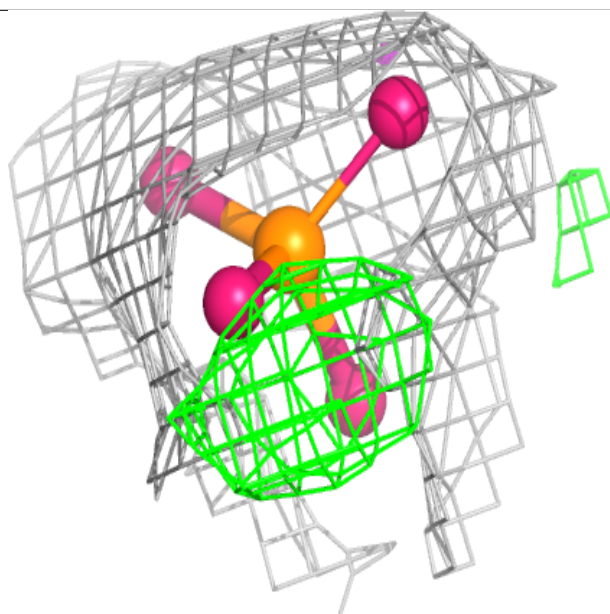
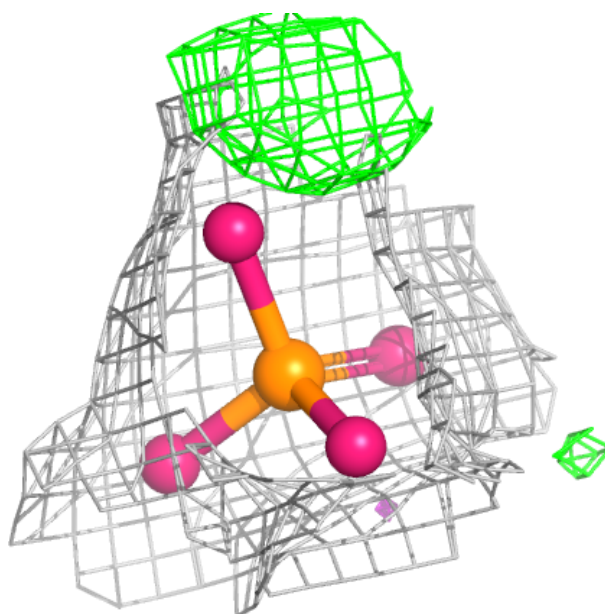
Electron density around PO4 M 405:

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



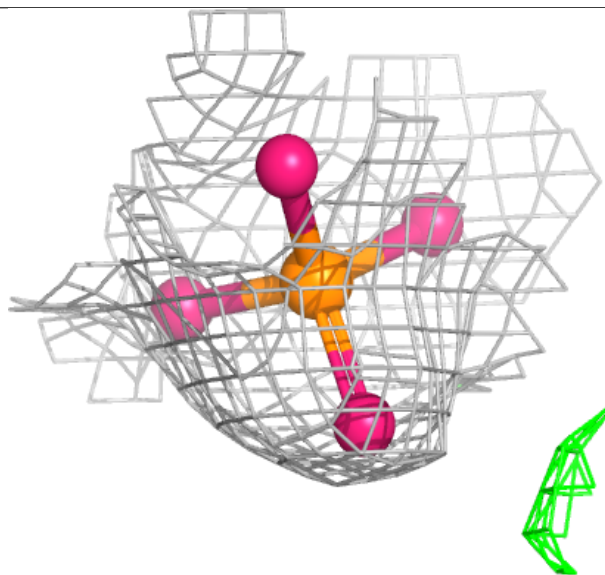
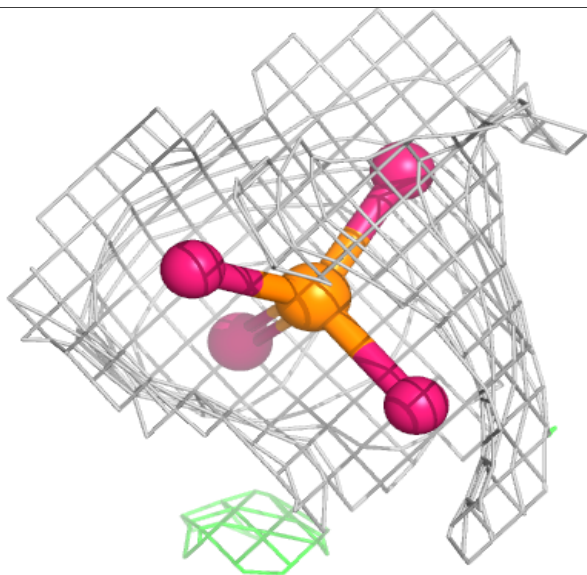
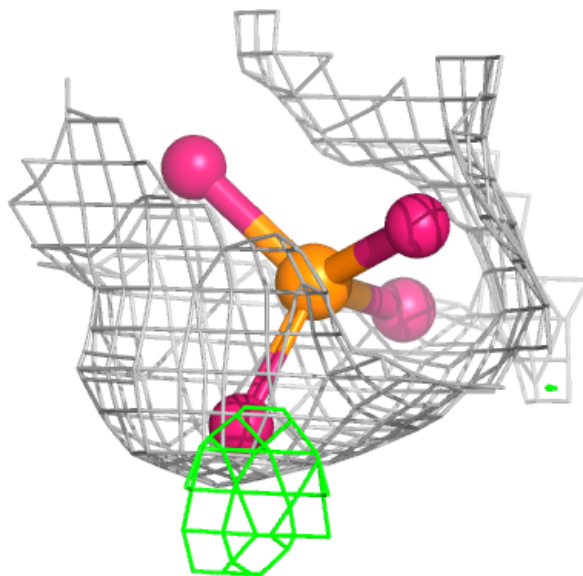
Electron density around PO4 N 405:

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



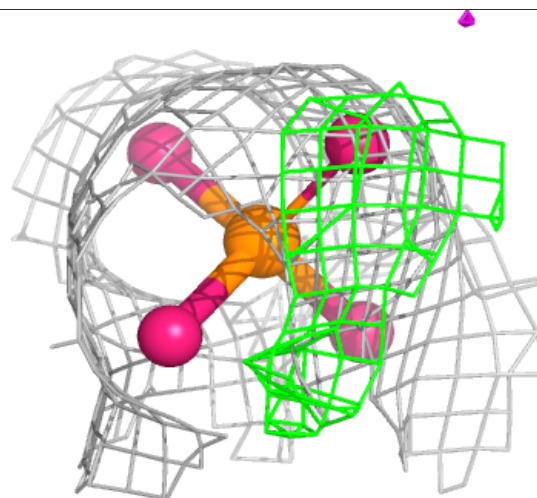
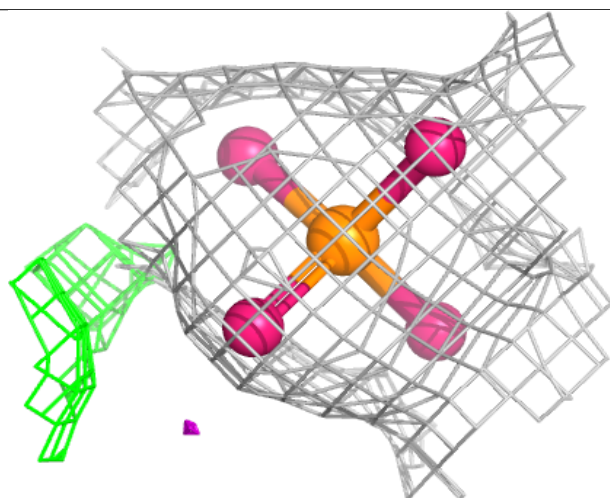
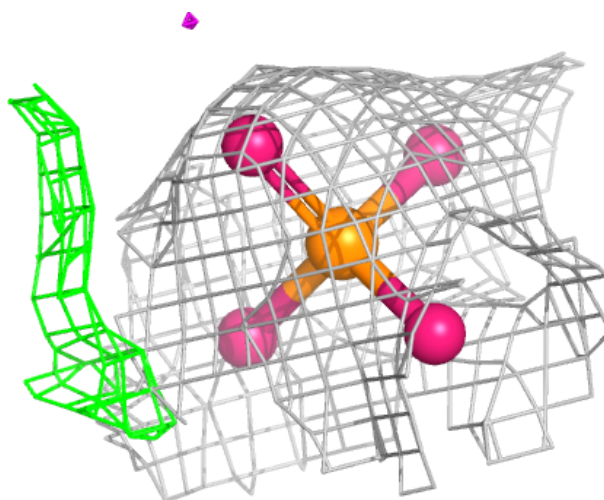
Electron density around PO4 S 405:

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



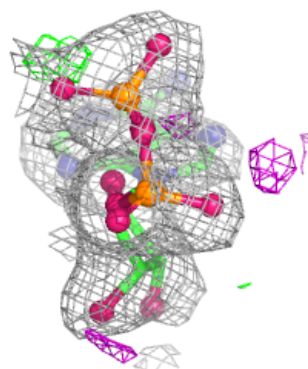
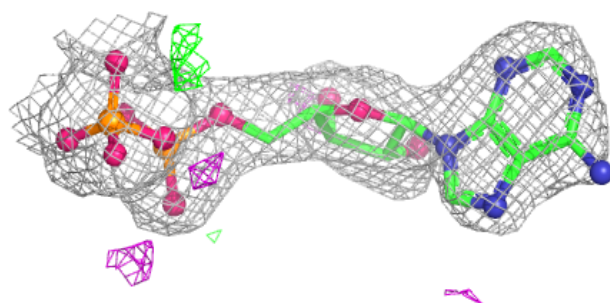
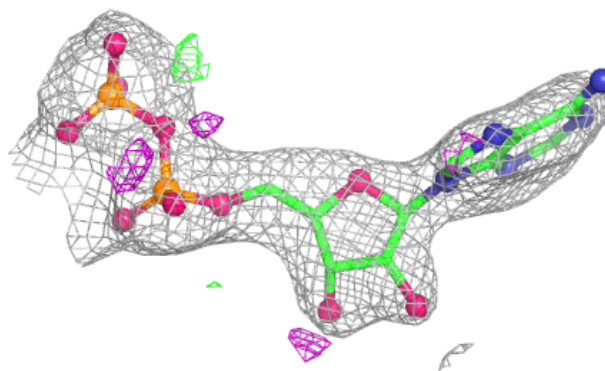
Electron density around PO4 T 405:

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

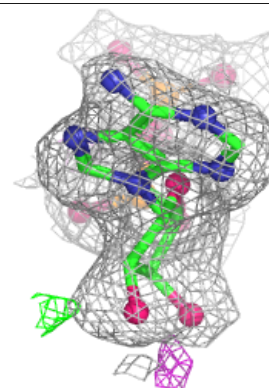
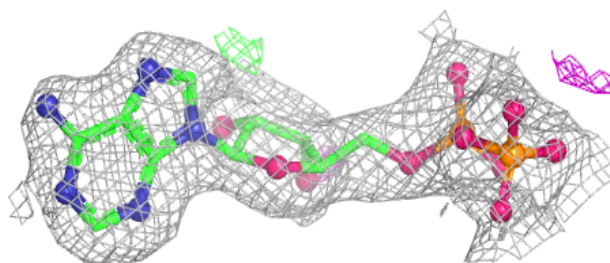
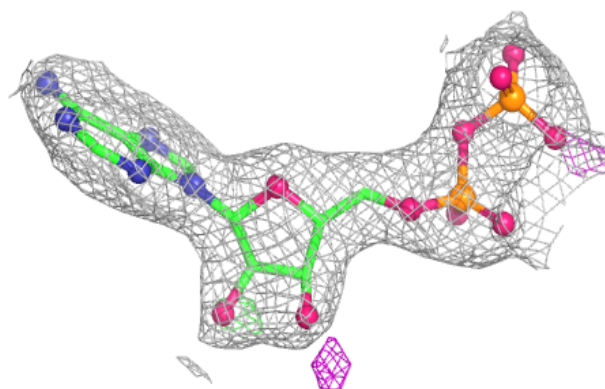


Electron density around ADP M 401:

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

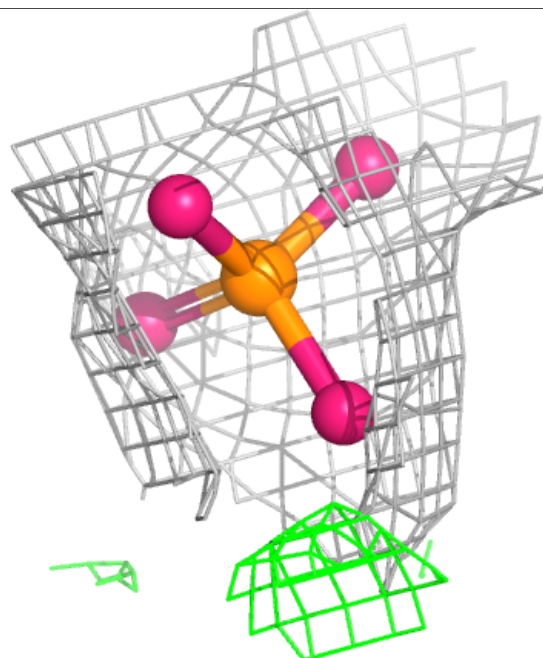
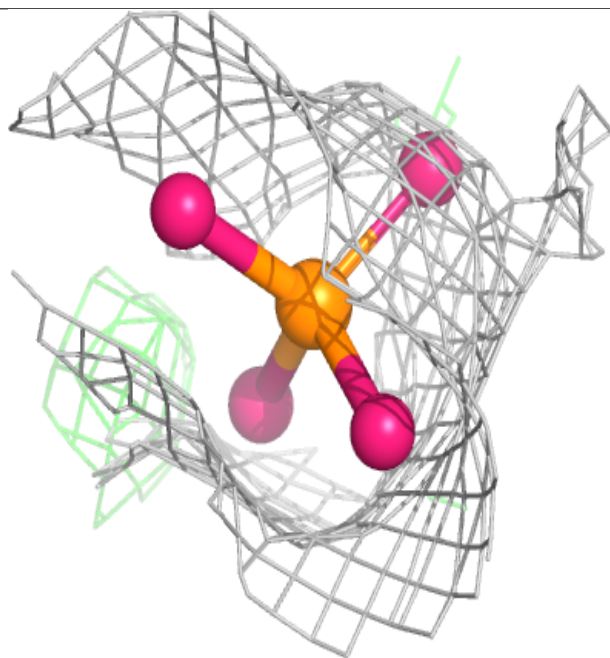
**Electron density around ADP D 401:**

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



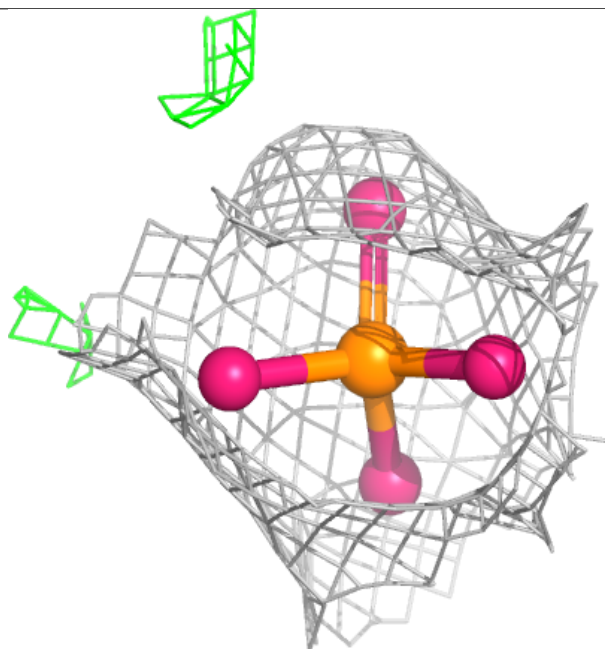
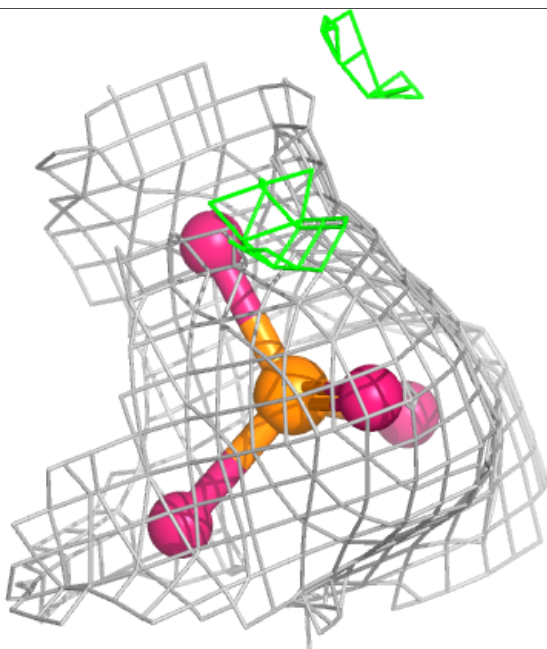
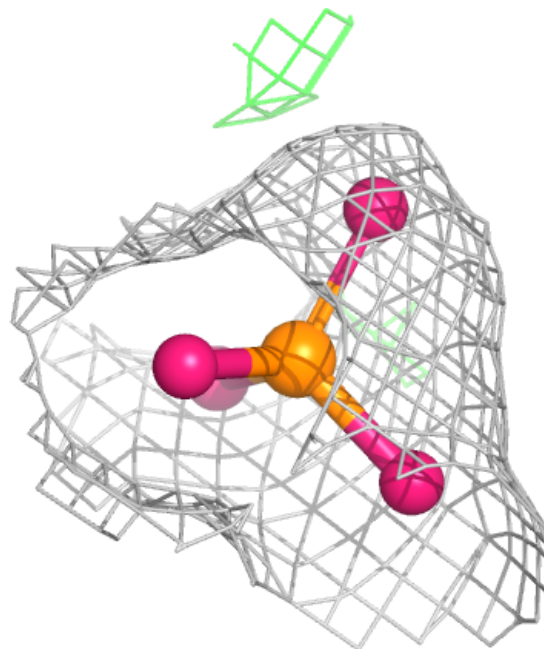
Electron density around PO4 Q 405:

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



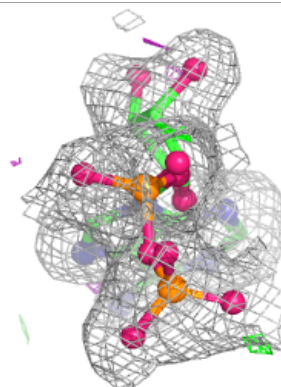
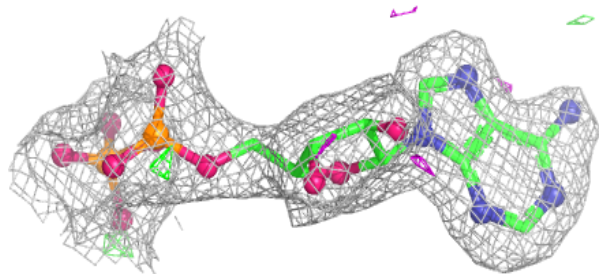
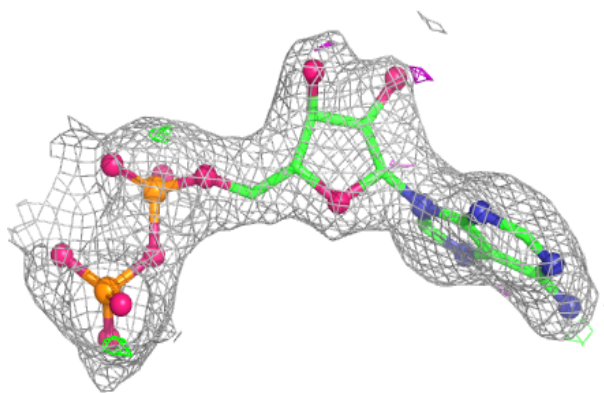
Electron density around PO4 R 405:

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

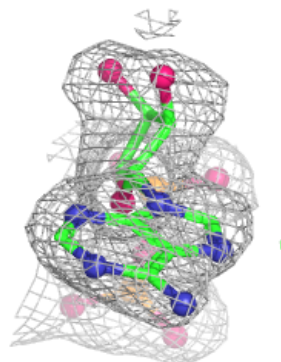
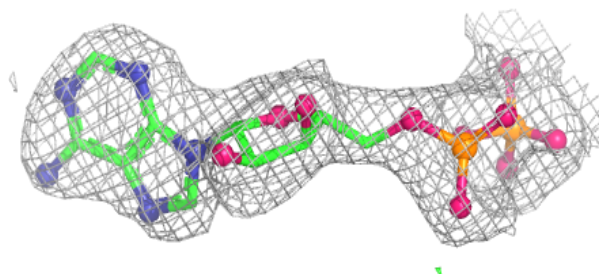
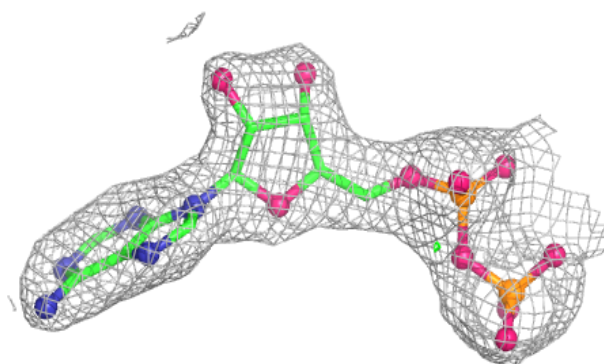


Electron density around ADP E 401:

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

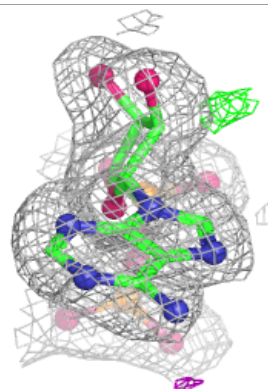
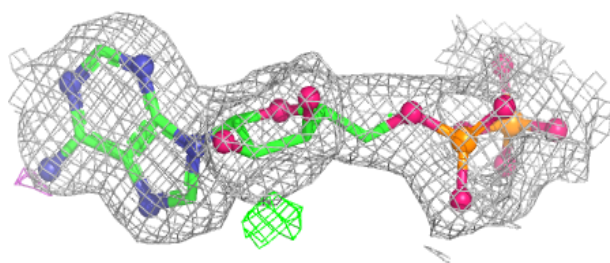
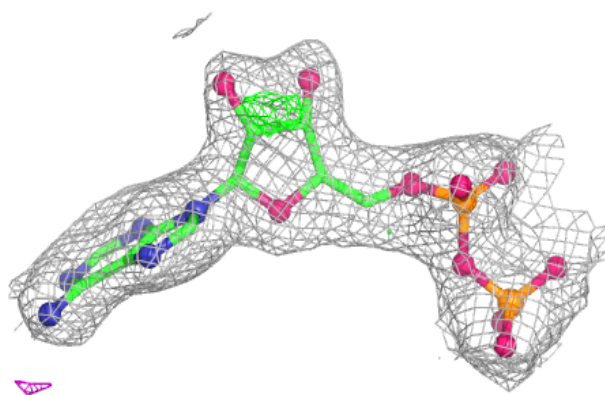
**Electron density around ADP O 401:**

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

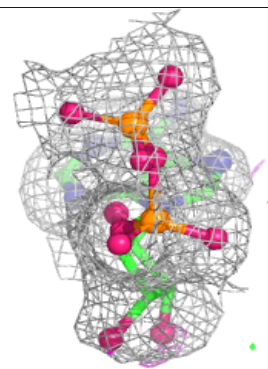
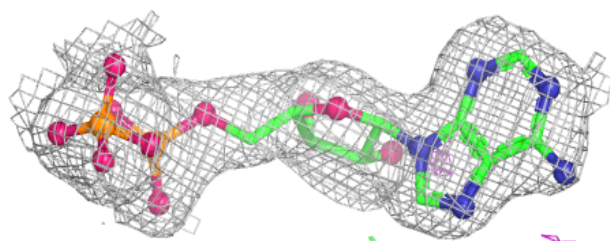
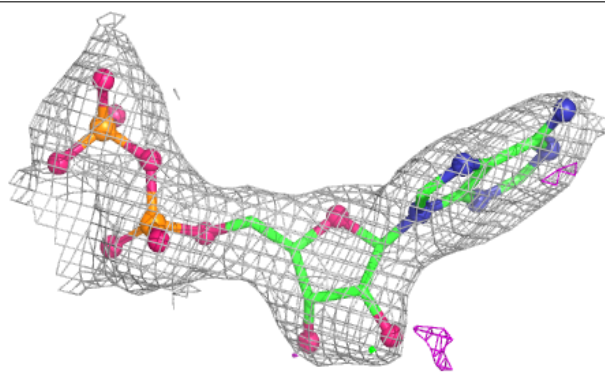


Electron density around ADP G 401:

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

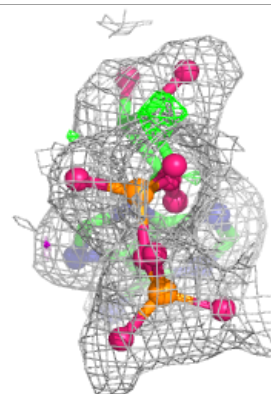
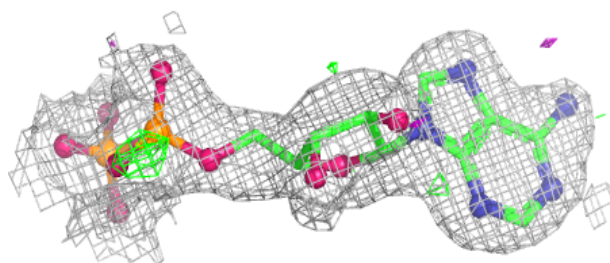
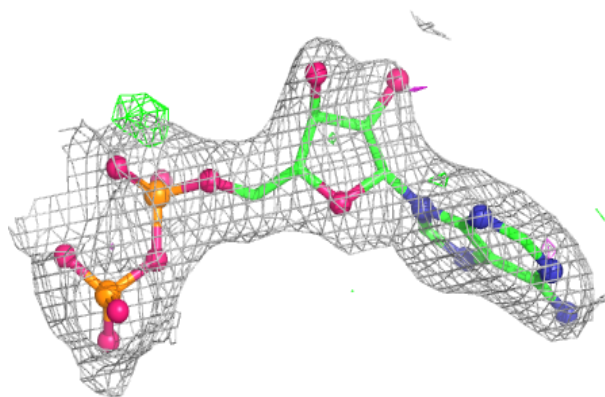
**Electron density around ADP H 401:**

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

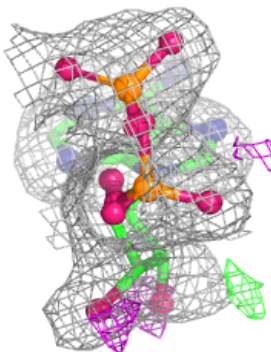
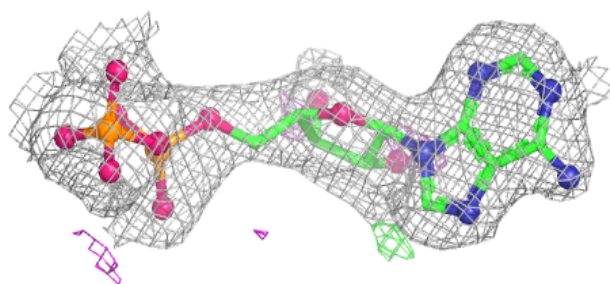
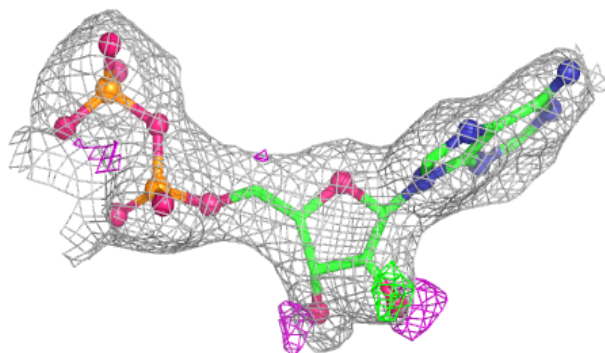


Electron density around ADP B 401:

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

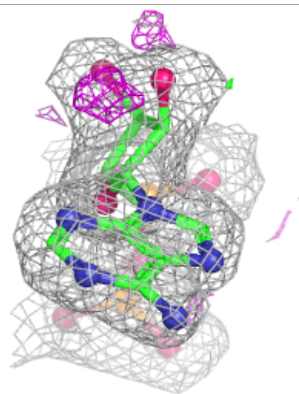
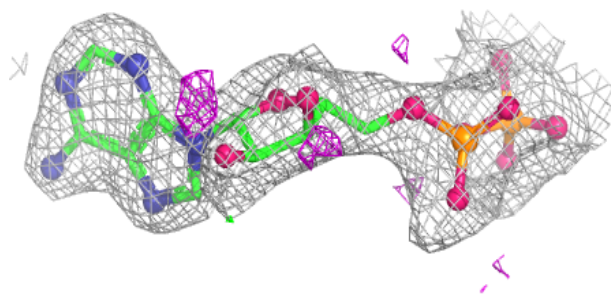
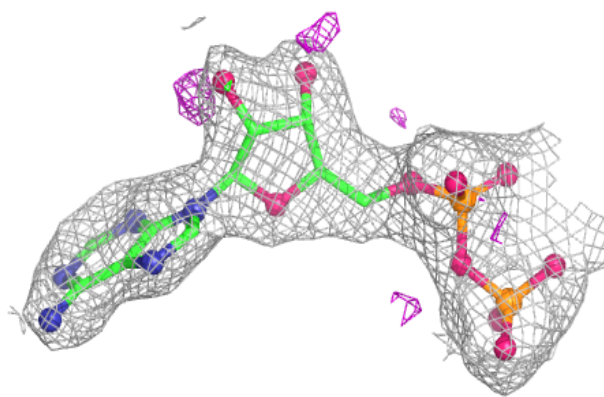
**Electron density around ADP C 401:**

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

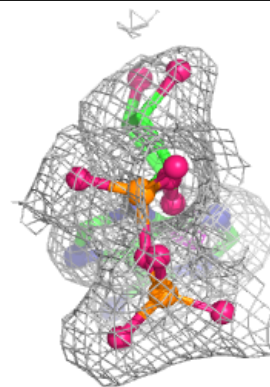
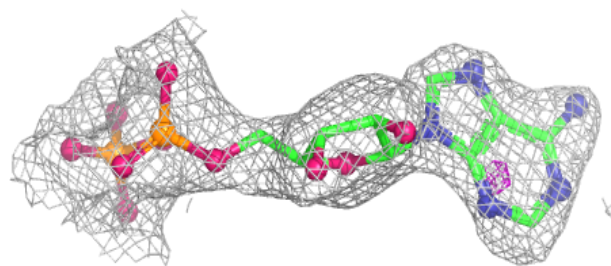
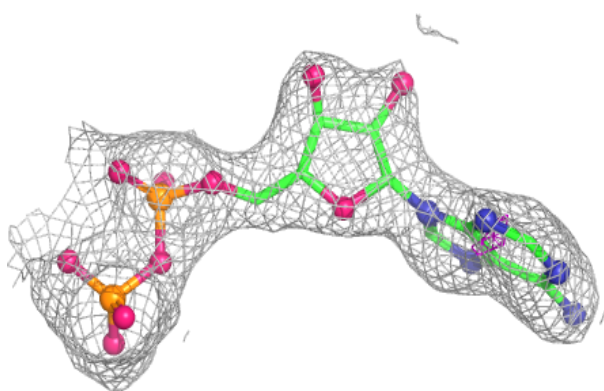


Electron density around ADP K 401:

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

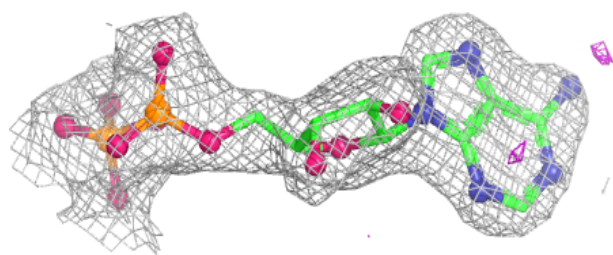
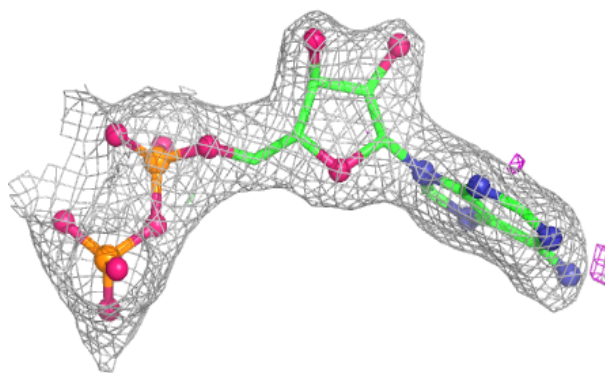
**Electron density around ADP L 401:**

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



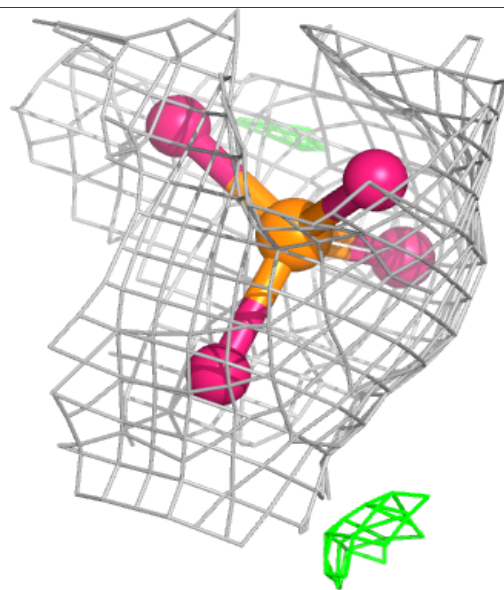
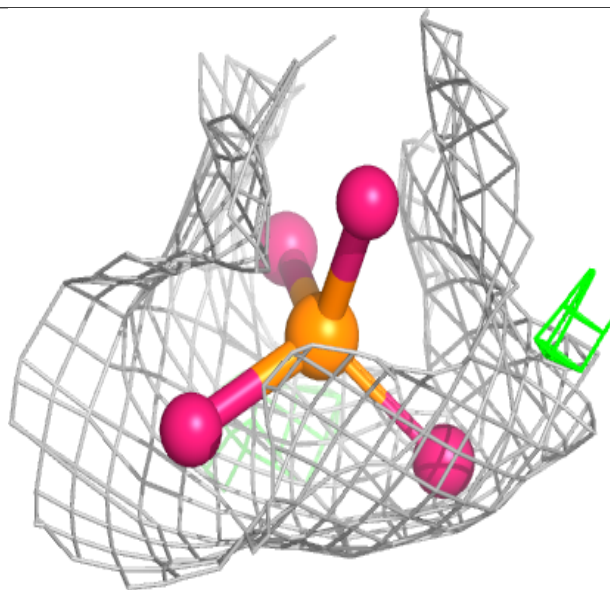
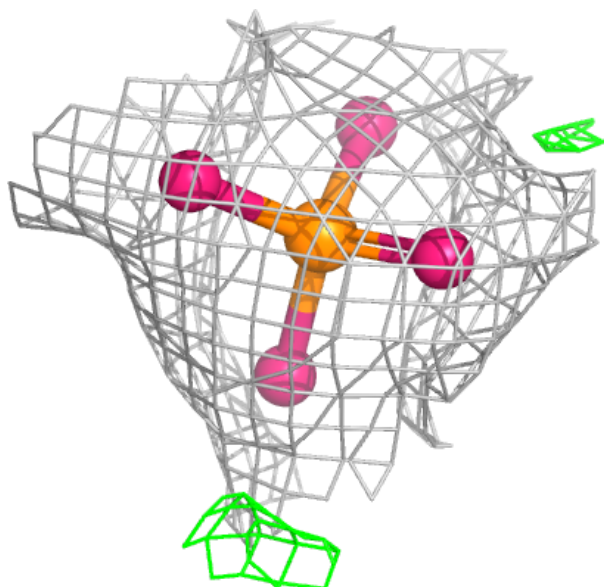
Electron density around ADP F 401:

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



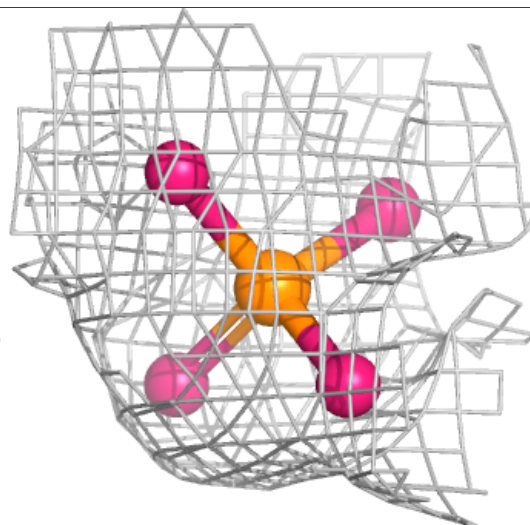
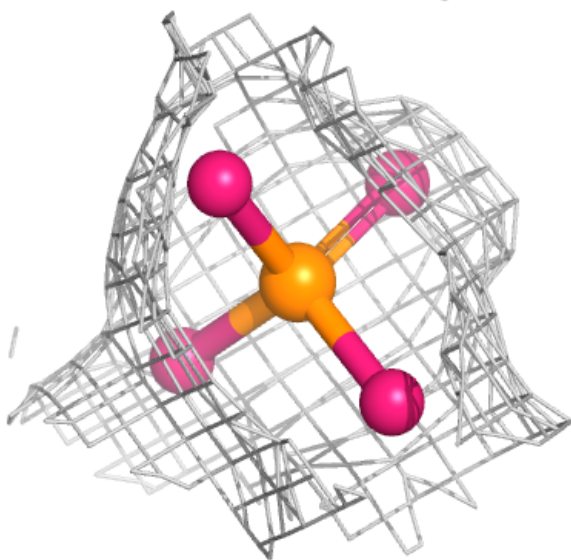
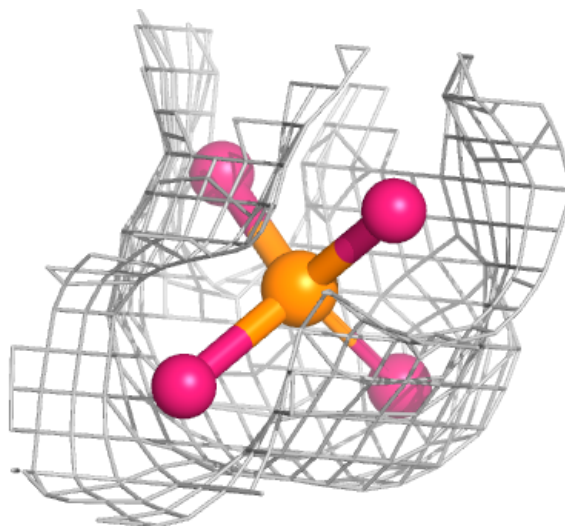
Electron density around PO4 O 405:

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



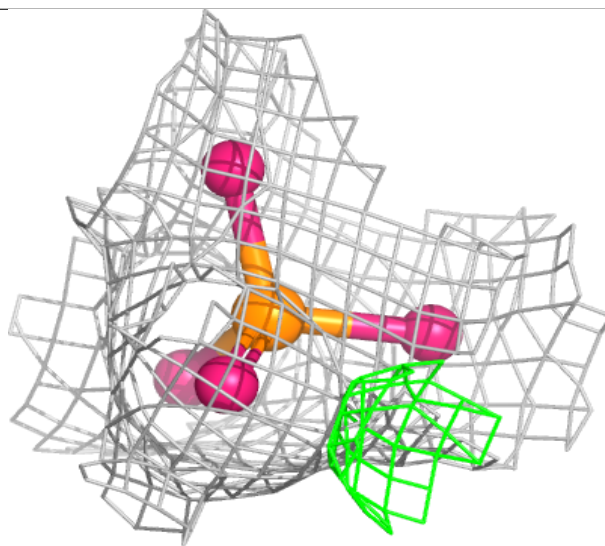
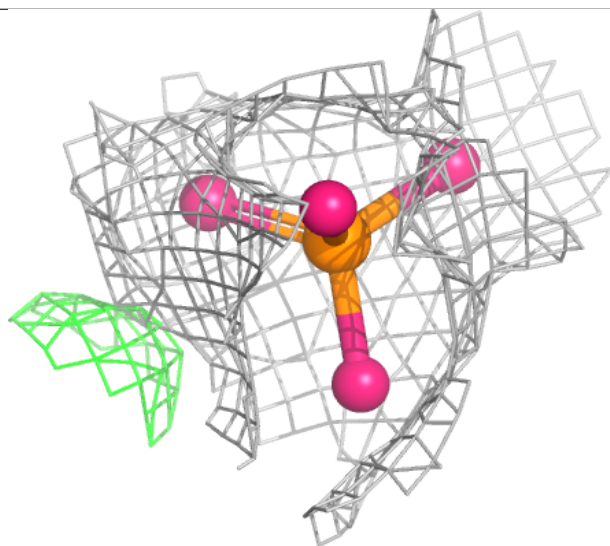
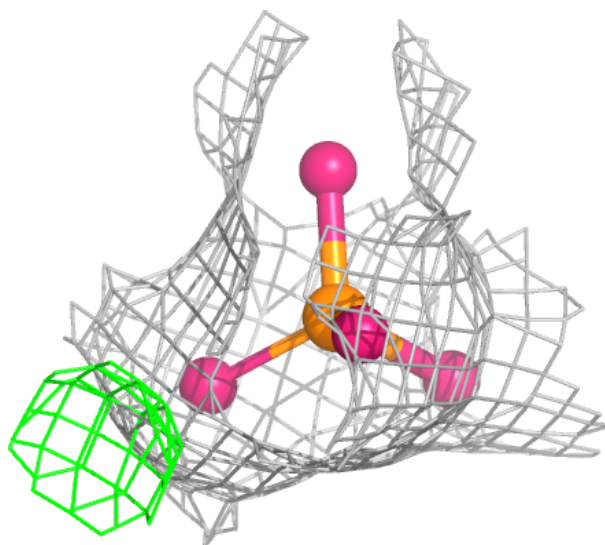
Electron density around PO4 P 405:

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



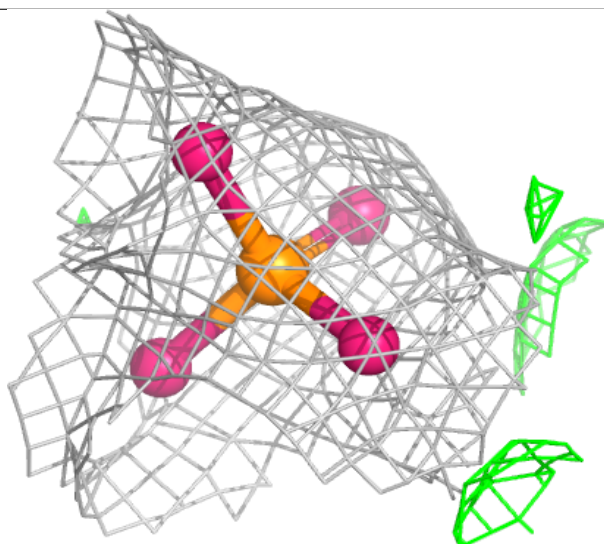
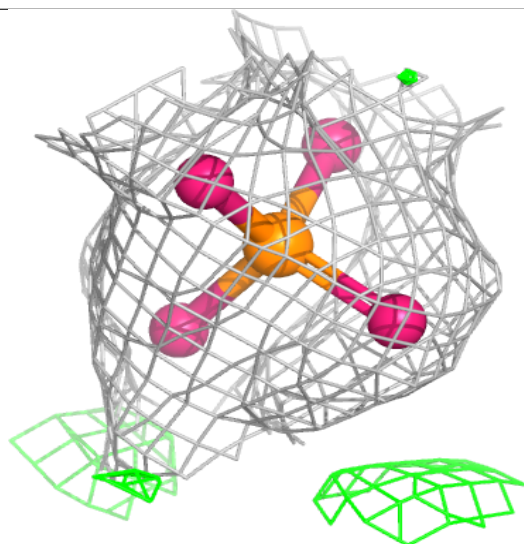
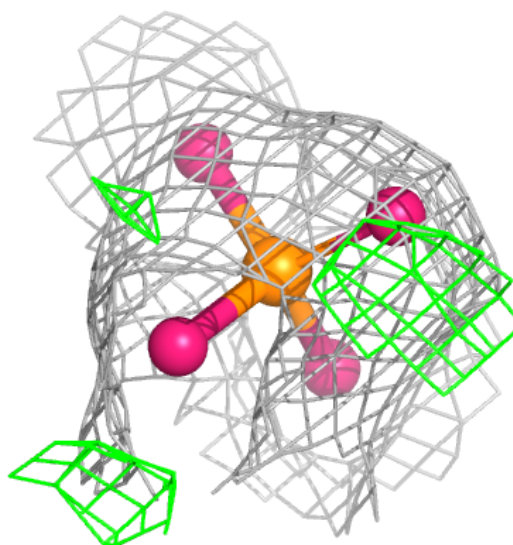
Electron density around PO4 F 405:

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



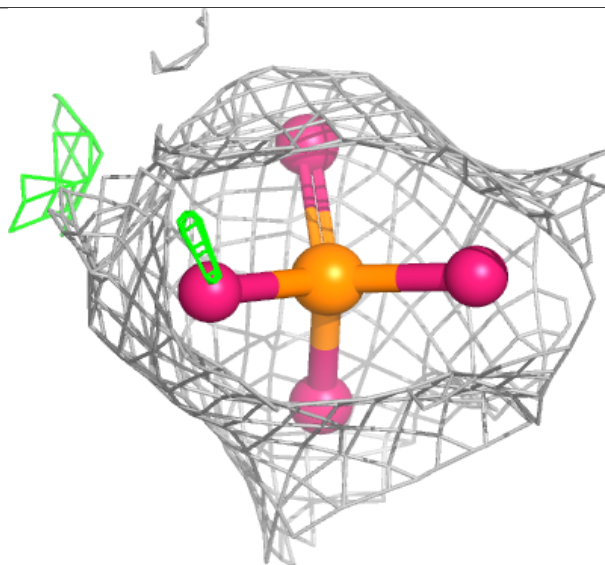
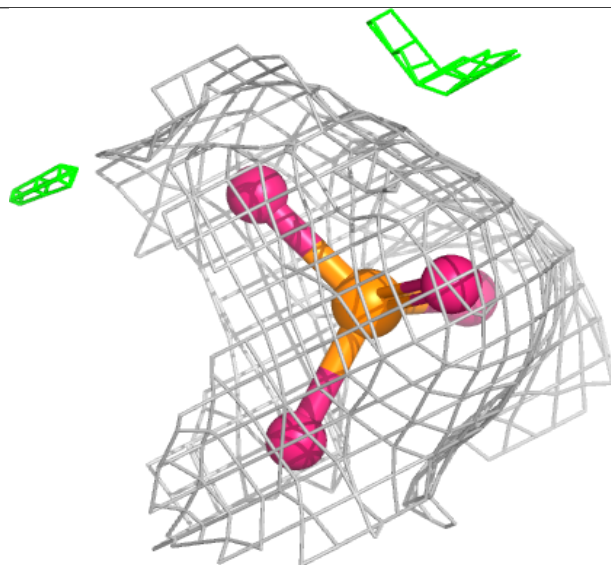
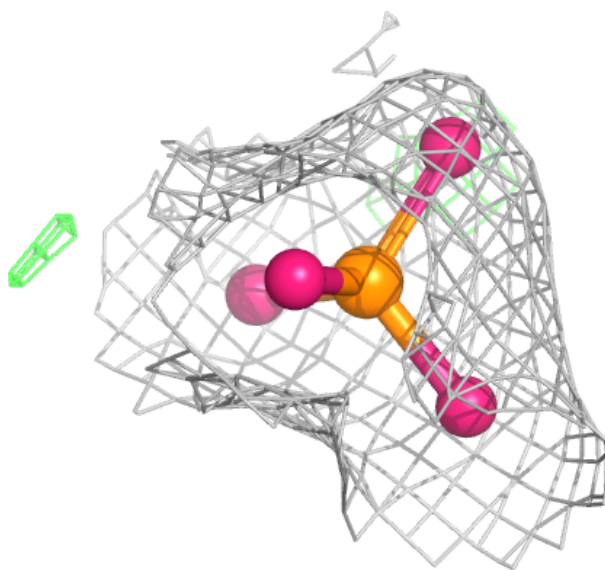
Electron density around PO4 J 405:

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



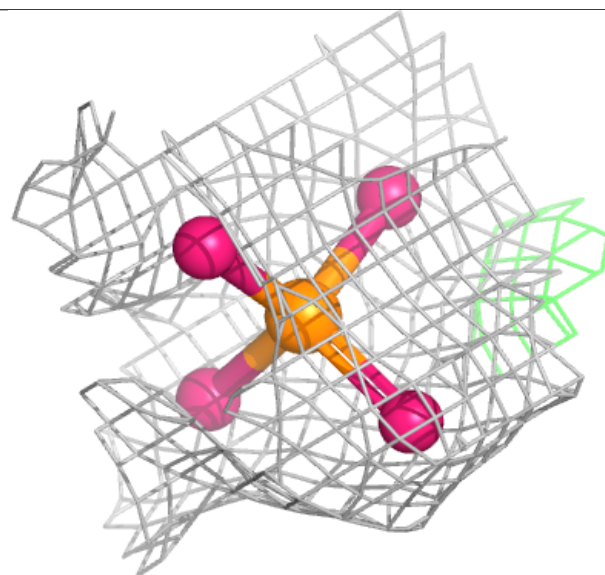
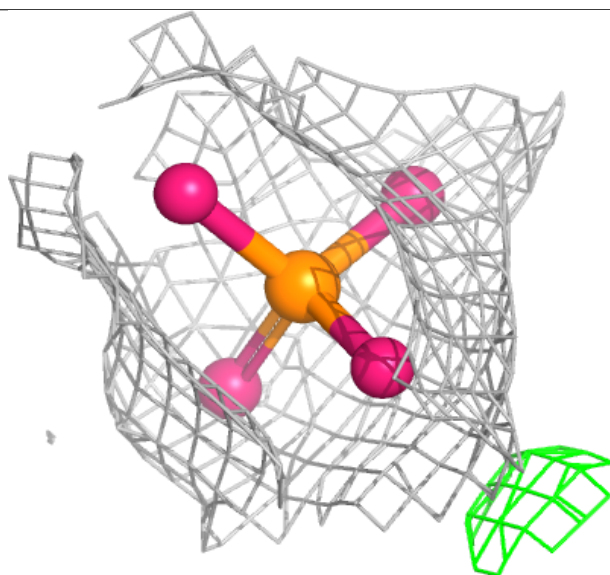
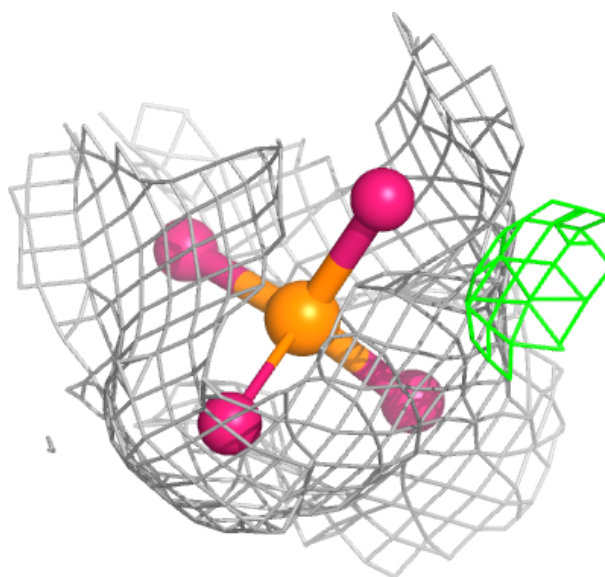
Electron density around PO4 K 405:

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



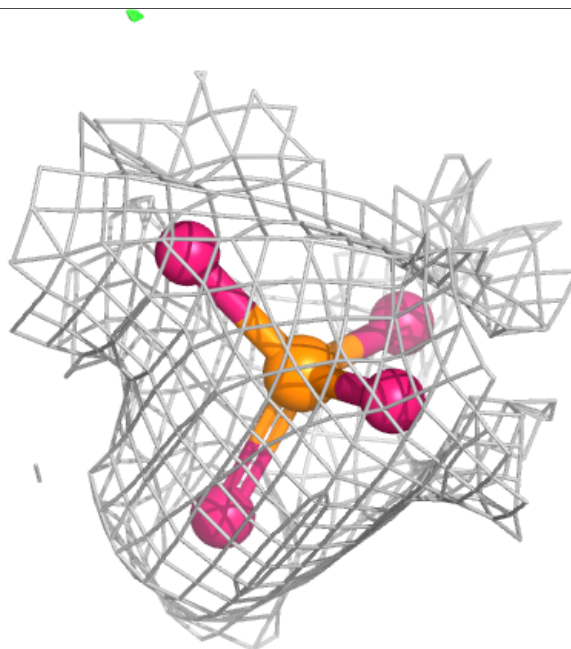
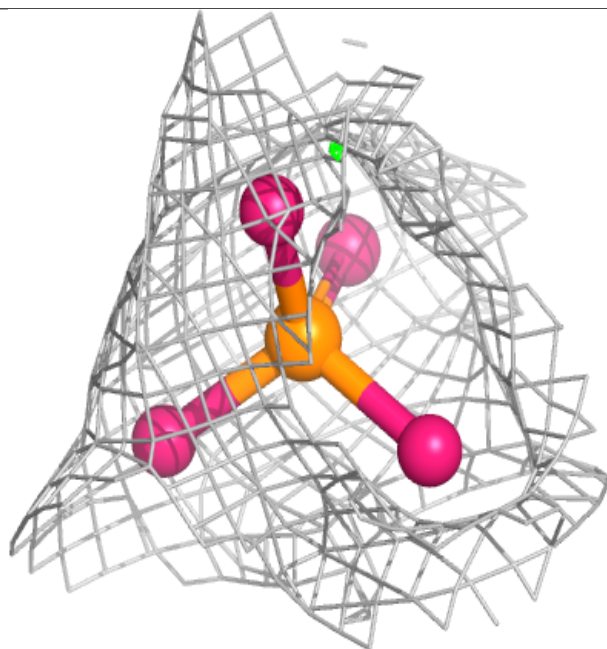
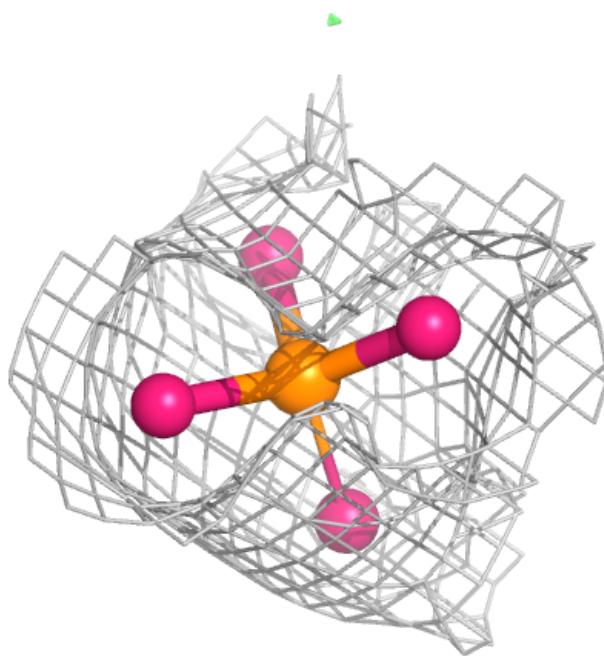
Electron density around PO4 L 405:

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



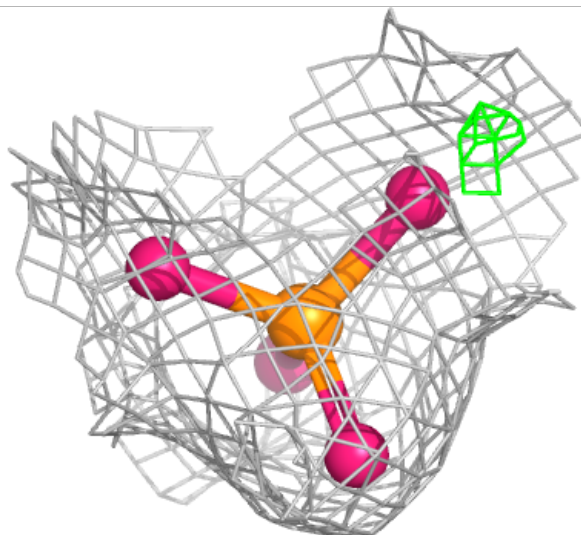
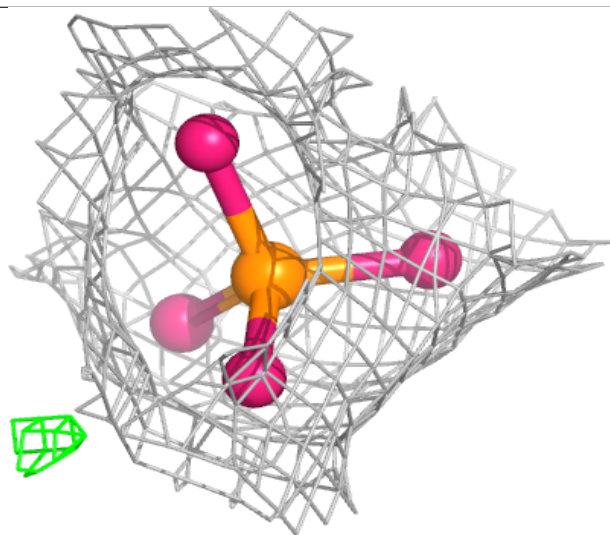
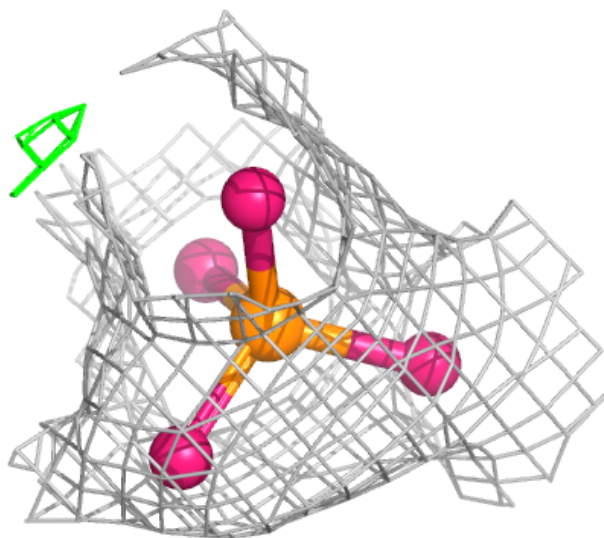
Electron density around PO4 A 405:

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



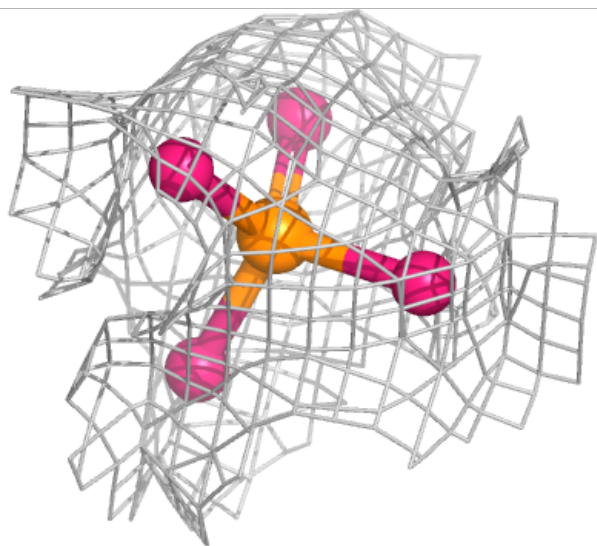
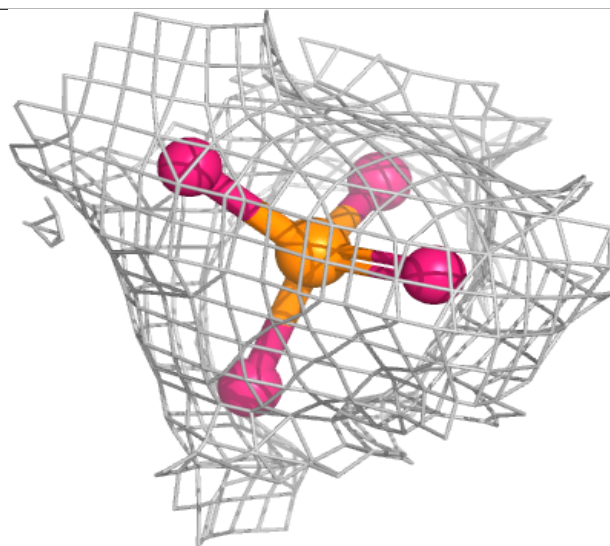
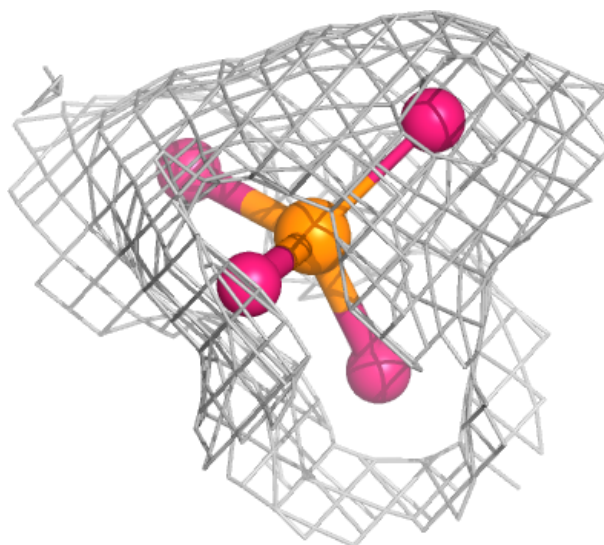
Electron density around PO4 B 405:

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



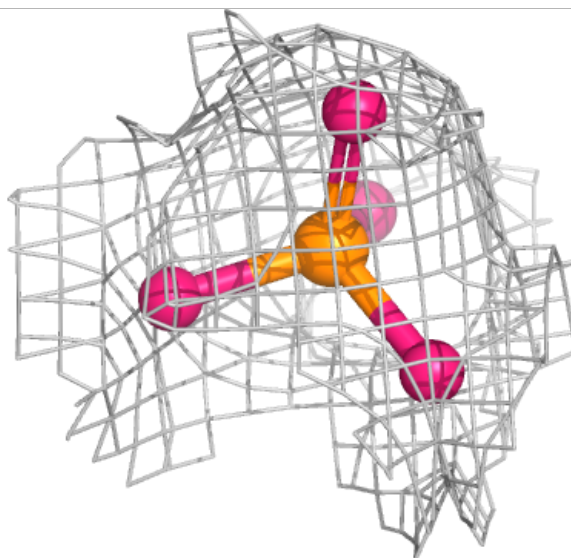
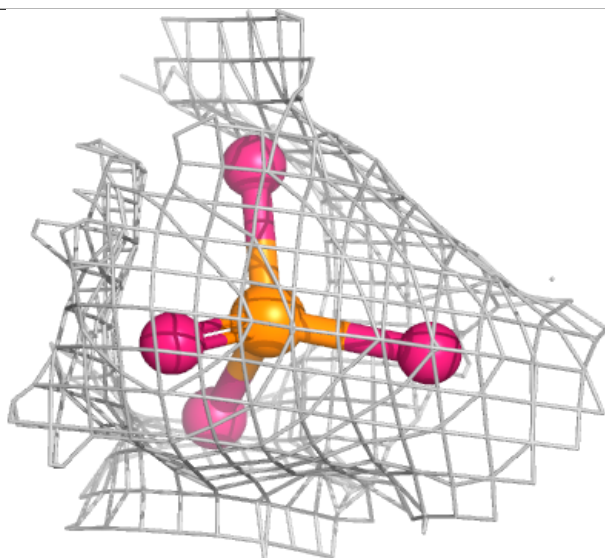
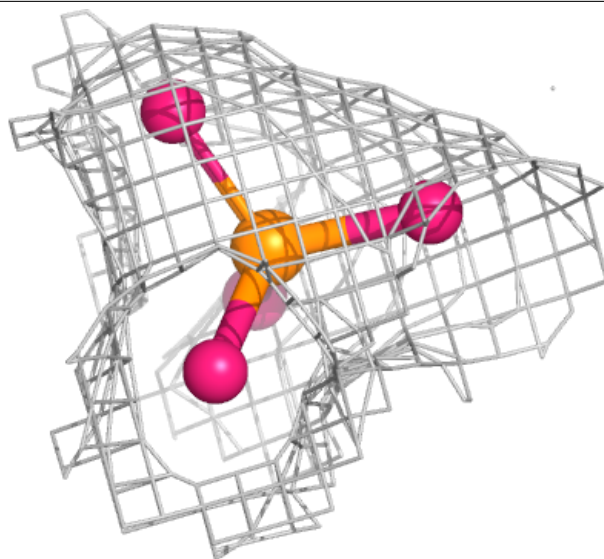
Electron density around PO4 C 405:

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



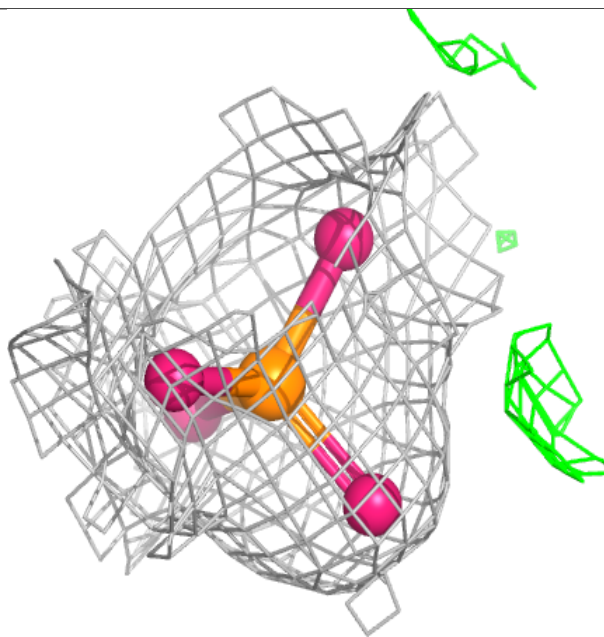
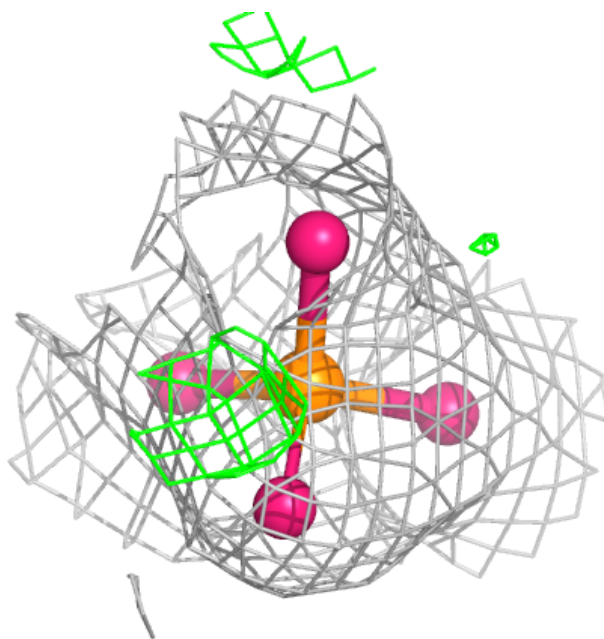
Electron density around PO4 D 405:

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



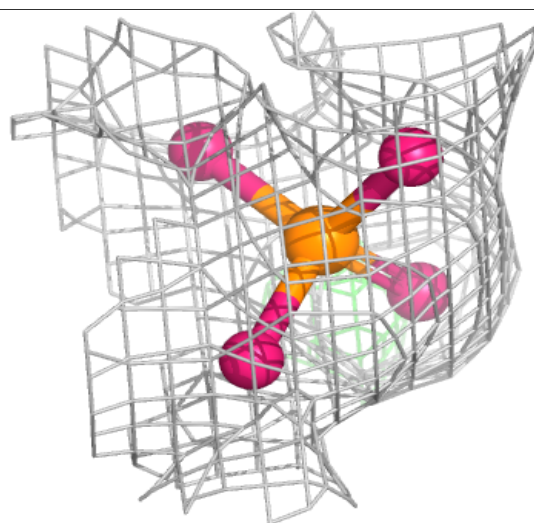
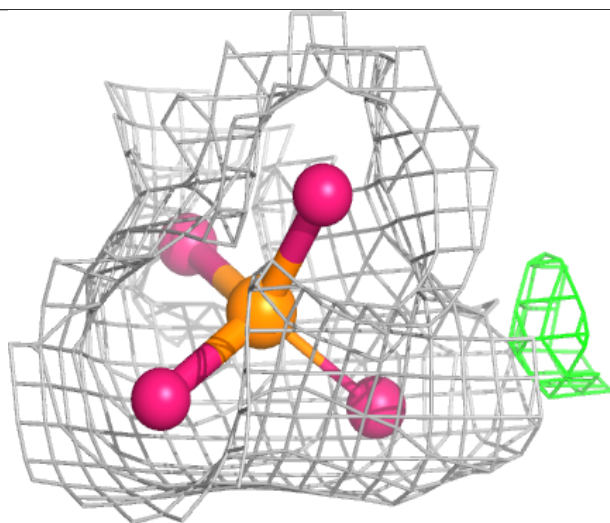
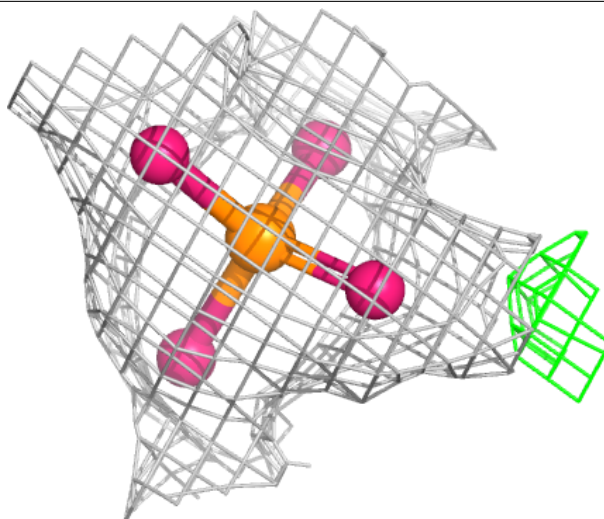
Electron density around PO4 E 405:

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



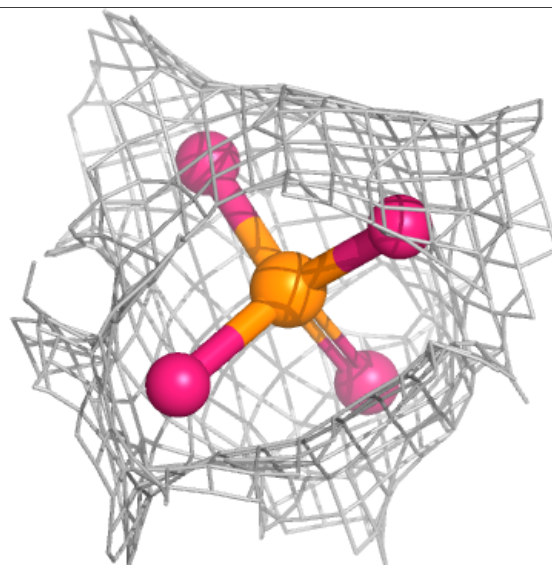
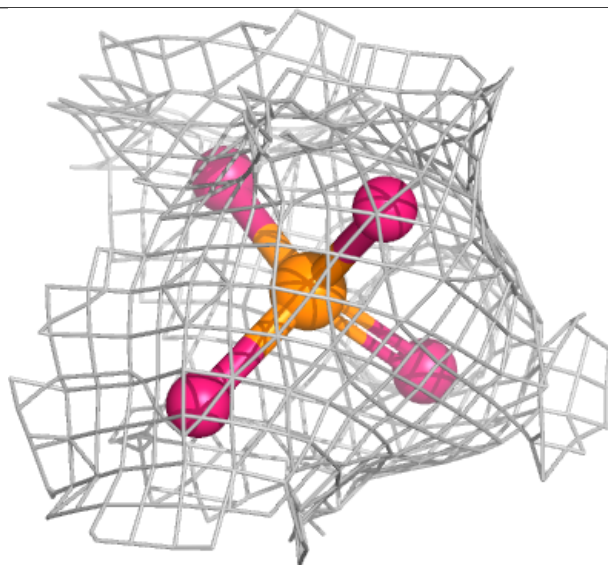
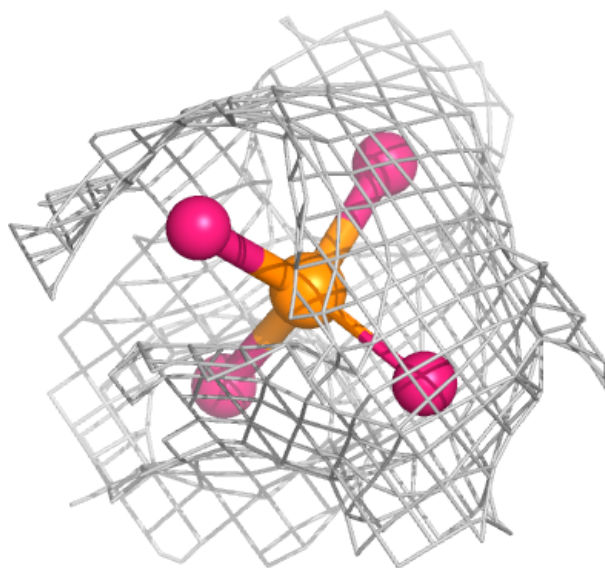
Electron density around PO4 G 405:

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



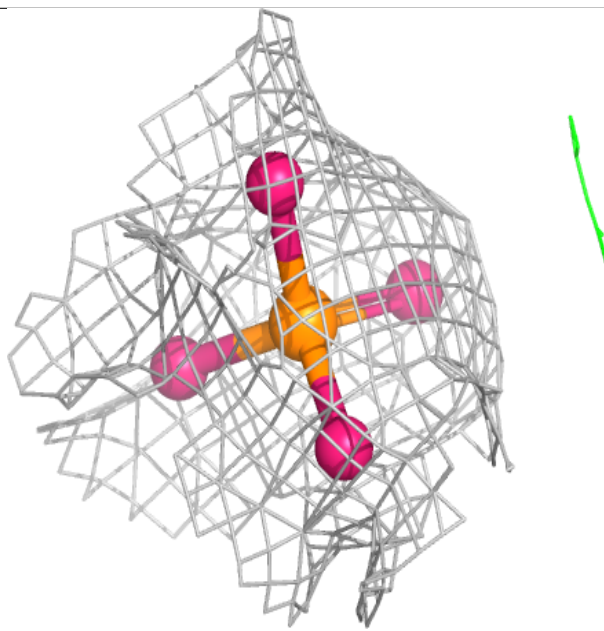
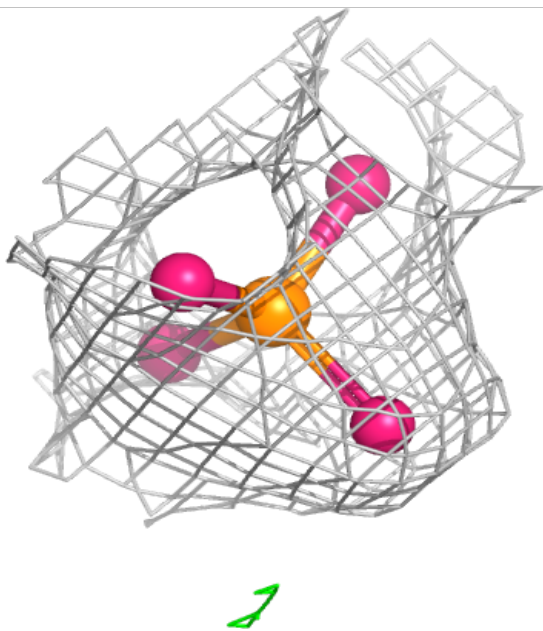
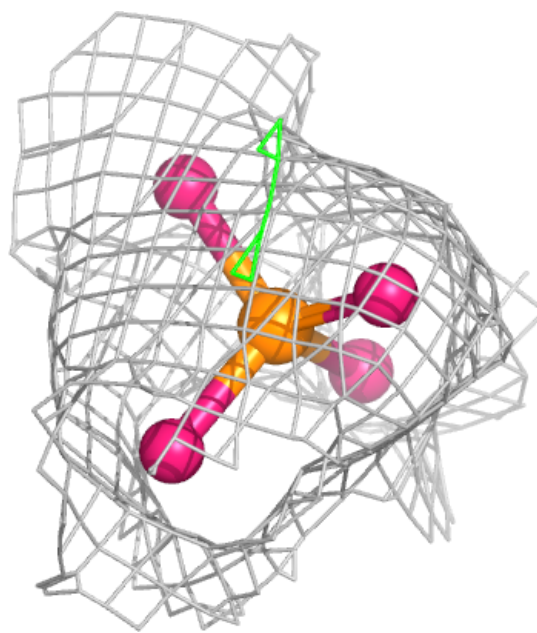
Electron density around PO4 H 405:

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



Electron density around PO4 I 405:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.