



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 12:52 PM BST

PDB ID : 3HQP  
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with ATP, Oxalate and fructose 2,6 biphosphate  
Authors : Morgan, H.P.; Walkinshaw, M.D.  
Deposited on : 2009-06-08  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

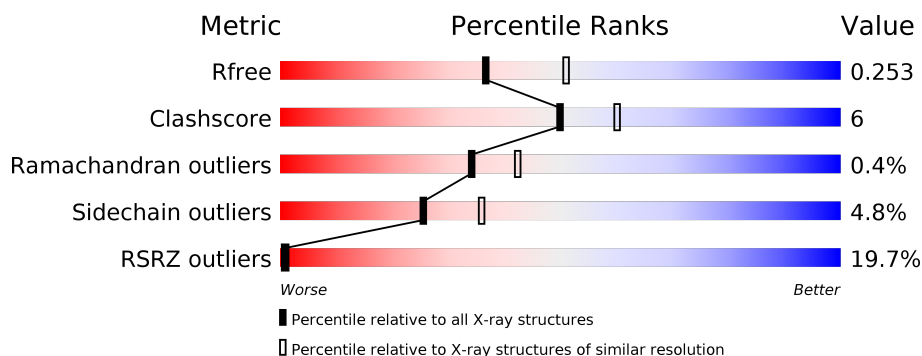
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	499	<div> <div>24%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	499	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
1	C	499	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	499	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	E	499	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	F	499	<div> <div>15%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	499	
1	H	499	
1	I	499	
1	J	499	
1	K	499	
1	L	499	
1	M	499	
1	N	499	
1	O	499	
1	P	499	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 65997 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	2	0
			3818	2379	674	739	26			
1	B	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	C	498	Total	C	N	O	S	0	2	0
			3815	2378	672	739	26			
1	D	498	Total	C	N	O	S	0	1	0
			3809	2374	673	736	26			
1	E	498	Total	C	N	O	S	0	1	0
			3808	2373	672	737	26			
1	F	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	G	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	H	498	Total	C	N	O	S	0	2	0
			3817	2379	675	737	26			
1	I	498	Total	C	N	O	S	0	2	0
			3816	2379	674	737	26			
1	J	498	Total	C	N	O	S	0	3	0
			3824	2383	676	739	26			
1	K	498	Total	C	N	O	S	0	2	0
			3816	2377	673	740	26			
1	L	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	M	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	N	498	Total	C	N	O	S	0	1	0
			3808	2373	671	738	26			
1	O	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	P	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			



There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA	SEE REMARK 999	UNP Q27686
A	405	SER	GLY	SEE REMARK 999	UNP Q27686
B	382	SER	GLY	SEE REMARK 999	UNP Q27686
B	389	TYR	SER	SEE REMARK 999	UNP Q27686
B	404	ARG	ALA	SEE REMARK 999	UNP Q27686
B	405	SER	GLY	SEE REMARK 999	UNP Q27686
C	382	SER	GLY	SEE REMARK 999	UNP Q27686
C	389	TYR	SER	SEE REMARK 999	UNP Q27686
C	404	ARG	ALA	SEE REMARK 999	UNP Q27686
C	405	SER	GLY	SEE REMARK 999	UNP Q27686
D	382	SER	GLY	SEE REMARK 999	UNP Q27686
D	389	TYR	SER	SEE REMARK 999	UNP Q27686
D	404	ARG	ALA	SEE REMARK 999	UNP Q27686
D	405	SER	GLY	SEE REMARK 999	UNP Q27686
E	382	SER	GLY	SEE REMARK 999	UNP Q27686
E	389	TYR	SER	SEE REMARK 999	UNP Q27686
E	404	ARG	ALA	SEE REMARK 999	UNP Q27686
E	405	SER	GLY	SEE REMARK 999	UNP Q27686
F	382	SER	GLY	SEE REMARK 999	UNP Q27686
F	389	TYR	SER	SEE REMARK 999	UNP Q27686
F	404	ARG	ALA	SEE REMARK 999	UNP Q27686
F	405	SER	GLY	SEE REMARK 999	UNP Q27686
G	382	SER	GLY	SEE REMARK 999	UNP Q27686
G	389	TYR	SER	SEE REMARK 999	UNP Q27686
G	404	ARG	ALA	SEE REMARK 999	UNP Q27686
G	405	SER	GLY	SEE REMARK 999	UNP Q27686
H	382	SER	GLY	SEE REMARK 999	UNP Q27686
H	389	TYR	SER	SEE REMARK 999	UNP Q27686
H	404	ARG	ALA	SEE REMARK 999	UNP Q27686
H	405	SER	GLY	SEE REMARK 999	UNP Q27686
I	382	SER	GLY	SEE REMARK 999	UNP Q27686
I	389	TYR	SER	SEE REMARK 999	UNP Q27686
I	404	ARG	ALA	SEE REMARK 999	UNP Q27686
I	405	SER	GLY	SEE REMARK 999	UNP Q27686
J	382	SER	GLY	SEE REMARK 999	UNP Q27686
J	389	TYR	SER	SEE REMARK 999	UNP Q27686
J	404	ARG	ALA	SEE REMARK 999	UNP Q27686
J	405	SER	GLY	SEE REMARK 999	UNP Q27686
K	382	SER	GLY	SEE REMARK 999	UNP Q27686
K	389	TYR	SER	SEE REMARK 999	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
K	404	ARG	ALA	SEE REMARK 999	UNP Q27686
K	405	SER	GLY	SEE REMARK 999	UNP Q27686
L	382	SER	GLY	SEE REMARK 999	UNP Q27686
L	389	TYR	SER	SEE REMARK 999	UNP Q27686
L	404	ARG	ALA	SEE REMARK 999	UNP Q27686
L	405	SER	GLY	SEE REMARK 999	UNP Q27686
M	382	SER	GLY	SEE REMARK 999	UNP Q27686
M	389	TYR	SER	SEE REMARK 999	UNP Q27686
M	404	ARG	ALA	SEE REMARK 999	UNP Q27686
M	405	SER	GLY	SEE REMARK 999	UNP Q27686
N	382	SER	GLY	SEE REMARK 999	UNP Q27686
N	389	TYR	SER	SEE REMARK 999	UNP Q27686
N	404	ARG	ALA	SEE REMARK 999	UNP Q27686
N	405	SER	GLY	SEE REMARK 999	UNP Q27686
O	382	SER	GLY	SEE REMARK 999	UNP Q27686
O	389	TYR	SER	SEE REMARK 999	UNP Q27686
O	404	ARG	ALA	SEE REMARK 999	UNP Q27686
O	405	SER	GLY	SEE REMARK 999	UNP Q27686
P	382	SER	GLY	SEE REMARK 999	UNP Q27686
P	389	TYR	SER	SEE REMARK 999	UNP Q27686
P	404	ARG	ALA	SEE REMARK 999	UNP Q27686
P	405	SER	GLY	SEE REMARK 999	UNP Q27686

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	K	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	H	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0
2	N	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	M	2	Total 2	Mg 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

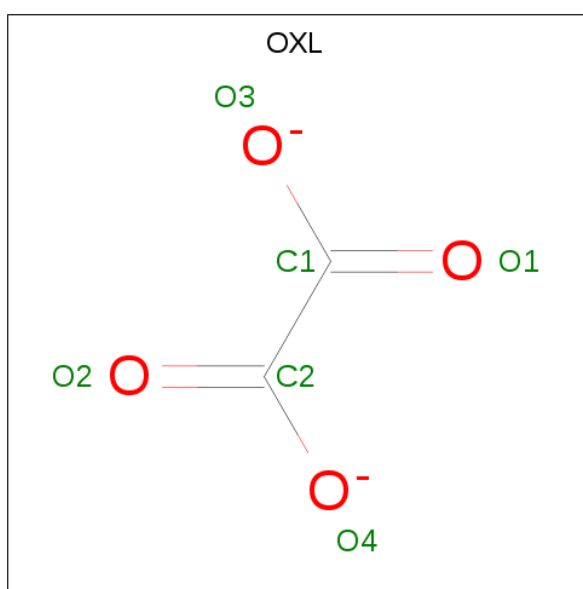
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total 2	K 2	0	0
3	G	2	Total 2	K 2	0	0
3	J	2	Total 2	K 2	0	0
3	D	2	Total 2	K 2	0	0
3	K	2	Total 2	K 2	0	0
3	E	2	Total 2	K 2	0	0
3	H	2	Total 2	K 2	0	0
3	B	2	Total 2	K 2	0	0
3	I	2	Total 2	K 2	0	0
3	C	2	Total 2	K 2	0	0
3	A	2	Total 2	K 2	0	0
3	N	2	Total 2	K 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	2	Total 2	K 2	0	0
3	L	2	Total 2	K 2	0	0
3	F	2	Total 2	K 2	0	0
3	M	2	Total 2	K 2	0	0

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula:  $C_2O_4$ ).



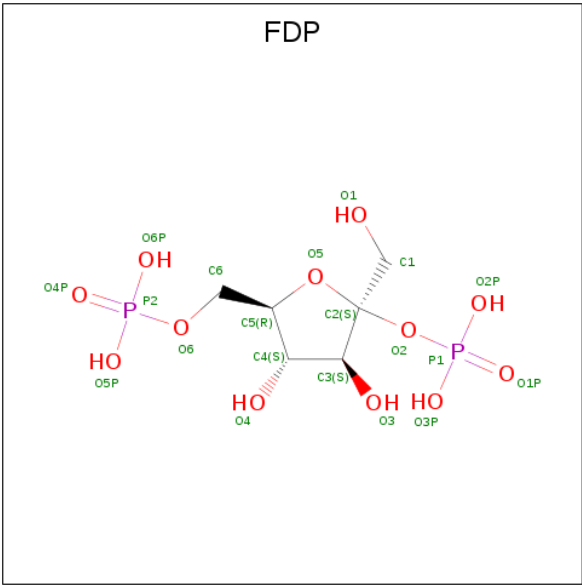
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 2	O 4	0	0
4	B	1	Total 6	C 2	O 4	0	0
4	C	1	Total 6	C 2	O 4	0	0
4	D	1	Total 6	C 2	O 4	0	0
4	E	1	Total 6	C 2	O 4	0	0
4	F	1	Total 6	C 2	O 4	0	0
4	G	1	Total 6	C 2	O 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	2	4		
4	I	1	Total	C	O	0	0
			6	2	4		
4	J	1	Total	C	O	0	0
			6	2	4		
4	K	1	Total	C	O	0	0
			6	2	4		
4	L	1	Total	C	O	0	0
			6	2	4		
4	M	1	Total	C	O	0	0
			6	2	4		
4	N	1	Total	C	O	0	0
			6	2	4		
4	P	1	Total	C	O	0	0
			6	2	4		

- Molecule 5 is 2,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FDP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



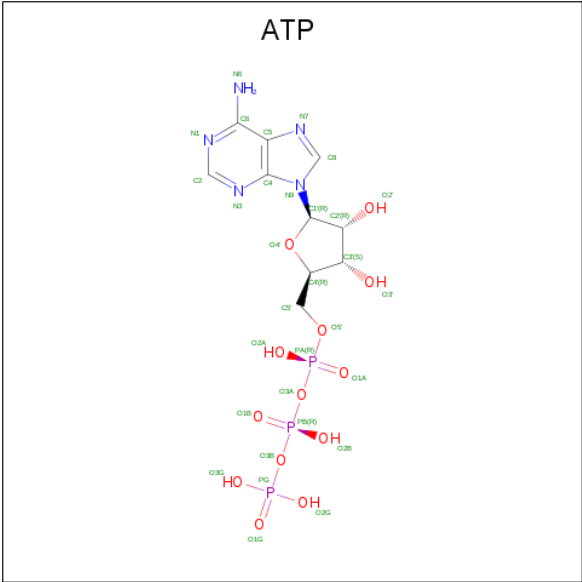
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			20	6	12	2		
5	B	1	Total	C	O	P	0	0
			20	6	12	2		
5	C	1	Total	C	O	P	0	0
			20	6	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	P	0	0
			20	6	12	2		
5	E	1	Total	C	O	P	0	0
			20	6	12	2		
5	F	1	Total	C	O	P	0	0
			20	6	12	2		
5	G	1	Total	C	O	P	0	0
			20	6	12	2		
5	H	1	Total	C	O	P	0	0
			20	6	12	2		
5	I	1	Total	C	O	P	0	0
			20	6	12	2		
5	J	1	Total	C	O	P	0	0
			20	6	12	2		
5	K	1	Total	C	O	P	0	0
			20	6	12	2		
5	L	1	Total	C	O	P	0	0
			20	6	12	2		
5	M	1	Total	C	O	P	0	0
			20	6	12	2		
5	N	1	Total	C	O	P	0	0
			20	6	12	2		
5	O	1	Total	C	O	P	0	0
			20	6	12	2		
5	P	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	167	Total	O	0	0
			167	167		
8	B	379	Total	O	0	0
			379	379		

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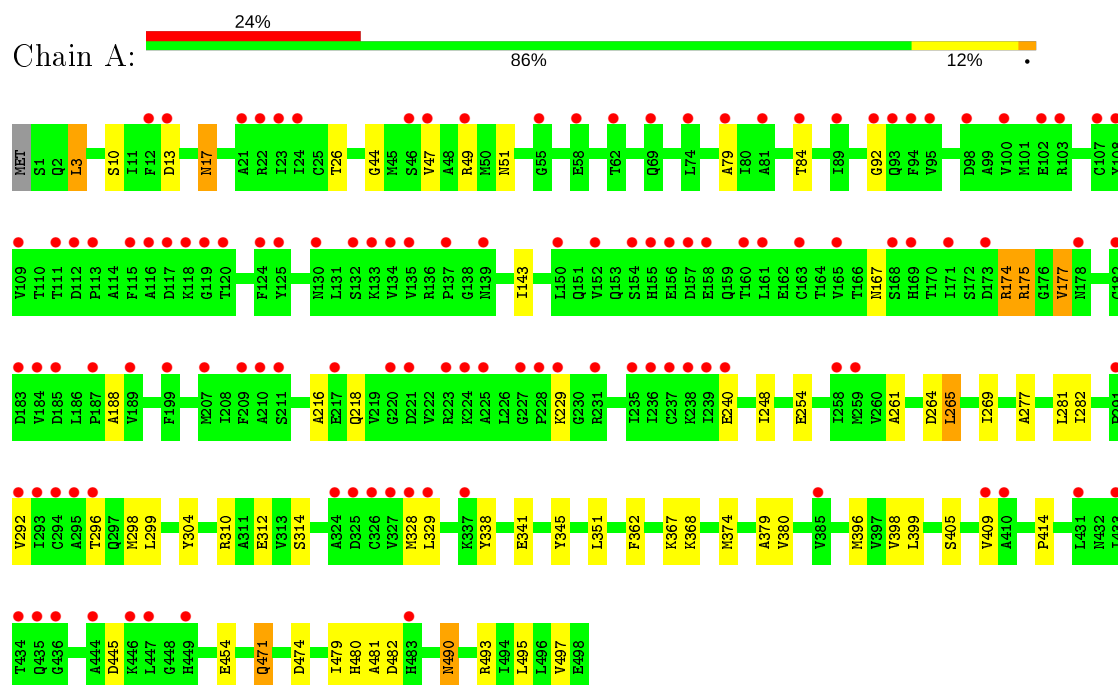
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	305	Total 305	O 305	0	0
8	D	400	Total 400	O 400	0	0
8	E	232	Total 232	O 232	0	0
8	F	187	Total 187	O 187	0	0
8	G	139	Total 139	O 139	0	0
8	H	215	Total 215	O 215	0	0
8	I	415	Total 415	O 415	0	0
8	J	499	Total 499	O 499	0	0
8	K	462	Total 462	O 462	0	0
8	L	316	Total 316	O 316	0	0
8	M	140	Total 140	O 140	0	0
8	N	103	Total 103	O 103	0	0
8	O	69	Total 69	O 69	0	0
8	P	72	Total 72	O 72	0	0

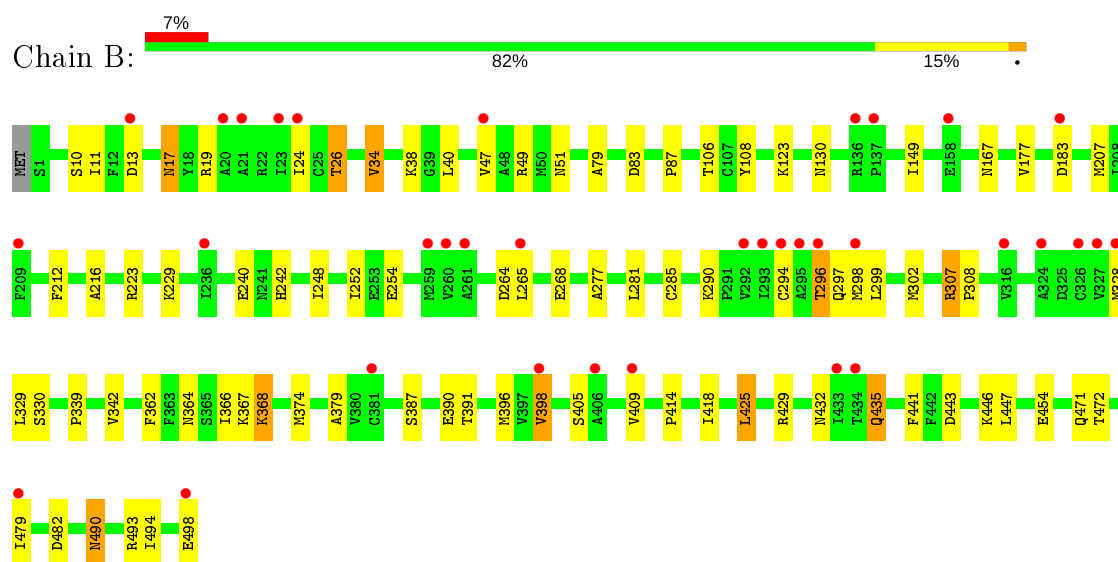
### 3 Residue-property plots [i](#)

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.

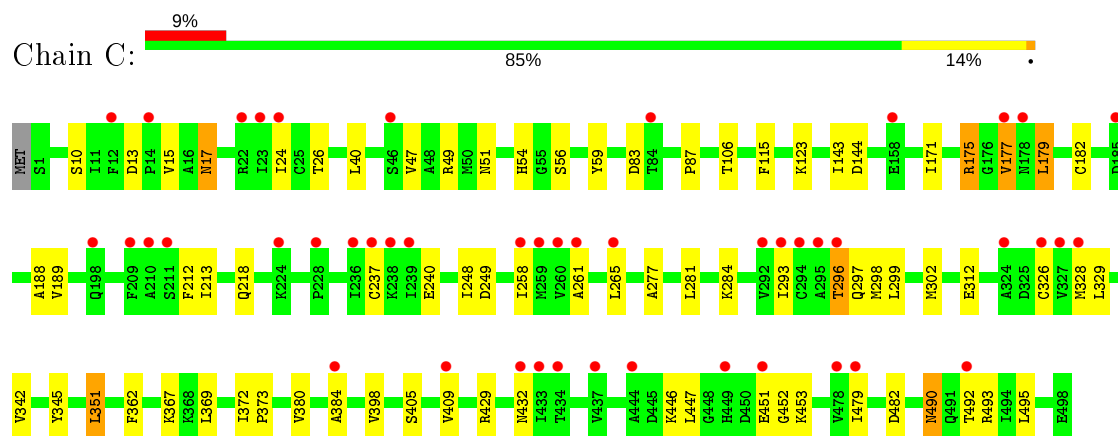
#### • Molecule 1: Pyruvate kinase



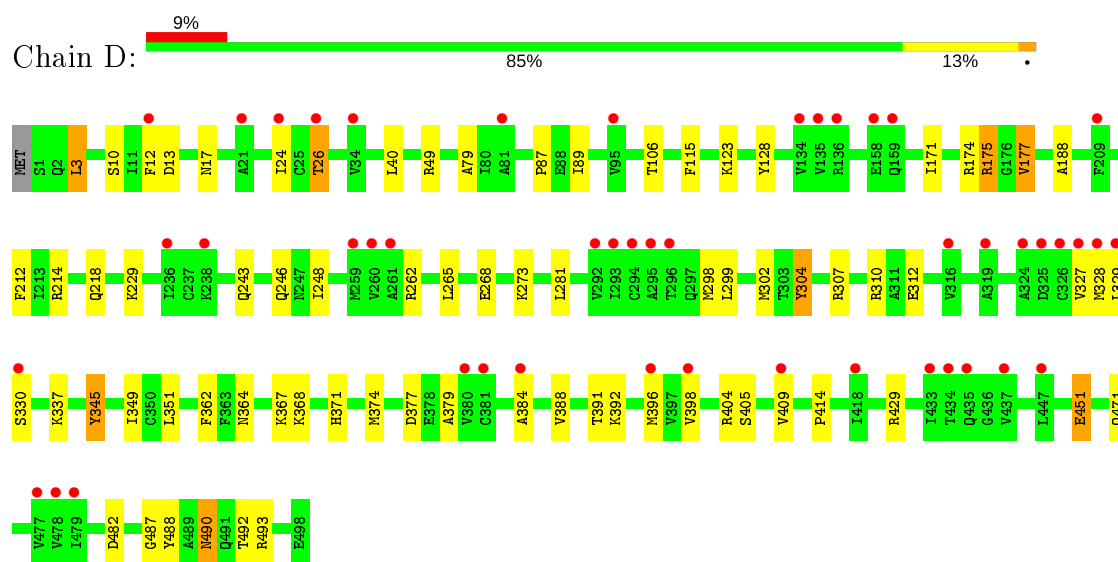
#### • Molecule 1: Pyruvate kinase



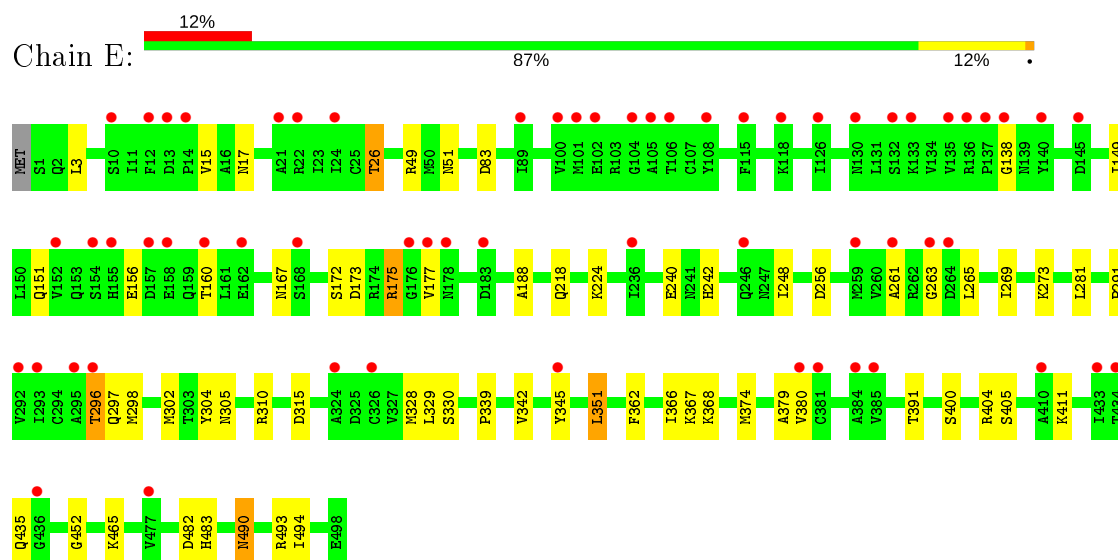
- Molecule 1: Pyruvate kinase



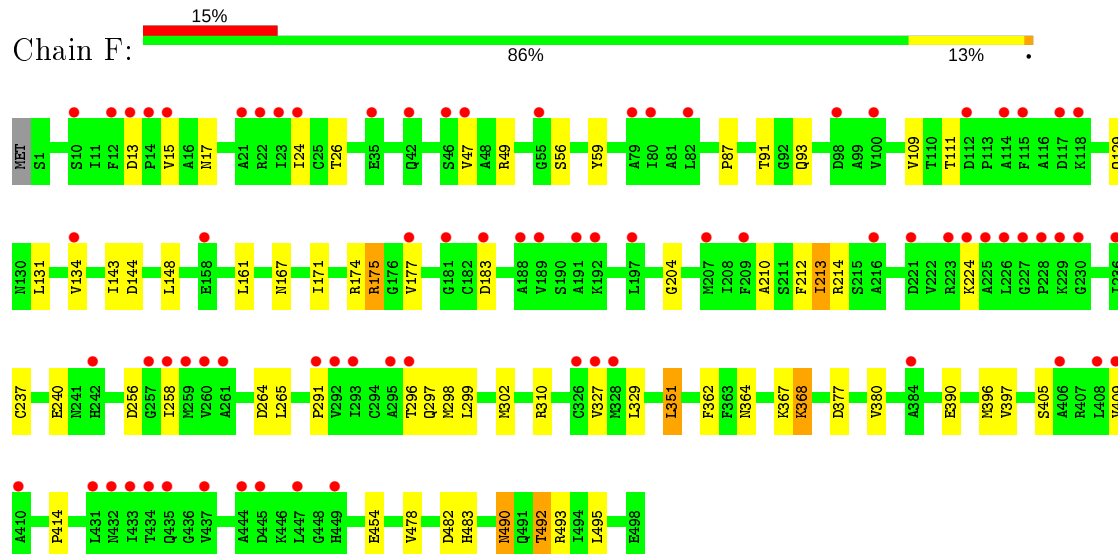
- Molecule 1: Pyruvate kinase



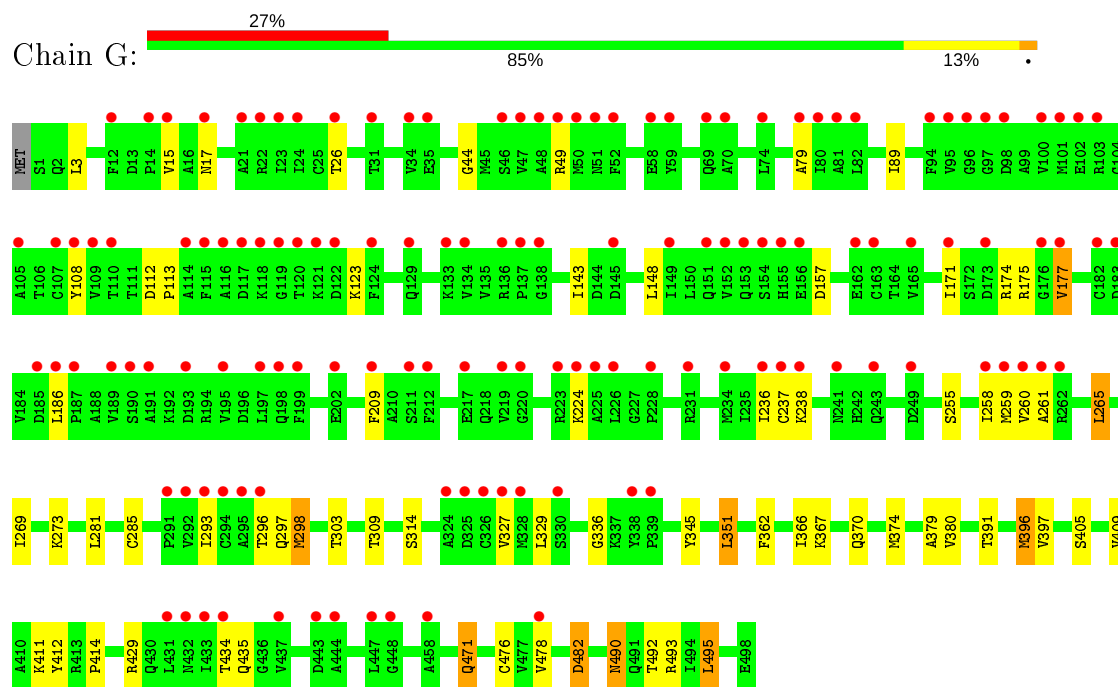
- Molecule 1: Pyruvate kinase



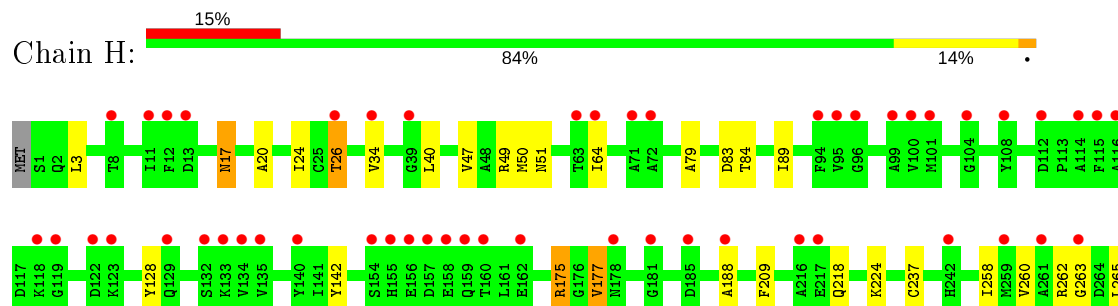
- Molecule 1: Pyruvate kinase

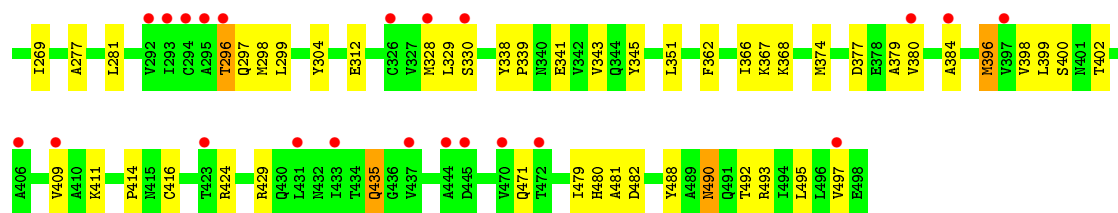


- Molecule 1: Pyruvate kinase

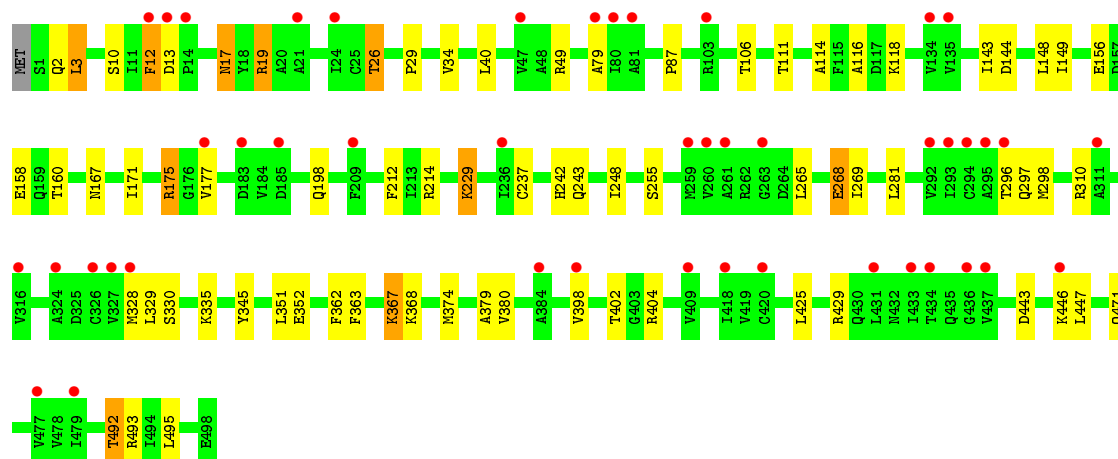
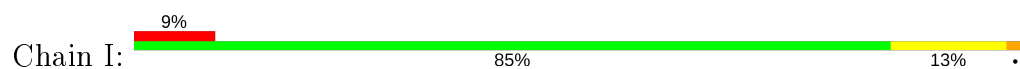


- Molecule 1: Pyruvate kinase

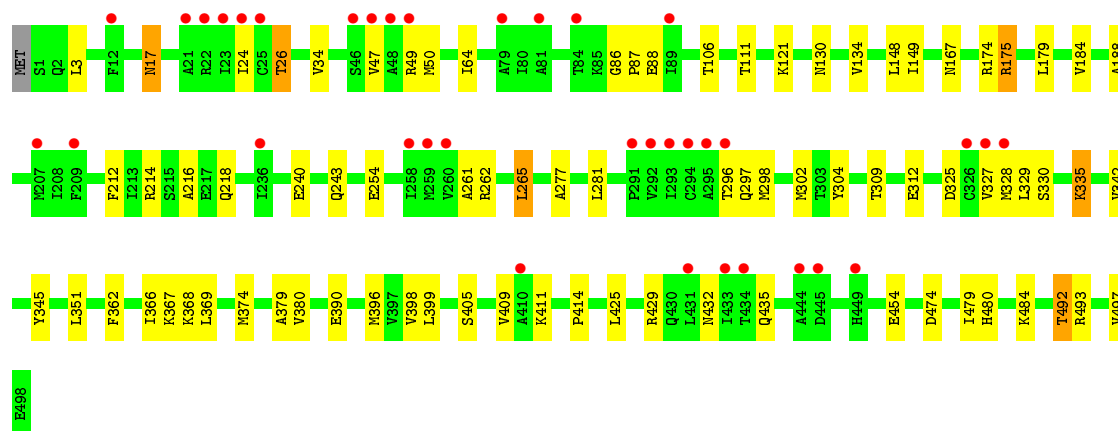
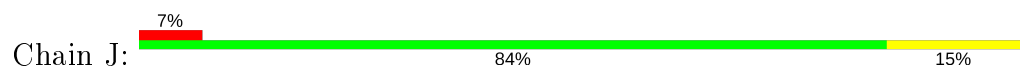




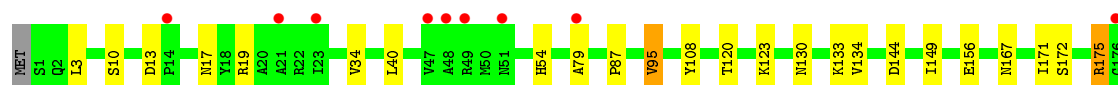
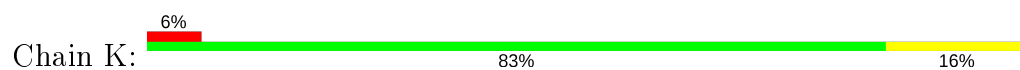
• Molecule 1: Pyruvate kinase

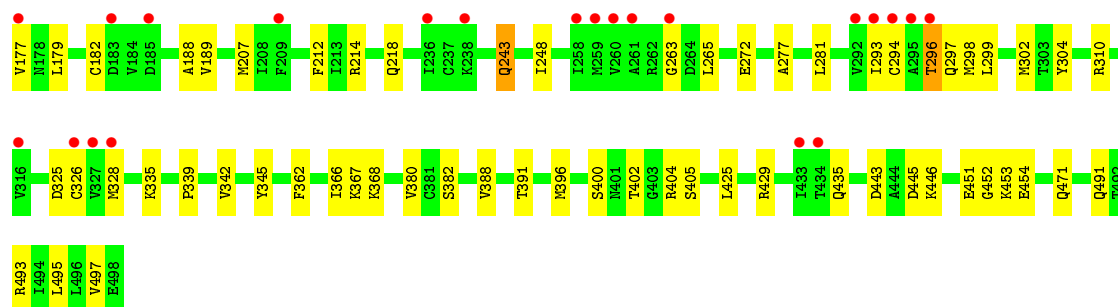


• Molecule 1: Pyruvate kinase

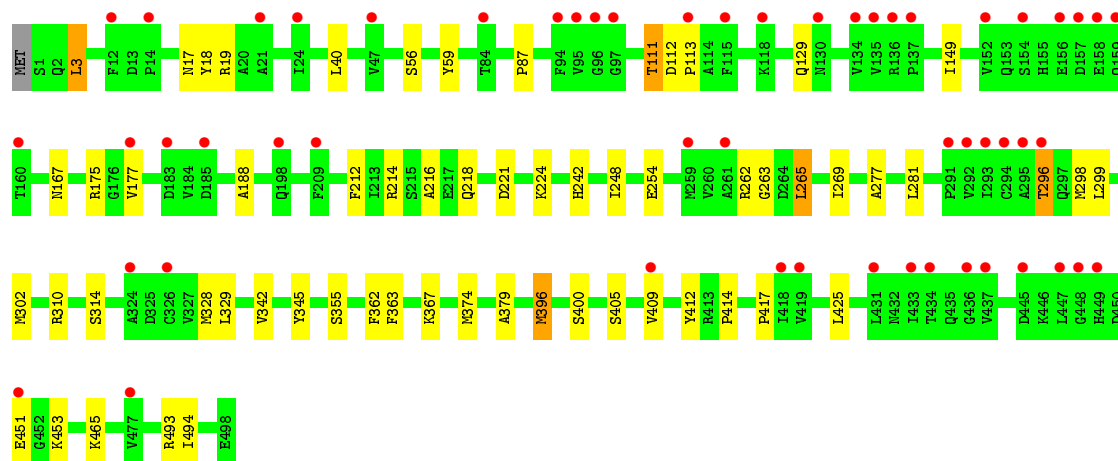
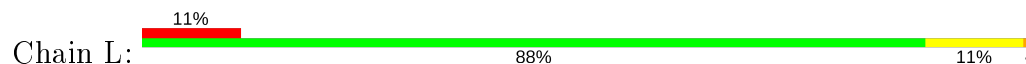


• Molecule 1: Pyruvate kinase

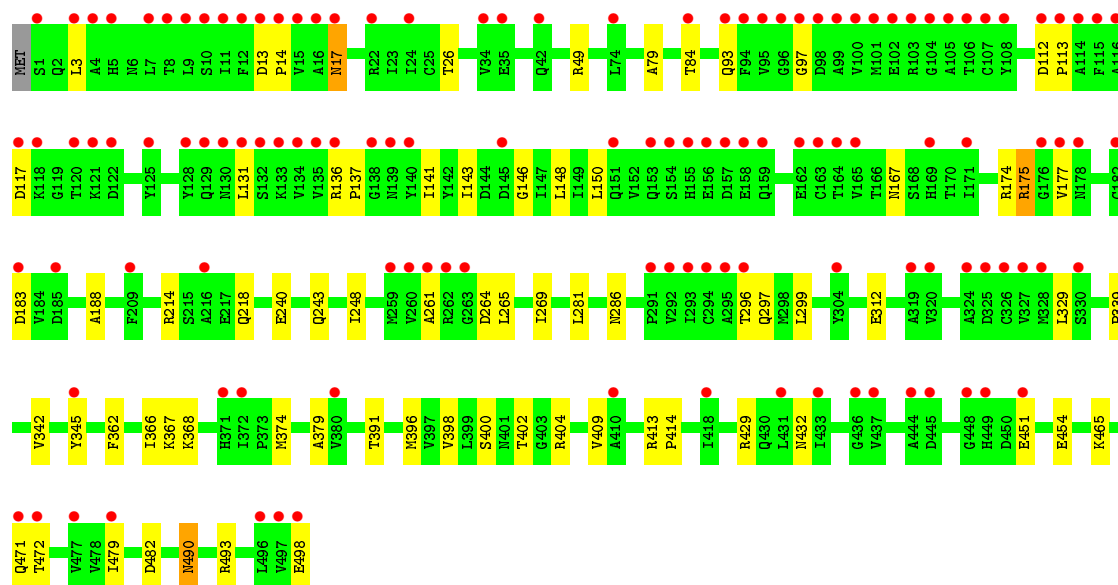
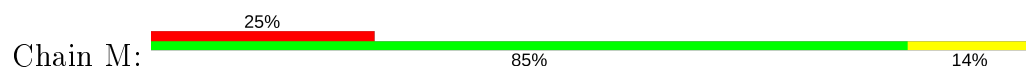




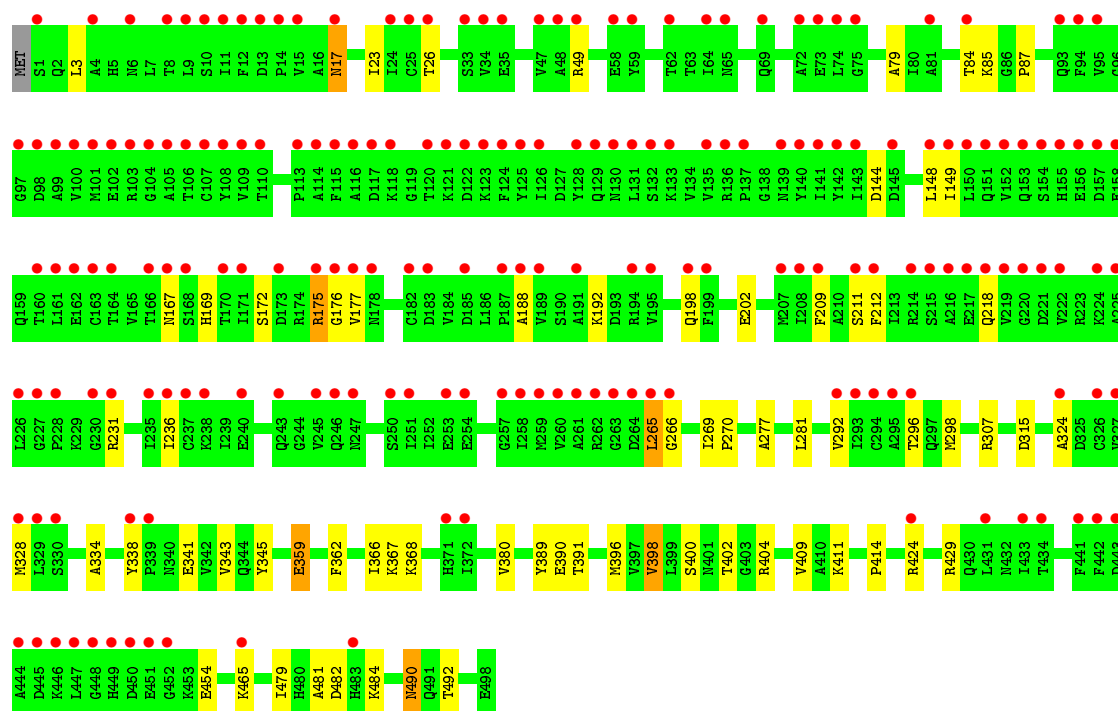
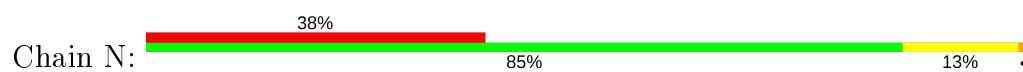
• Molecule 1: Pyruvate kinase



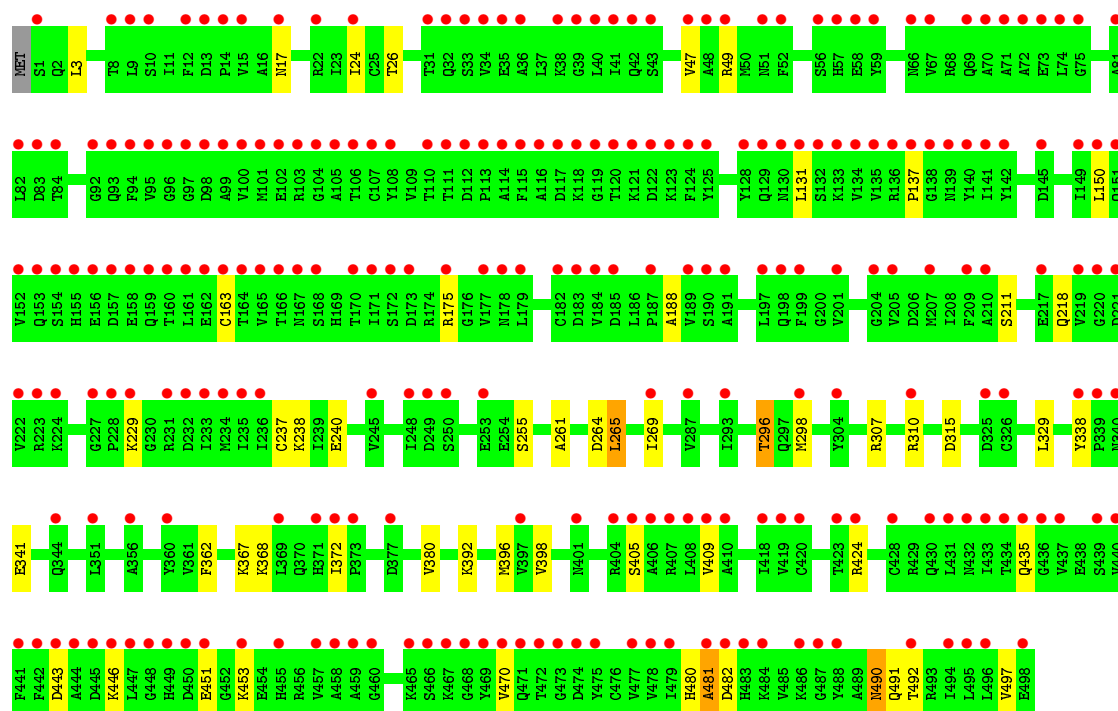
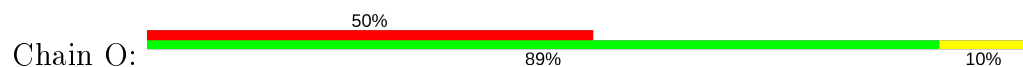
• Molecule 1: Pyruvate kinase



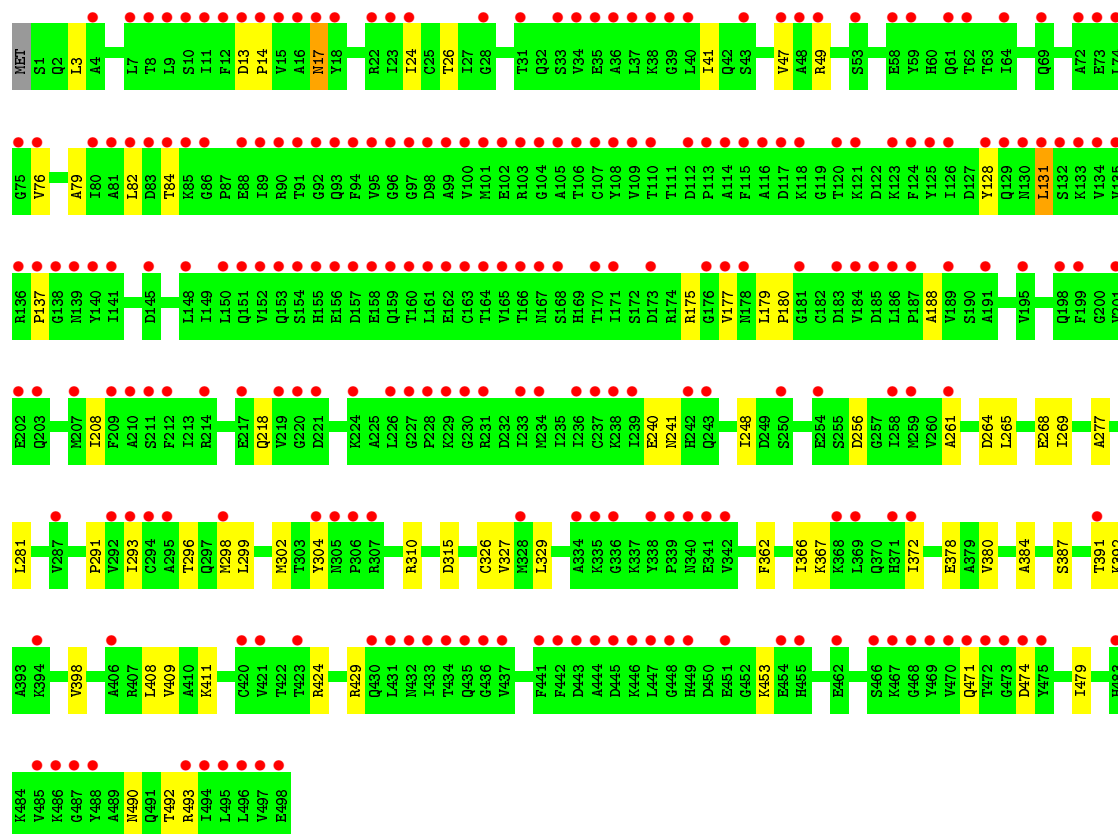
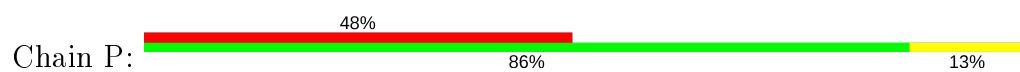
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.49Å 151.14Å 160.32Å 89.73° 80.17° 71.64°	Depositor
Resolution (Å)	34.46 – 2.30 34.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (34.46-2.30) 94.6 (34.09-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.198 , 0.252 0.201 , 0.253	Depositor DCC
$R_{free}$ test set	23579 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	65997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG, K, OXL, FDP, ATP

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	0.34	0/3876	0.50	0/5247
1	B	0.39	0/3856	0.55	0/5220
1	C	0.36	0/3872	0.53	0/5242
1	D	0.40	0/3867	0.55	0/5235
1	E	0.36	0/3865	0.51	0/5232
1	F	0.36	0/3856	0.51	0/5220
1	G	0.33	0/3856	0.49	0/5220
1	H	0.37	0/3874	0.51	0/5244
1	I	0.44	0/3874	0.59	1/5245 (0.0%)
1	J	0.44	0/3882	0.58	0/5256
1	K	0.45	0/3873	0.59	0/5243
1	L	0.41	0/3856	0.56	0/5220
1	M	0.35	0/3856	0.49	0/5220
1	N	0.35	0/3865	0.48	0/5232
1	O	0.34	0/3856	0.47	0/5220
1	P	0.33	0/3856	0.46	0/5220
All	All	0.38	0/61840	0.53	1/83716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	19	ARG	NE-CZ-NH1	-5.07	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3818	0	3813	48	0
1	B	3799	0	3801	66	0
1	C	3815	0	3814	51	0
1	D	3809	0	3807	57	0
1	E	3808	0	3808	38	0
1	F	3799	0	3801	50	0
1	G	3799	0	3801	40	0
1	H	3817	0	3821	46	0
1	I	3816	0	3815	48	0
1	J	3824	0	3820	58	0
1	K	3816	0	3811	49	0
1	L	3799	0	3802	35	0
1	M	3799	0	3802	42	0
1	N	3808	0	3807	39	0
1	O	3799	0	3802	37	0
1	P	3799	0	3802	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	P	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	1	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	0	0
4	F	6	0	0	0	0
4	G	6	0	0	0	0
4	H	6	0	0	0	0
4	I	6	0	0	0	0
4	J	6	0	0	0	0
4	K	6	0	0	0	0
4	L	6	0	0	0	0
4	M	6	0	0	1	0
4	N	6	0	0	0	0
4	P	6	0	0	0	0
5	A	20	0	10	0	0
5	B	20	0	10	0	0
5	C	20	0	10	0	0
5	D	20	0	10	2	0
5	E	20	0	10	0	0
5	F	20	0	10	0	0
5	G	20	0	10	0	0
5	H	20	0	10	0	0
5	I	20	0	9	1	0
5	J	20	0	10	0	0
5	K	20	0	10	0	0
5	L	20	0	10	0	0
5	M	20	0	10	0	0
5	N	20	0	10	2	0
5	O	20	0	10	1	0
5	P	20	0	10	1	0
6	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	31	0	12	0	0
6	C	31	0	12	3	0
6	D	31	0	12	3	0
6	E	31	0	12	1	0
6	F	31	0	12	1	0
6	G	31	0	12	1	0
6	H	31	0	12	1	0
6	I	31	0	12	0	0
6	J	31	0	12	0	0
6	K	31	0	12	2	0
6	L	31	0	12	0	0
6	M	31	0	12	0	0
6	N	31	0	12	0	0
6	P	31	0	12	0	0
7	E	6	0	8	0	0
7	G	6	0	8	0	0
7	I	12	0	16	1	0
7	J	6	0	8	1	0
7	O	6	0	8	0	0
8	A	167	0	0	1	0
8	B	379	0	0	7	0
8	C	305	0	0	0	0
8	D	400	0	0	4	0
8	E	232	0	0	0	0
8	F	187	0	0	1	0
8	G	139	0	0	1	0
8	H	215	0	0	1	0
8	I	415	0	0	6	0
8	J	499	0	0	5	0
8	K	462	0	0	1	0
8	L	316	0	0	2	0
8	M	140	0	0	0	0
8	N	103	0	0	0	0
8	O	69	0	0	0	0
8	P	72	0	0	0	0
All	All	65997	0	61314	710	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 6.

The worst 5 of 710 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:K:388:VAL:HG21	1:K:396:MET:HE1	1.34	1.09
1:C:26:THR:HG22	1:C:49:ARG:HD3	1.40	1.04
1:J:298:MET:HE3	1:J:327:VAL:HB	1.39	1.01
1:K:388:VAL:HG21	1:K:396:MET:CE	1.90	0.99
1:J:398[A]:VAL:HG11	1:J:409:VAL:HG21	1.50	0.92

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	498/499 (100%)	481 (97%)	14 (3%)	3 (1%)	25	31
1	B	496/499 (99%)	486 (98%)	8 (2%)	2 (0%)	34	42
1	C	498/499 (100%)	482 (97%)	15 (3%)	1 (0%)	47	58
1	D	497/499 (100%)	483 (97%)	14 (3%)	0	100	100
1	E	497/499 (100%)	477 (96%)	19 (4%)	1 (0%)	47	58
1	F	496/499 (99%)	480 (97%)	14 (3%)	2 (0%)	34	42
1	G	496/499 (99%)	465 (94%)	27 (5%)	4 (1%)	19	23
1	H	498/499 (100%)	477 (96%)	20 (4%)	1 (0%)	47	58
1	I	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	47	58
1	J	499/499 (100%)	483 (97%)	15 (3%)	1 (0%)	47	58
1	K	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	47	58
1	L	496/499 (99%)	477 (96%)	18 (4%)	1 (0%)	47	58
1	M	496/499 (99%)	472 (95%)	20 (4%)	4 (1%)	19	23
1	N	497/499 (100%)	476 (96%)	20 (4%)	1 (0%)	47	58
1	O	496/499 (99%)	466 (94%)	27 (5%)	3 (1%)	25	31
1	P	496/499 (99%)	469 (95%)	25 (5%)	2 (0%)	34	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7952/7984 (100%)	7646 (96%)	278 (4%)	28 (0%)	34	42

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	481	ALA
1	O	296	THR
1	A	174	ARG
1	I	296	THR
1	J	296	THR

### 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	418/417 (100%)	397 (95%)	21 (5%)	24	34
1	B	416/417 (100%)	395 (95%)	21 (5%)	24	34
1	C	418/417 (100%)	401 (96%)	17 (4%)	30	43
1	D	417/417 (100%)	395 (95%)	22 (5%)	22	31
1	E	417/417 (100%)	398 (95%)	19 (5%)	27	38
1	F	416/417 (100%)	398 (96%)	18 (4%)	29	40
1	G	416/417 (100%)	396 (95%)	20 (5%)	25	36
1	H	418/417 (100%)	394 (94%)	24 (6%)	20	28
1	I	418/417 (100%)	391 (94%)	27 (6%)	17	23
1	J	419/417 (100%)	398 (95%)	21 (5%)	24	34
1	K	418/417 (100%)	392 (94%)	26 (6%)	18	25
1	L	416/417 (100%)	400 (96%)	16 (4%)	33	47
1	M	416/417 (100%)	397 (95%)	19 (5%)	27	38
1	N	417/417 (100%)	397 (95%)	20 (5%)	25	36
1	O	416/417 (100%)	401 (96%)	15 (4%)	35	49
1	P	416/417 (100%)	400 (96%)	16 (4%)	33	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6672/6672 (100%)	6350 (95%)	322 (5%)	25 36

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	224	LYS
1	I	367	LYS
1	O	296	THR
1	H	345	TYR
1	I	12	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	297	GLN
1	I	178	ASN
1	N	344	GLN
1	G	386	ASN
1	H	297	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 62 are monoatomic - leaving 52 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
7	GOL	E	499	-	5,5,5	0.39	0	5,5,5	0.30	0
5	FDP	N	700	-	19,20,20	1.13	2 (10%)	30,32,32	1.16	1 (3%)
7	GOL	O	499	-	5,5,5	0.38	0	5,5,5	0.23	0
6	ATP	P	1001	3,2	26,33,33	0.99	1 (3%)	31,52,52	1.46	5 (16%)
5	FDP	M	700	-	19,20,20	0.74	0	30,32,32	1.10	3 (10%)
4	OXL	N	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	L	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	H	1001	3,2	26,33,33	0.97	1 (3%)	31,52,52	1.31	4 (12%)
5	FDP	E	700	-	19,20,20	1.21	2 (10%)	30,32,32	1.08	2 (6%)
6	ATP	L	1001	3,2	26,33,33	1.06	3 (11%)	31,52,52	1.36	5 (16%)
5	FDP	A	700	-	19,20,20	0.87	0	30,32,32	1.30	3 (10%)
6	ATP	B	1001	3,2	26,33,33	0.92	1 (3%)	31,52,52	1.32	3 (9%)
4	OXL	I	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	F	1001	3,2	26,33,33	1.05	3 (11%)	31,52,52	1.30	3 (9%)
5	FDP	H	700	-	19,20,20	0.92	1 (5%)	30,32,32	1.38	4 (13%)
7	GOL	G	499	-	5,5,5	0.38	0	5,5,5	0.25	0
4	OXL	A	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	E	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	J	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	O	700	-	19,20,20	1.02	0	30,32,32	1.01	1 (3%)
7	GOL	J	499	-	5,5,5	0.37	0	5,5,5	0.32	0
6	ATP	I	1001	3,2	26,33,33	1.07	3 (11%)	31,52,52	1.34	6 (19%)
6	ATP	J	1001	3,2	26,33,33	1.03	2 (7%)	31,52,52	1.27	2 (6%)
5	FDP	G	700	-	19,20,20	1.24	2 (10%)	30,32,32	1.33	3 (10%)
6	ATP	M	1001	3,2	26,33,33	1.01	2 (7%)	31,52,52	1.32	4 (12%)
4	OXL	F	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	C	700	-	19,20,20	0.91	0	30,32,32	1.51	5 (16%)
4	OXL	D	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	E	1001	3,2	26,33,33	1.03	3 (11%)	31,52,52	1.34	4 (12%)
6	ATP	D	1001	3,2	26,33,33	1.02	2 (7%)	31,52,52	1.47	6 (19%)
5	FDP	D	700	-	19,20,20	1.13	1 (5%)	30,32,32	1.36	3 (10%)
4	OXL	P	510	2	0,5,5	0.00	-	0,6,6	0.00	-
7	GOL	I	499	-	5,5,5	0.37	0	5,5,5	0.28	0
4	OXL	H	510	2	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FDP	K	700	-	19,20,20	1.13	3 (15%)	30,32,32	1.47	7 (23%)
4	OXL	B	510	2	0,5,5	0.00	-	0,6,6	0.00	-
7	GOL	I	501	-	5,5,5	0.41	0	5,5,5	0.35	0
6	ATP	N	1001	3,2	26,33,33	1.02	2 (7%)	31,52,52	1.50	5 (16%)
6	ATP	A	1001	3,2	26,33,33	1.01	2 (7%)	31,52,52	1.34	5 (16%)
4	OXL	K	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	G	1001	2	26,33,33	0.99	2 (7%)	31,52,52	1.39	4 (12%)
5	FDP	J	700	-	19,20,20	1.08	2 (10%)	30,32,32	1.36	4 (13%)
5	FDP	F	700	-	19,20,20	1.17	2 (10%)	30,32,32	1.38	4 (13%)
5	FDP	B	700	-	19,20,20	1.50	3 (15%)	30,32,32	1.54	6 (20%)
4	OXL	G	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	C	1001	3,2	26,33,33	1.03	3 (11%)	31,52,52	1.34	4 (12%)
5	FDP	I	700	-	19,20,20	1.58	3 (15%)	30,32,32	1.44	3 (10%)
5	FDP	P	700	-	19,20,20	1.17	1 (5%)	30,32,32	0.80	1 (3%)
5	FDP	L	700	-	19,20,20	1.04	1 (5%)	30,32,32	1.39	4 (13%)
6	ATP	K	1001	3,2	26,33,33	0.97	1 (3%)	31,52,52	1.19	3 (9%)
4	OXL	M	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	C	510	2	0,5,5	0.00	-	0,6,6	0.00	-

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
7	GOL	E	499	-	-	2/4/4/4	-
5	FDP	N	700	-	-	5/12/34/34	0/1/1/1
7	GOL	O	499	-	-	4/4/4/4	-
6	ATP	P	1001	3,2	-	2/18/38/38	0/3/3/3
5	FDP	M	700	-	-	3/12/34/34	0/1/1/1
4	OXL	N	510	2	-	0/0/4/4	-
4	OXL	L	510	2	-	0/0/4/4	-
6	ATP	H	1001	3,2	-	7/18/38/38	0/3/3/3
5	FDP	E	700	-	-	2/12/34/34	0/1/1/1
6	ATP	L	1001	3,2	-	7/18/38/38	0/3/3/3
5	FDP	A	700	-	-	3/12/34/34	0/1/1/1
6	ATP	B	1001	3,2	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OXL	I	510	2	-	0/0/4/4	-
6	ATP	F	1001	3,2	-	1/18/38/38	0/3/3/3
5	FDP	H	700	-	-	2/12/34/34	0/1/1/1
7	GOL	G	499	-	-	0/4/4/4	-
4	OXL	A	510	2	-	0/0/4/4	-
4	OXL	E	510	2	-	0/0/4/4	-
4	OXL	J	510	2	-	0/0/4/4	-
5	FDP	O	700	-	-	8/12/34/34	0/1/1/1
7	GOL	J	499	-	-	4/4/4/4	-
6	ATP	I	1001	3,2	-	2/18/38/38	0/3/3/3
6	ATP	J	1001	3,2	-	2/18/38/38	0/3/3/3
5	FDP	G	700	-	-	0/12/34/34	0/1/1/1
6	ATP	M	1001	3,2	-	2/18/38/38	0/3/3/3
4	OXL	F	510	2	-	0/0/4/4	-
5	FDP	C	700	-	-	1/12/34/34	0/1/1/1
4	OXL	D	510	2	-	0/0/4/4	-
6	ATP	E	1001	3,2	-	2/18/38/38	0/3/3/3
6	ATP	D	1001	3,2	-	6/18/38/38	0/3/3/3
5	FDP	D	700	-	-	1/12/34/34	0/1/1/1
4	OXL	P	510	2	-	0/0/4/4	-
7	GOL	I	499	-	-	2/4/4/4	-
4	OXL	H	510	2	-	0/0/4/4	-
5	FDP	K	700	-	-	0/12/34/34	0/1/1/1
4	OXL	B	510	2	-	0/0/4/4	-
7	GOL	I	501	-	-	4/4/4/4	-
6	ATP	N	1001	3,2	-	4/18/38/38	0/3/3/3
6	ATP	A	1001	3,2	-	7/18/38/38	0/3/3/3
4	OXL	K	510	2	-	0/0/4/4	-
6	ATP	G	1001	2	-	6/18/38/38	0/3/3/3
5	FDP	J	700	-	-	1/12/34/34	0/1/1/1
5	FDP	F	700	-	-	7/12/34/34	0/1/1/1
5	FDP	B	700	-	-	1/12/34/34	0/1/1/1
4	OXL	G	510	2	-	0/0/4/4	-
6	ATP	C	1001	3,2	-	2/18/38/38	0/3/3/3
5	FDP	I	700	-	-	1/12/34/34	0/1/1/1
5	FDP	P	700	-	-	8/12/34/34	0/1/1/1
5	FDP	L	700	-	-	2/12/34/34	0/1/1/1
6	ATP	K	1001	3,2	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OXL	M	510	2	-	0/0/4/4	-
4	OXL	C	510	2	-	0/0/4/4	-

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	700	FDP	P2-O6	-4.52	1.45	1.60
5	I	700	FDP	P1-O2P	-3.84	1.40	1.54
5	I	700	FDP	O3-C3	-3.16	1.36	1.42
5	E	700	FDP	P2-O6	-2.98	1.50	1.60
5	D	700	FDP	O5-C5	2.90	1.50	1.43

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FDP	O2-C2-C3	3.96	120.92	108.18
5	I	700	FDP	O2-C2-C3	3.91	120.74	108.18
6	B	1001	ATP	N3-C2-N1	-3.91	122.57	128.68
5	B	700	FDP	O2-C2-C3	3.89	120.67	108.18
5	L	700	FDP	O2-C2-C3	3.81	120.44	108.18

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	O	499	GOL	O1-C1-C2-C3
7	O	499	GOL	C1-C2-C3-O3
6	I	1001	ATP	PB-O3B-PG-O3G
6	E	1001	ATP	PB-O3B-PG-O3G
5	N	700	FDP	O1-C1-C2-C3

There are no ring outliers.

16 monomers are involved in 24 short contacts:

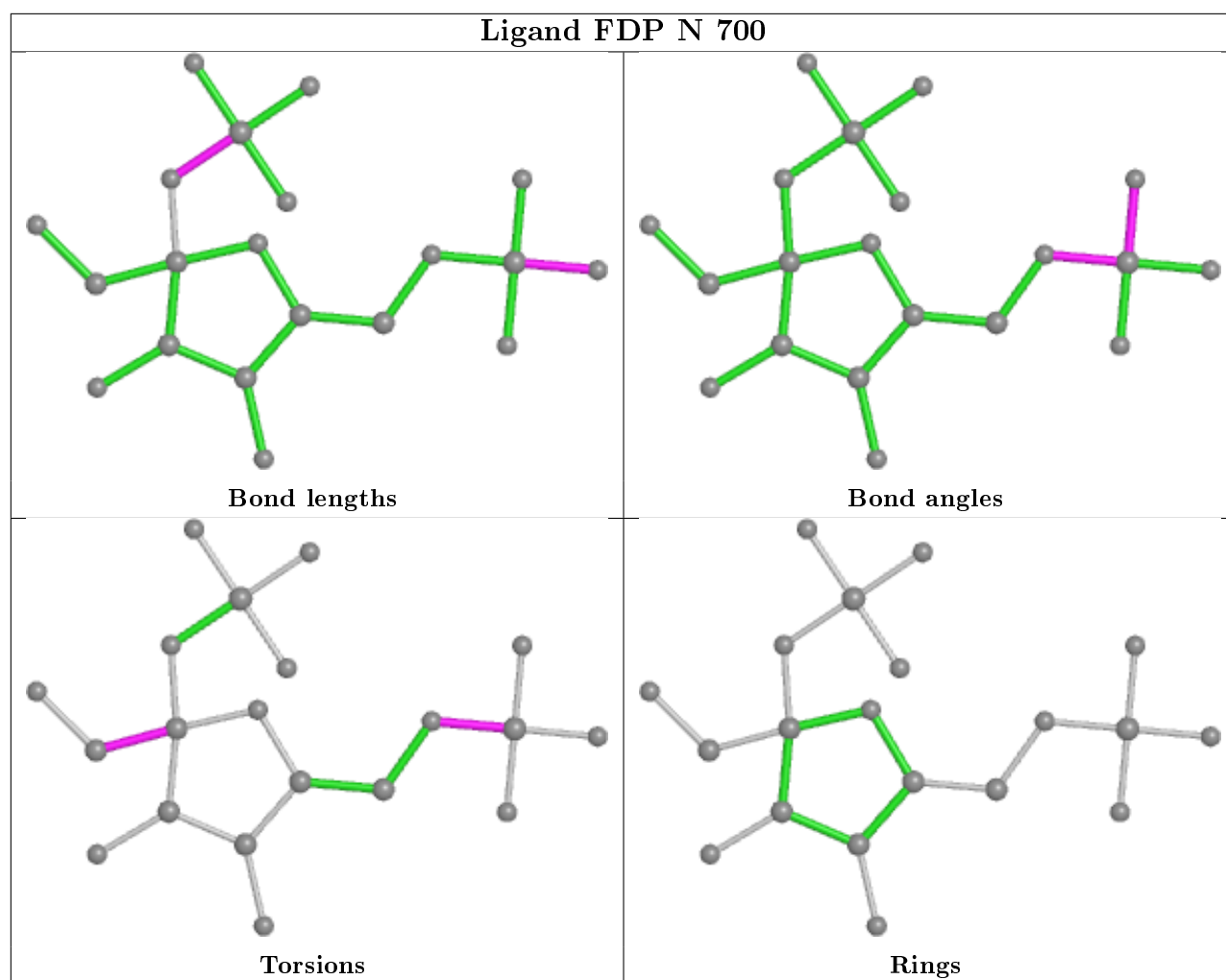
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	700	FDP	2	0
6	H	1001	ATP	1	0
6	F	1001	ATP	1	0
5	O	700	FDP	1	0
7	J	499	GOL	1	0
6	E	1001	ATP	1	0

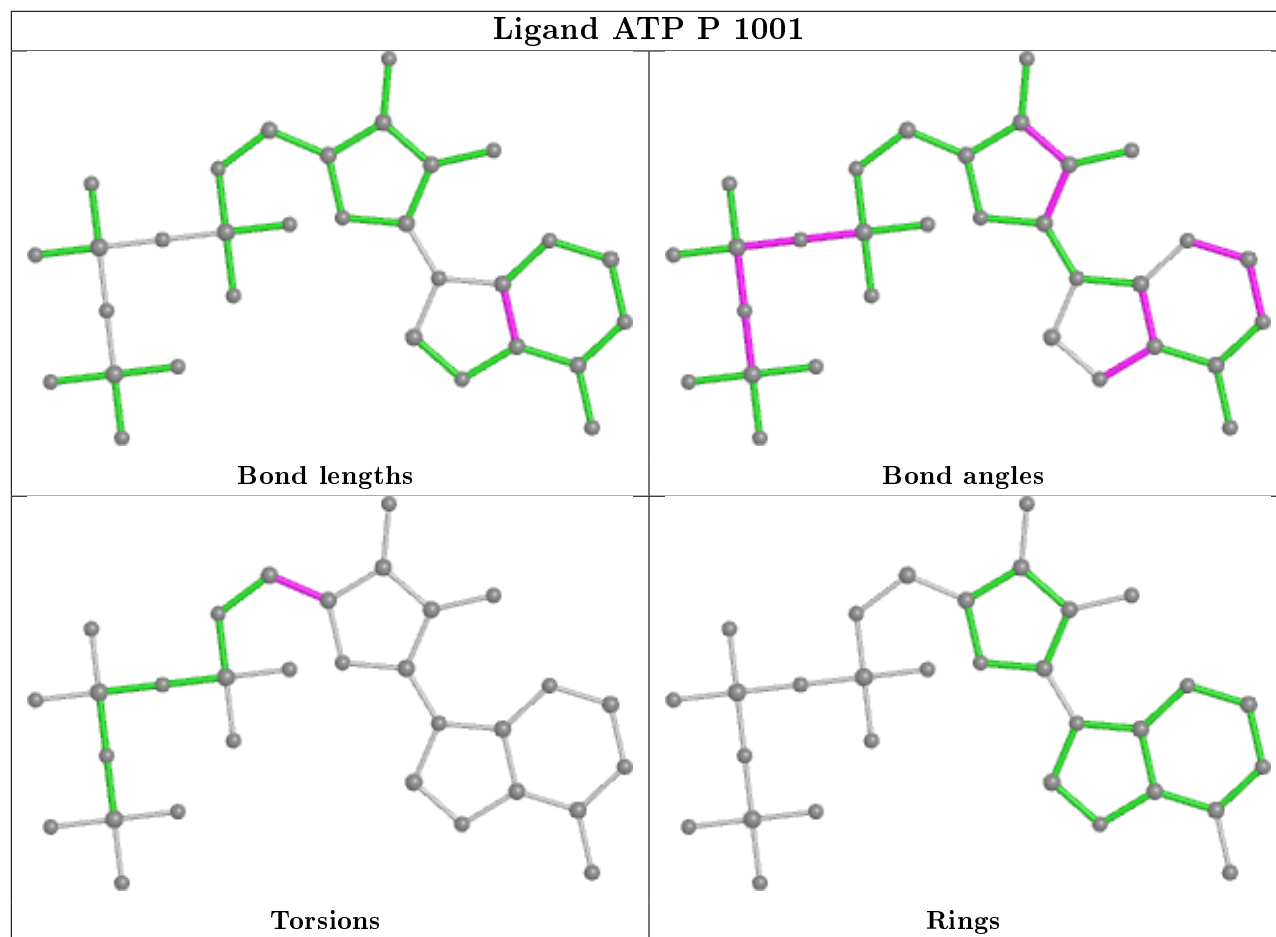
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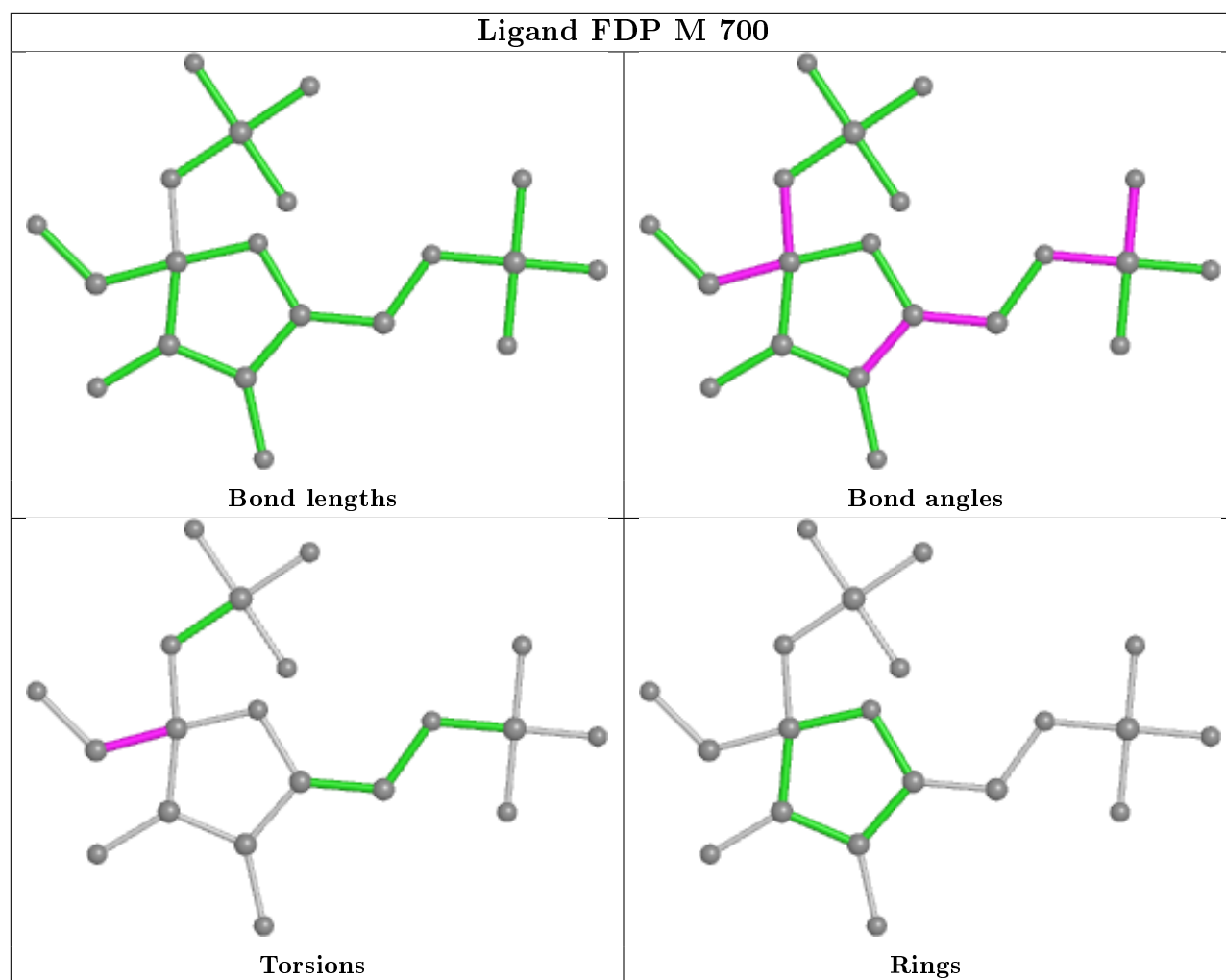
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1001	ATP	3	0
5	D	700	FDP	2	0
7	I	499	GOL	1	0
6	A	1001	ATP	2	0
6	G	1001	ATP	1	0
6	C	1001	ATP	3	0
5	I	700	FDP	1	0
5	P	700	FDP	1	0
6	K	1001	ATP	2	0
4	M	510	OXL	1	0

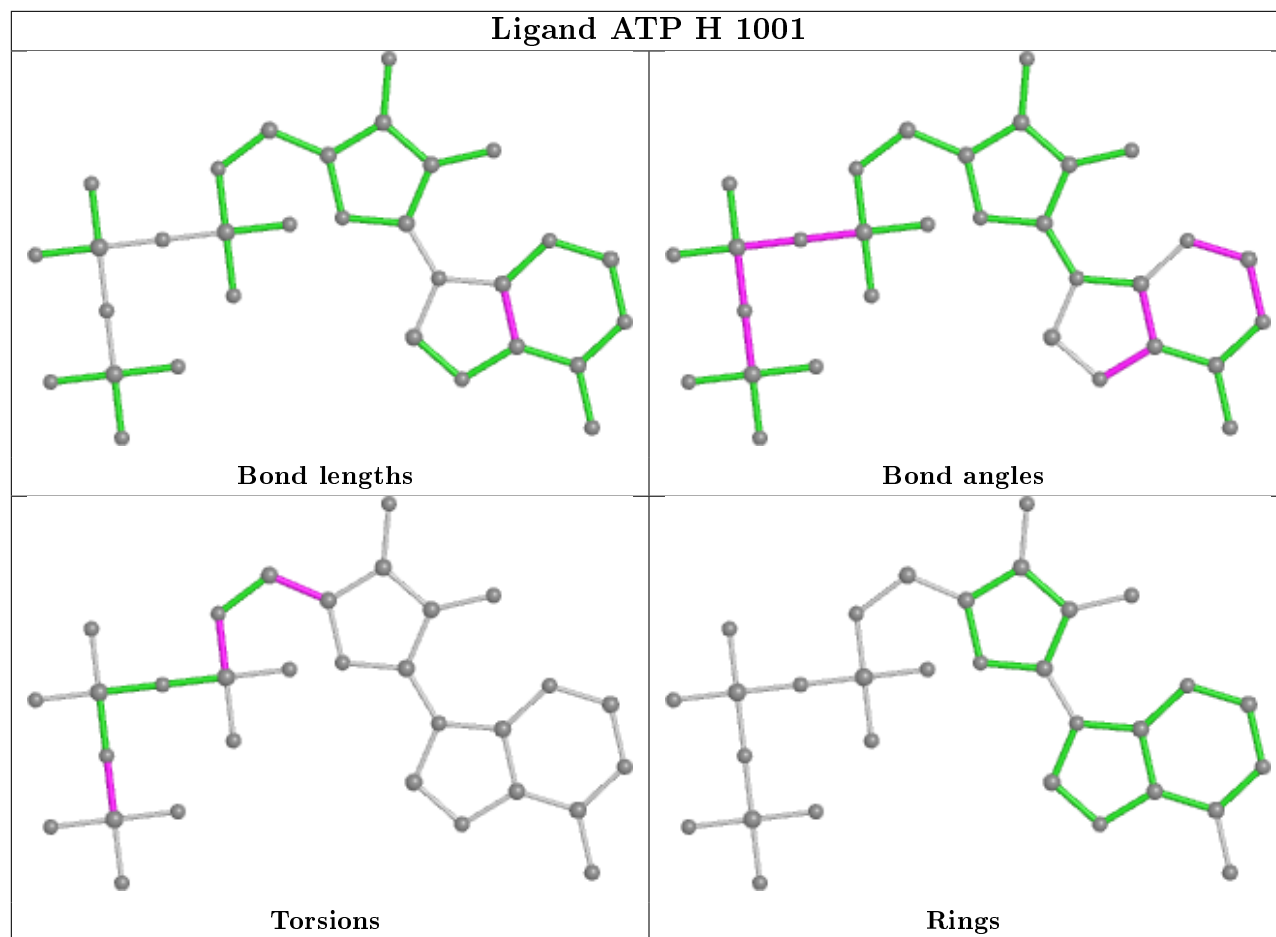
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



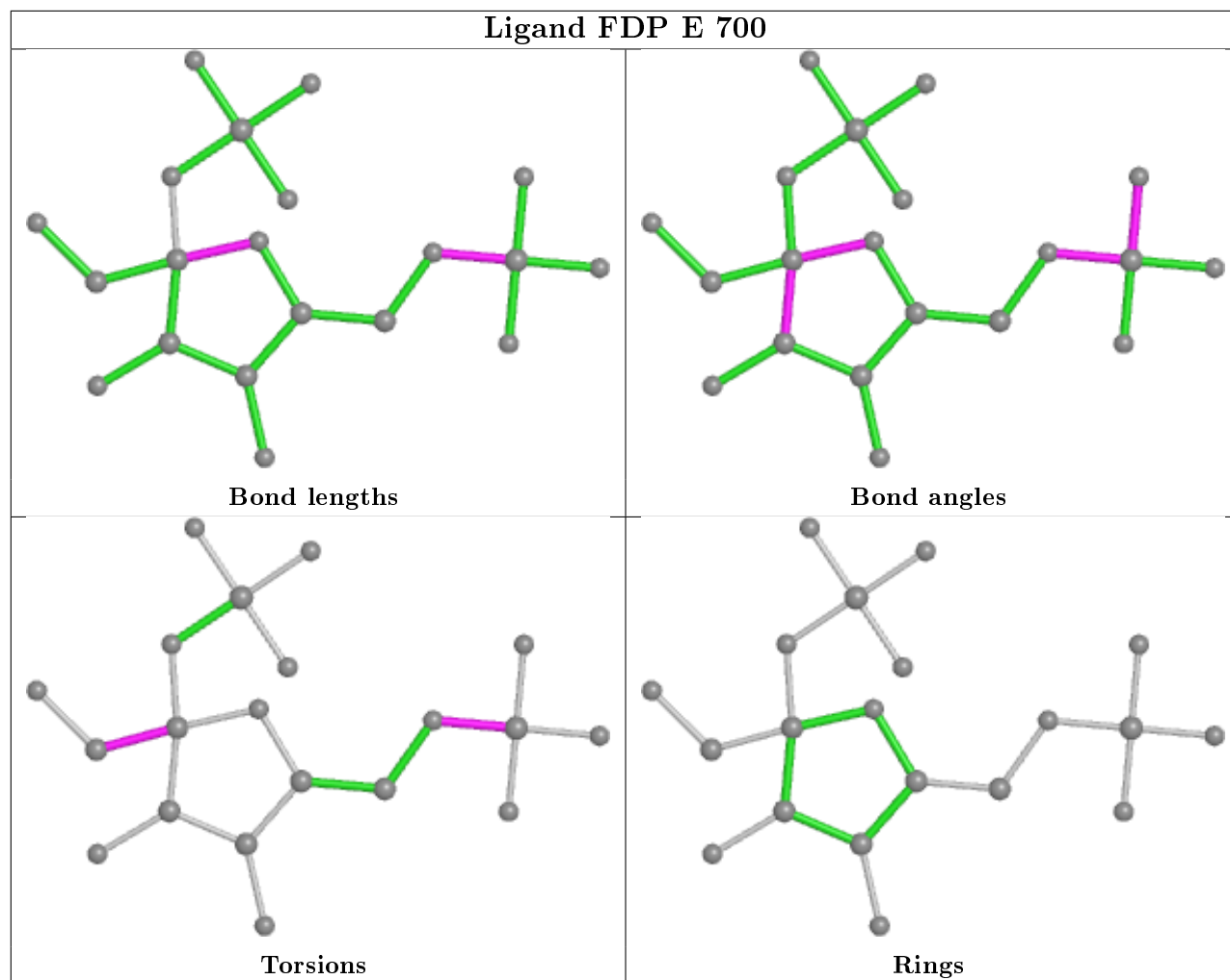


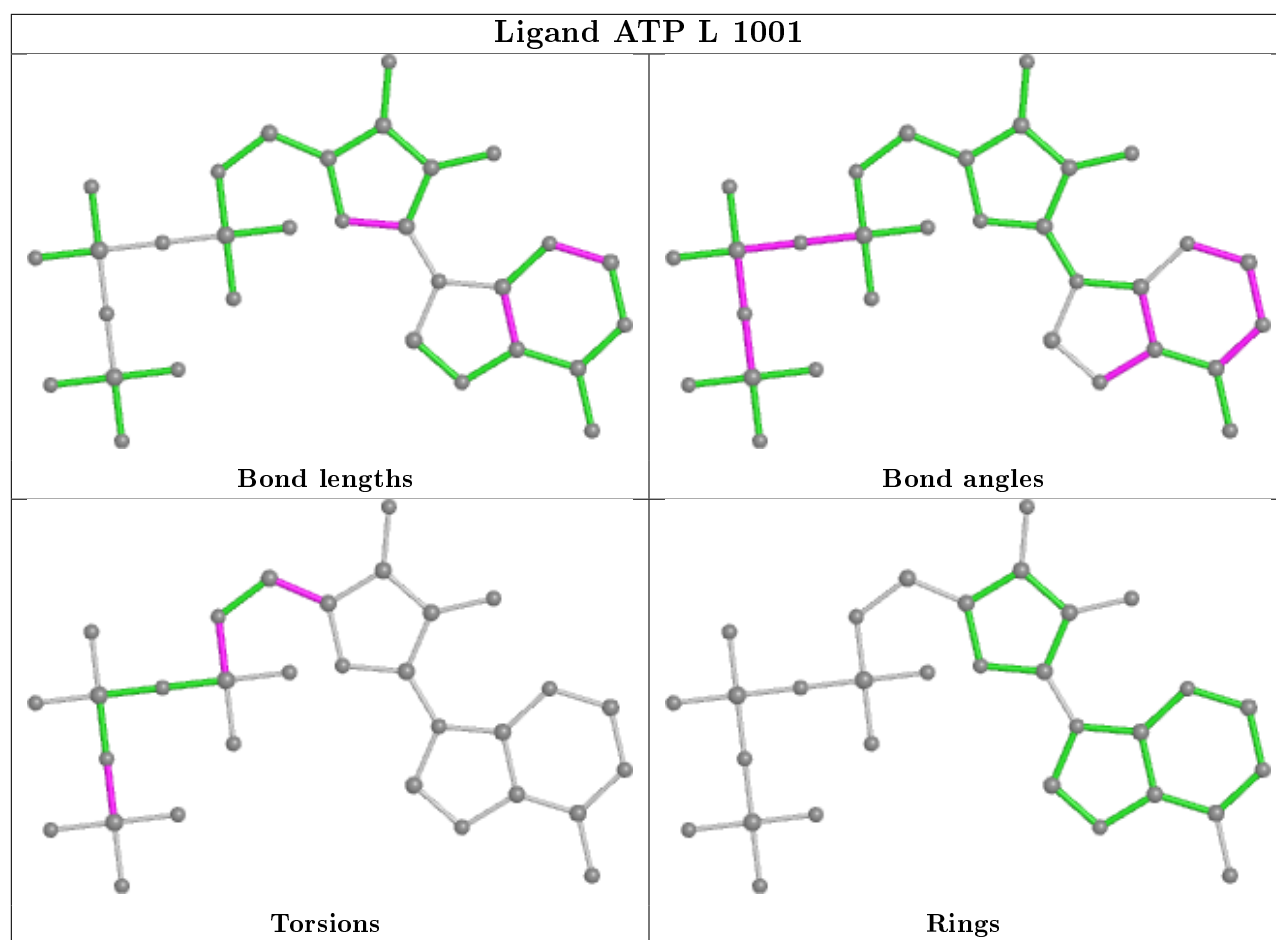


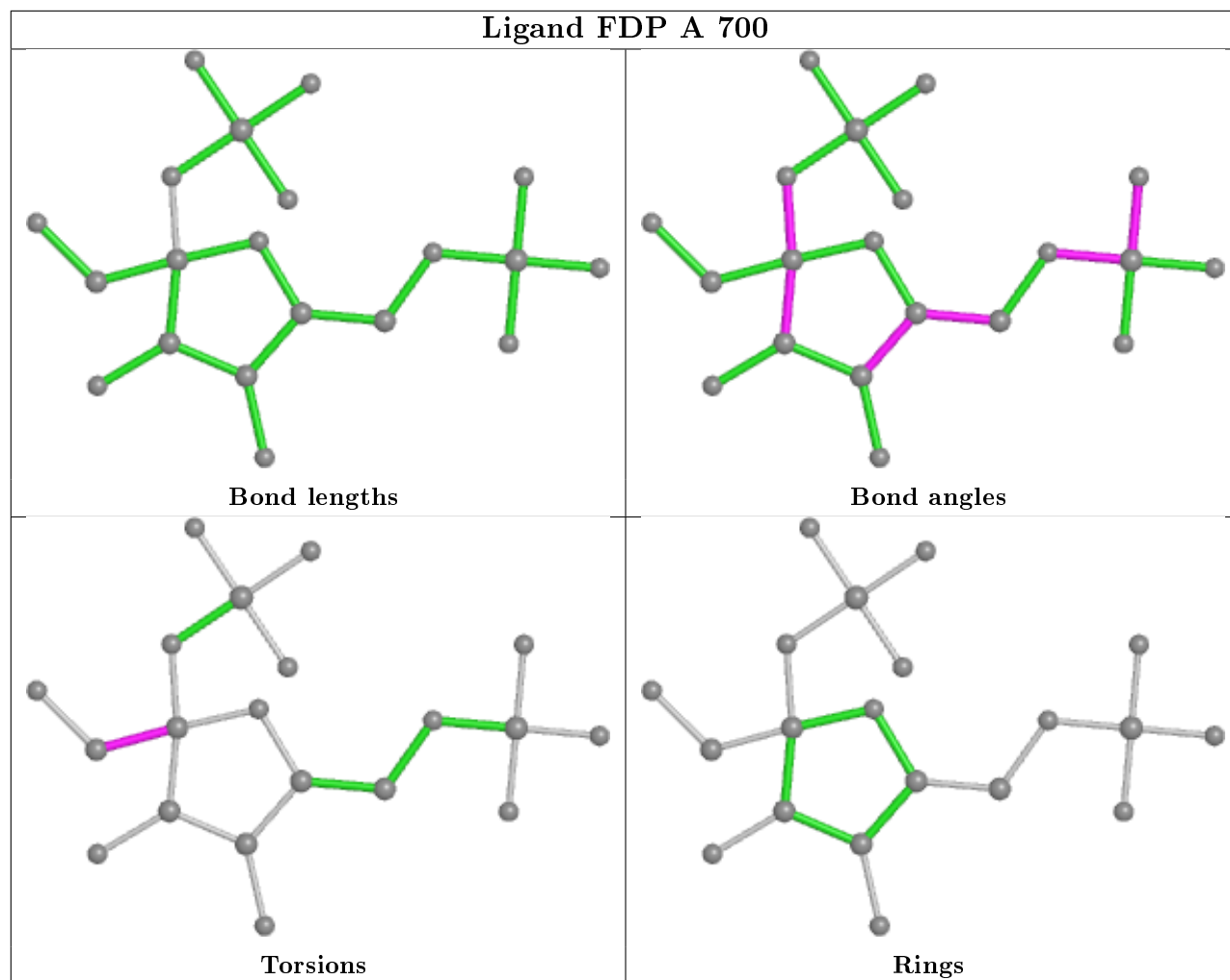


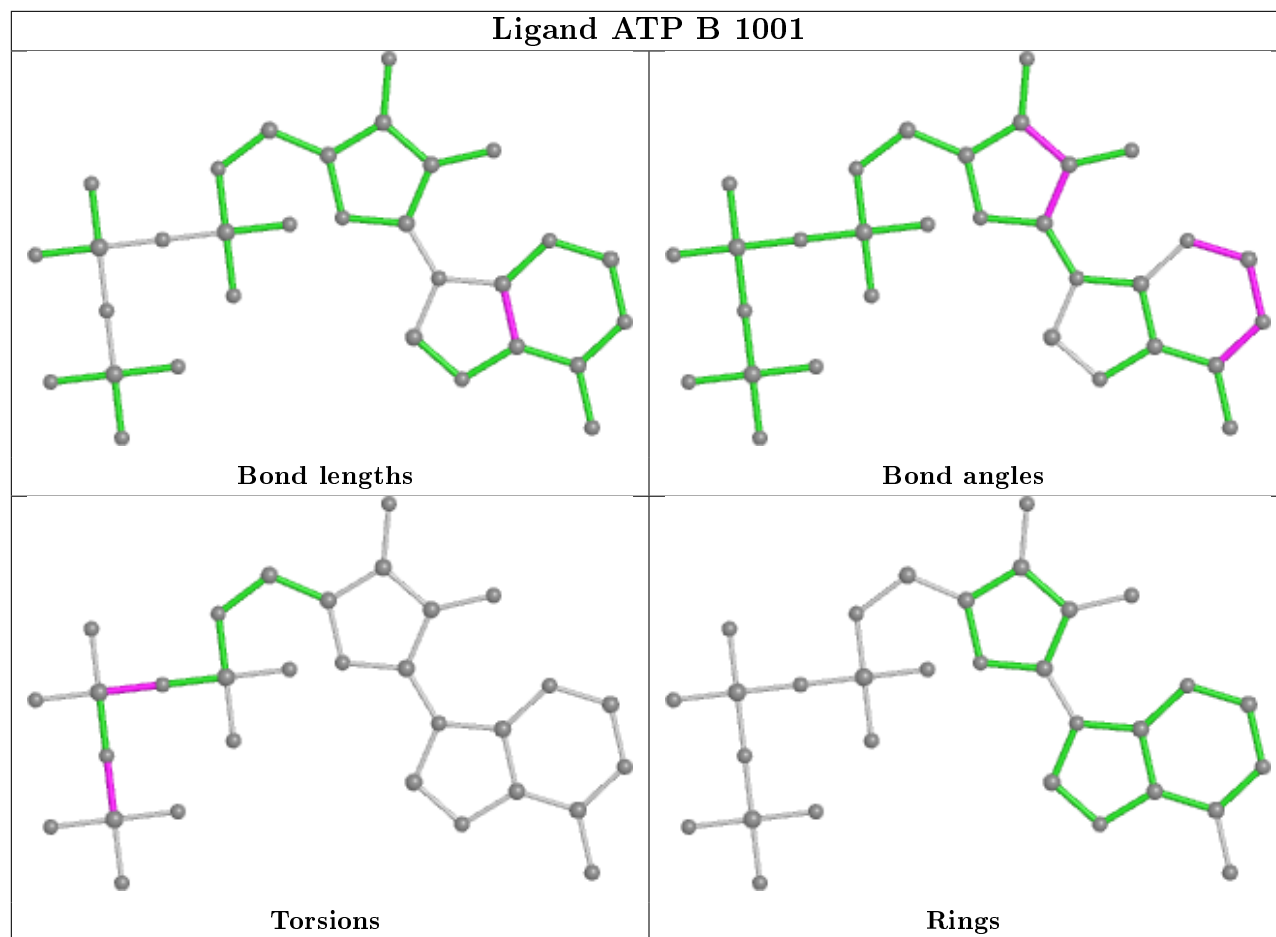


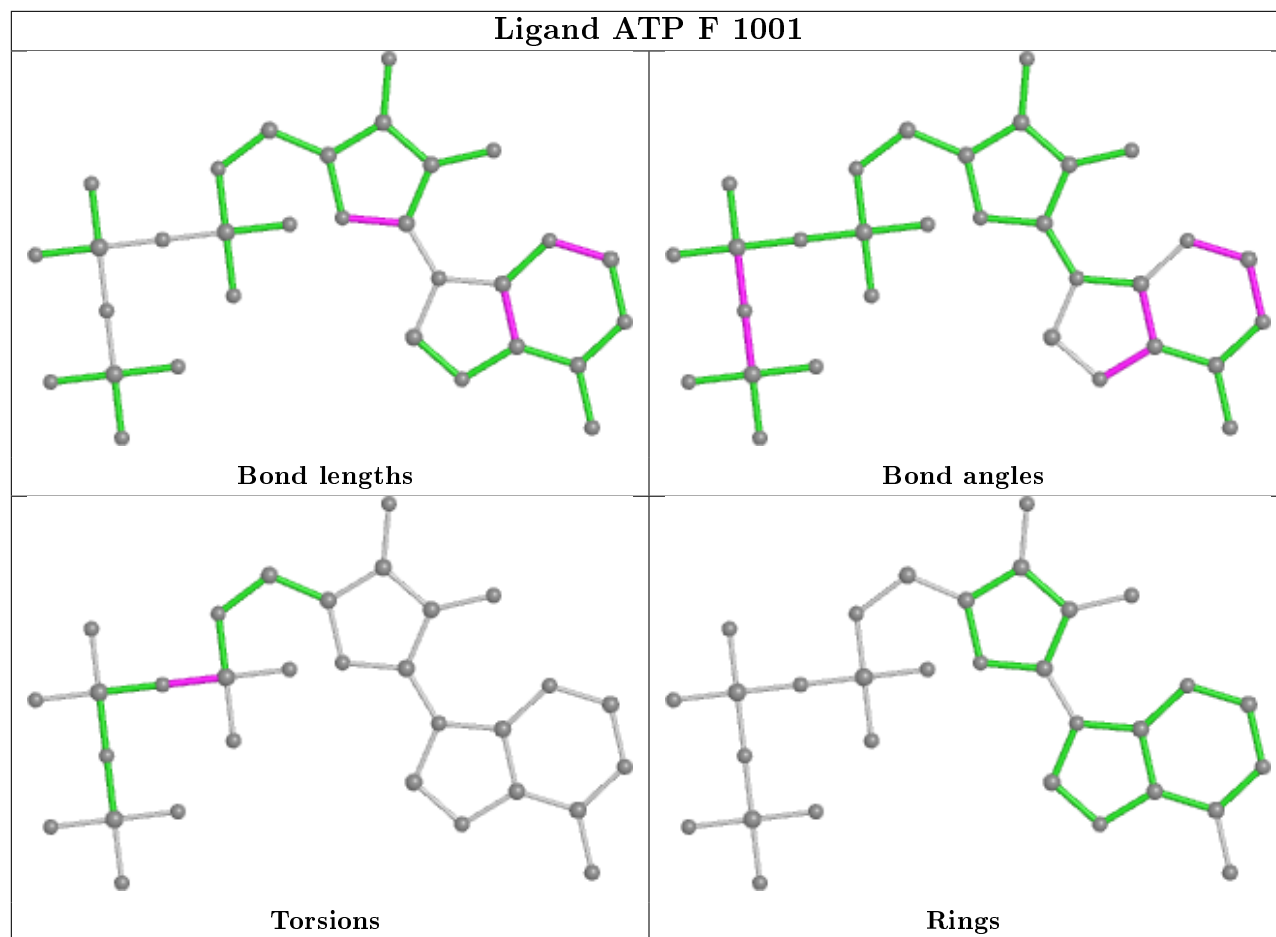
## Ligand FDP E 700

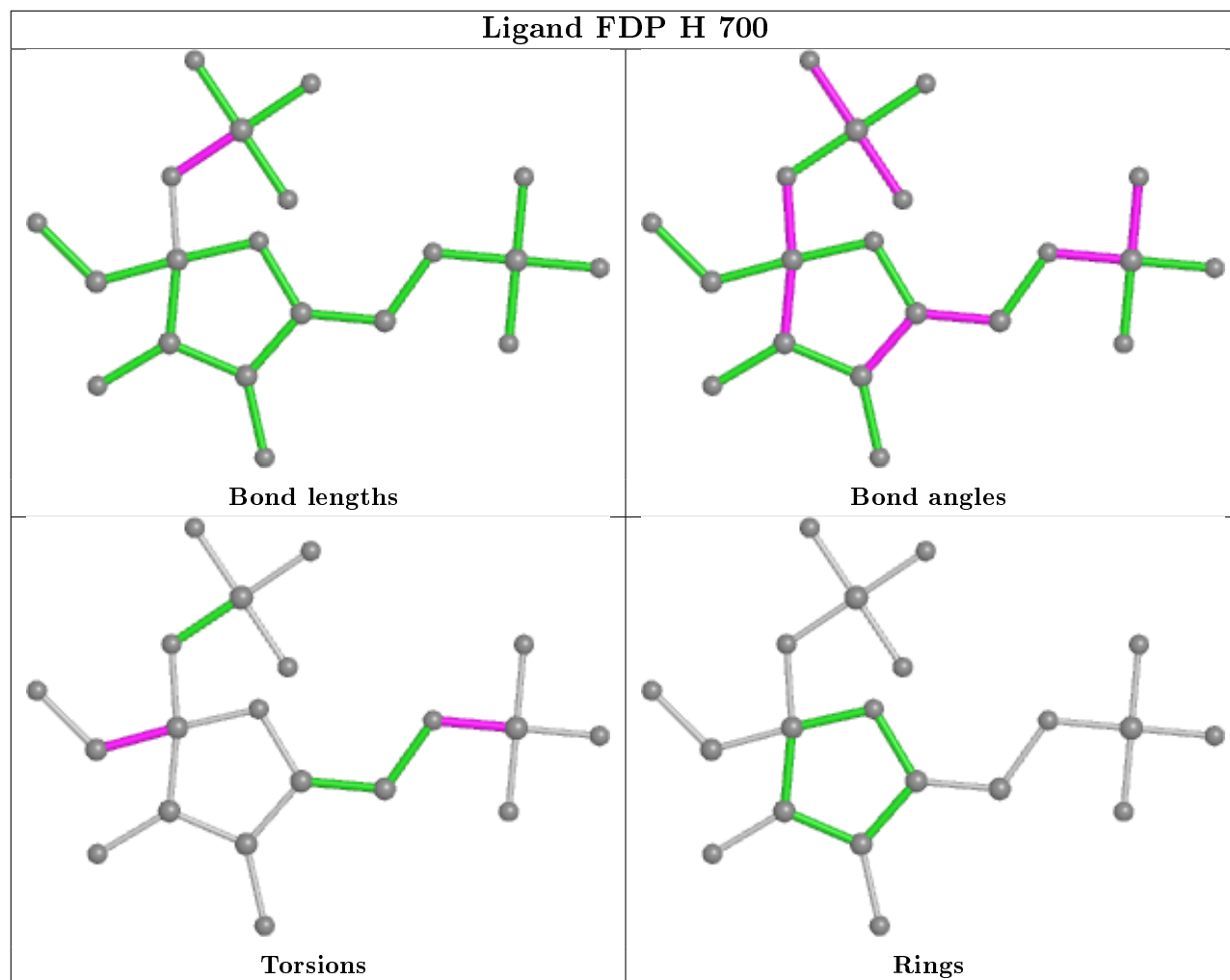


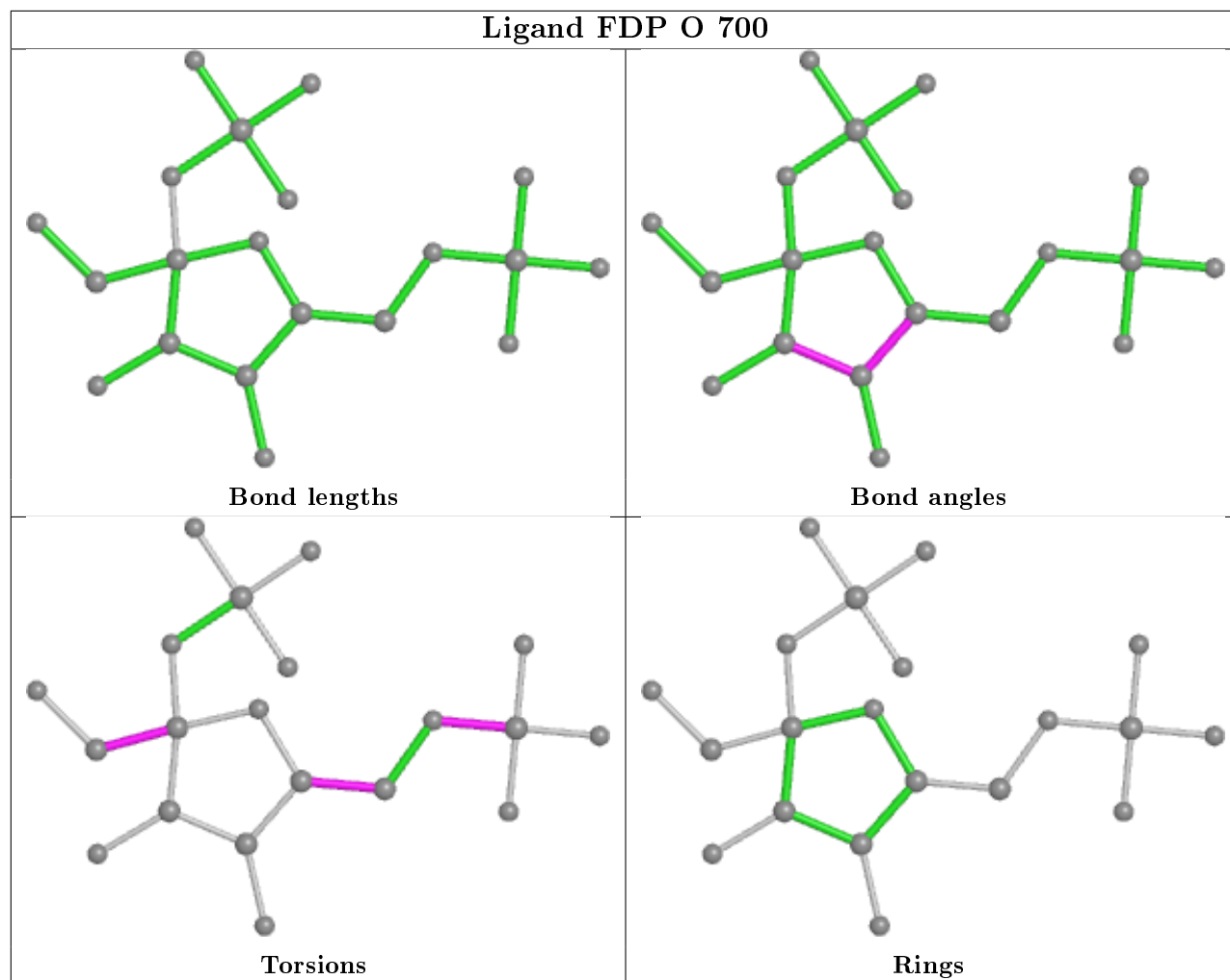




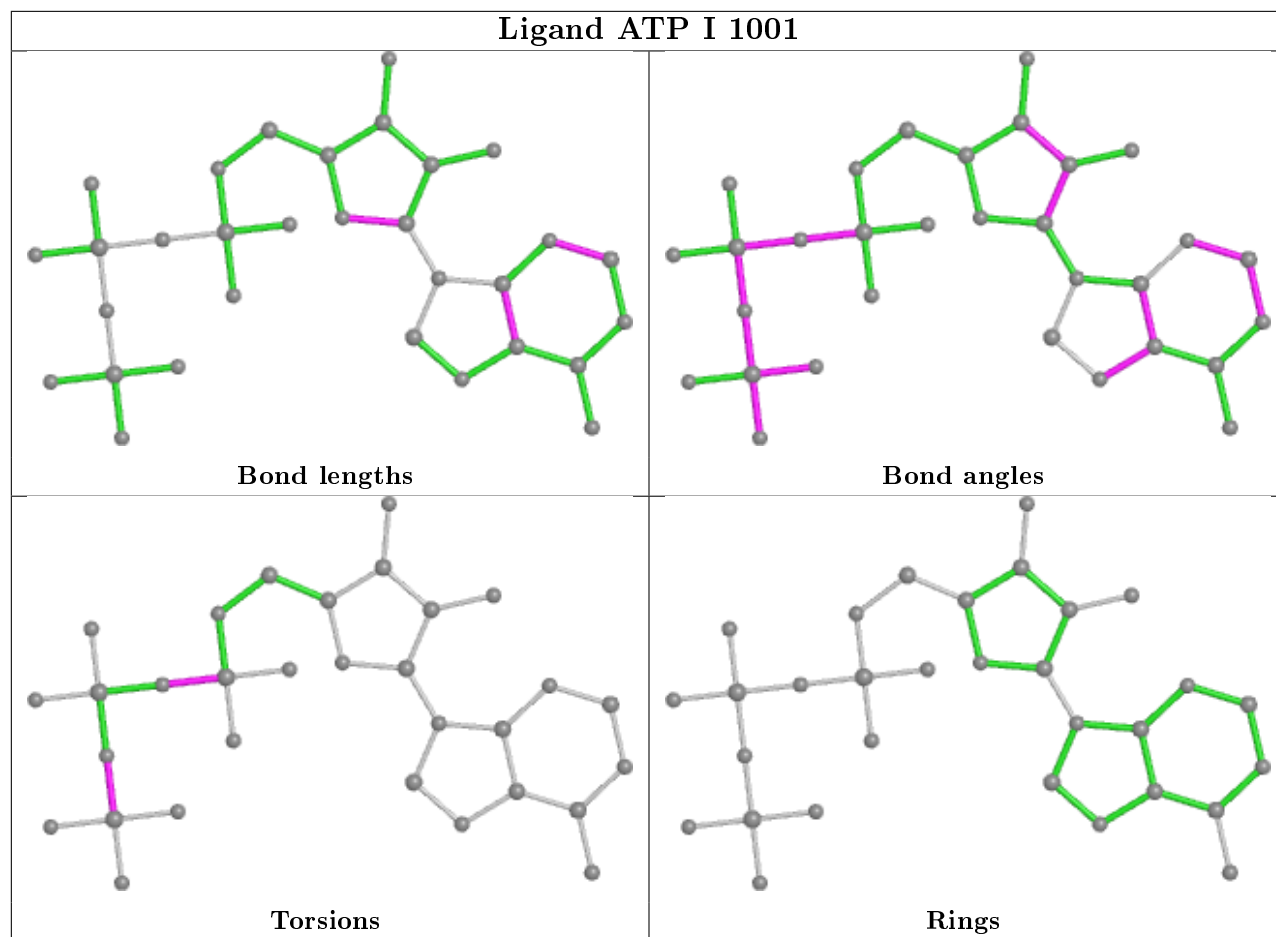


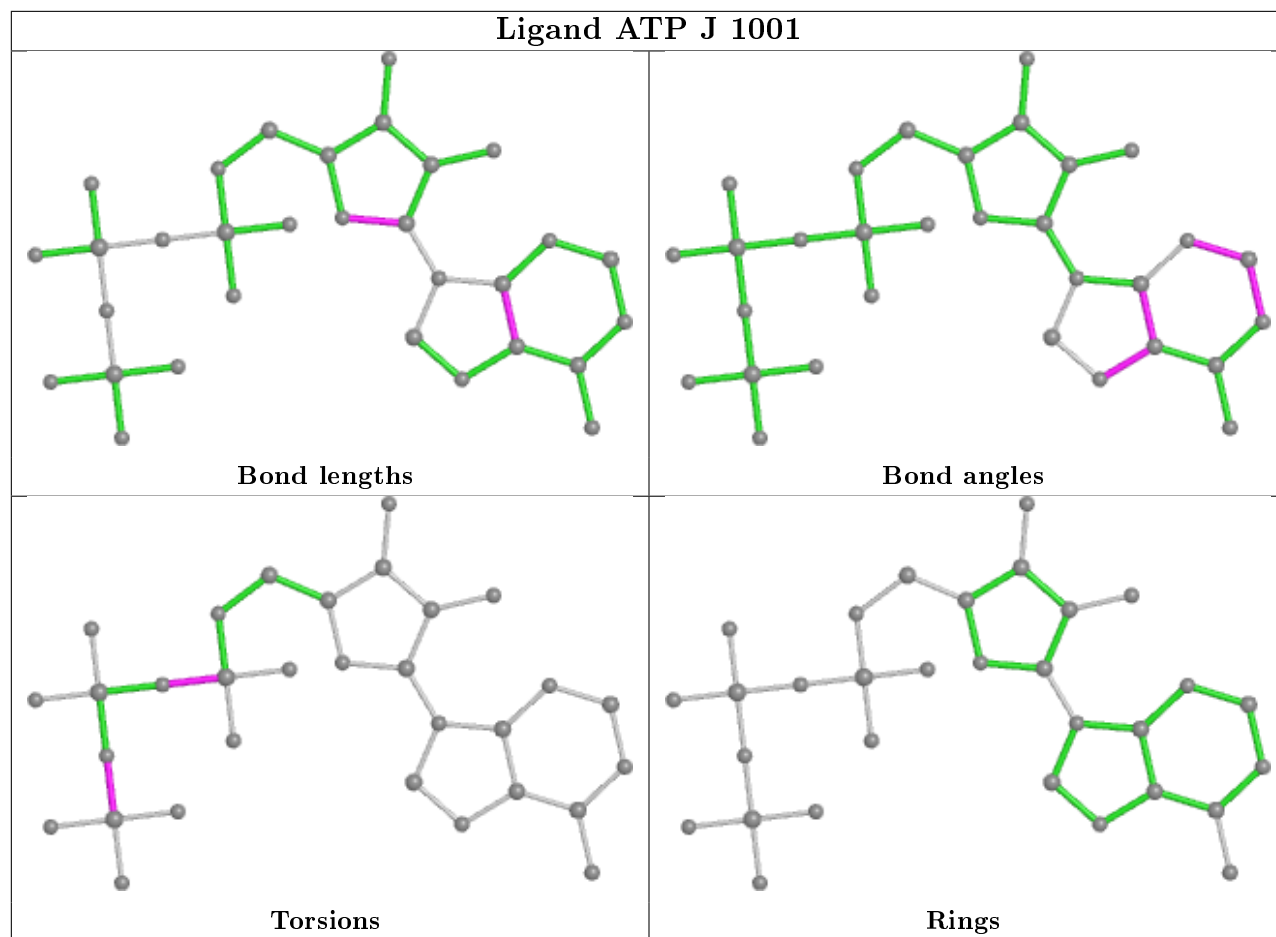


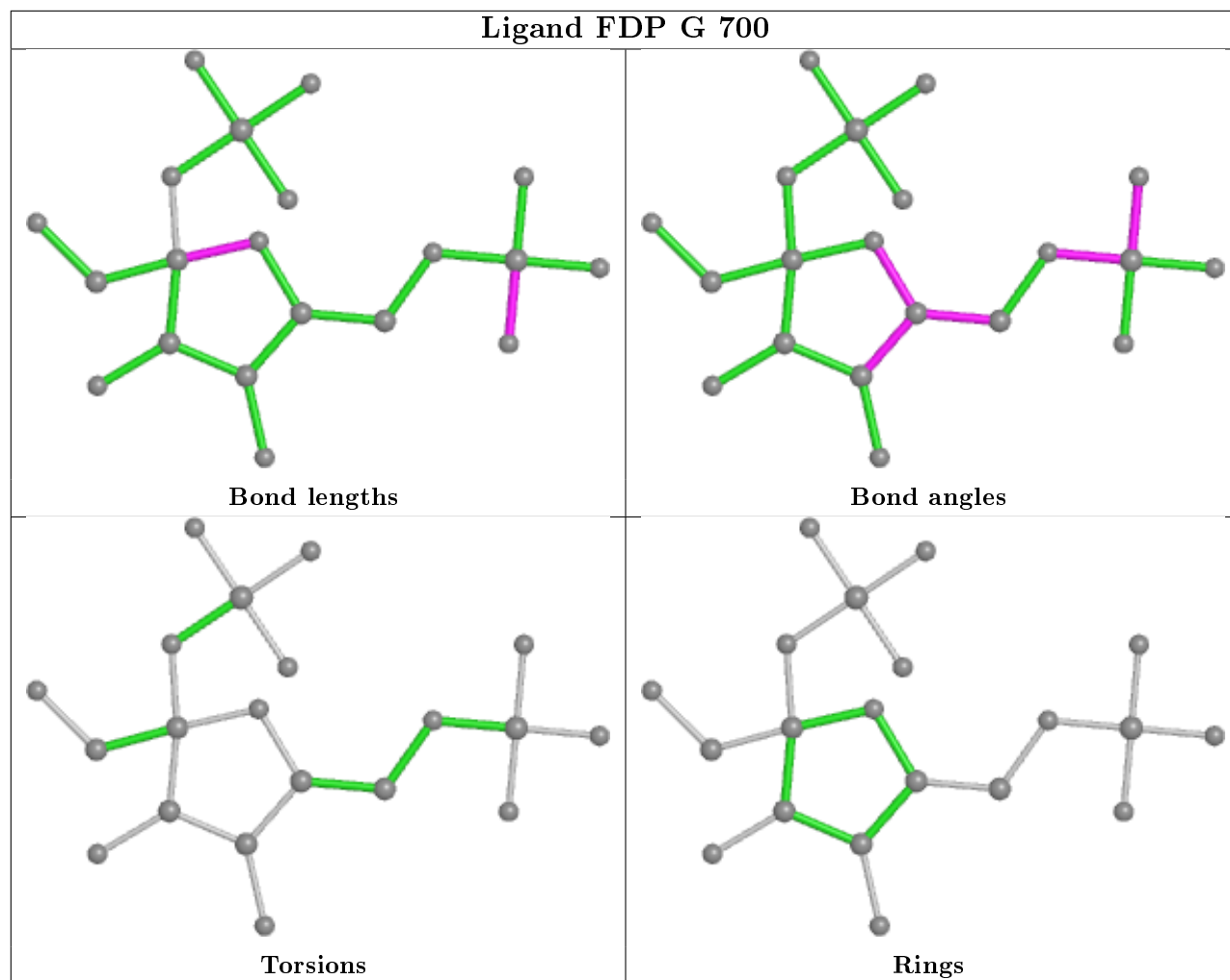


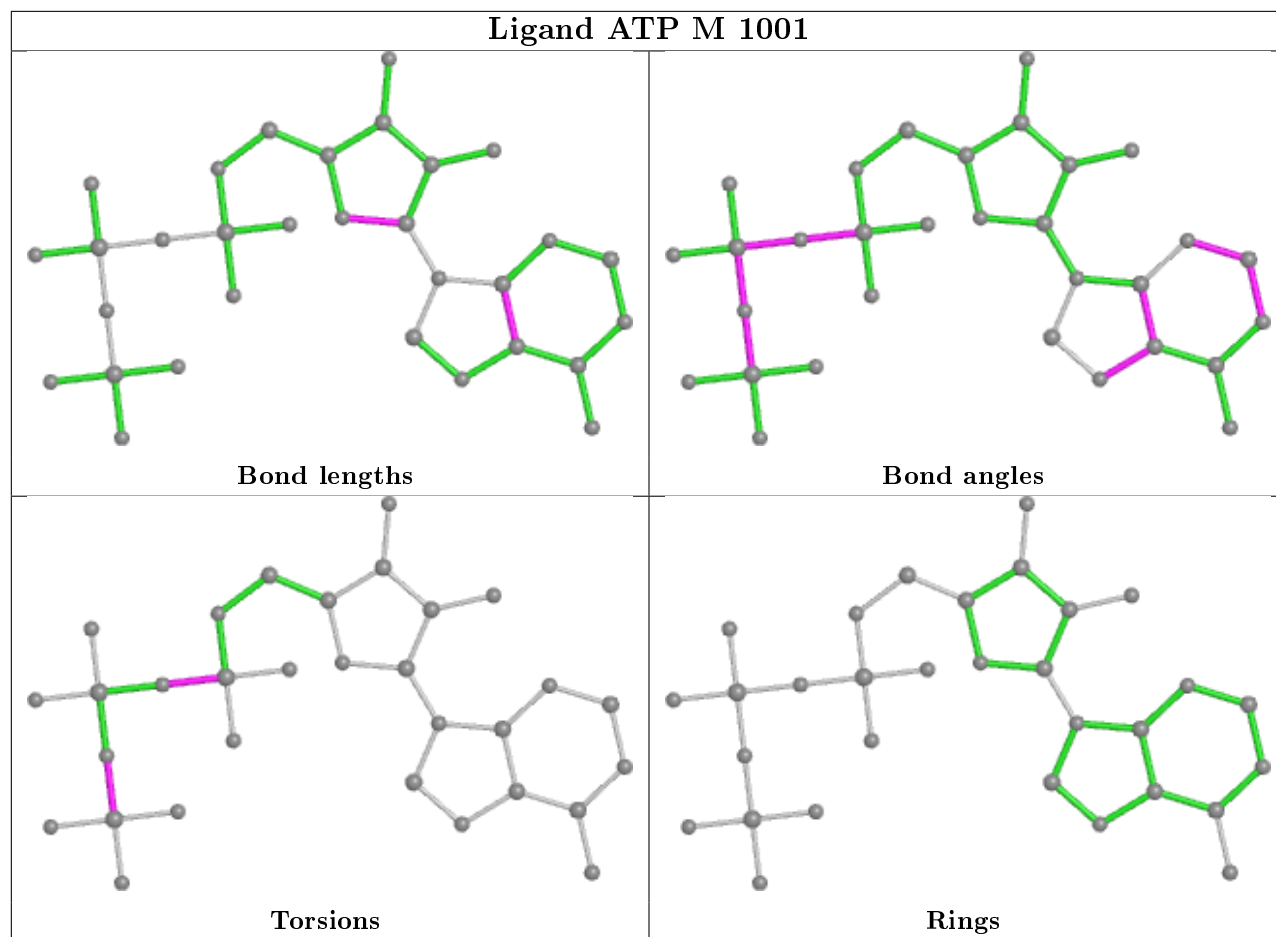


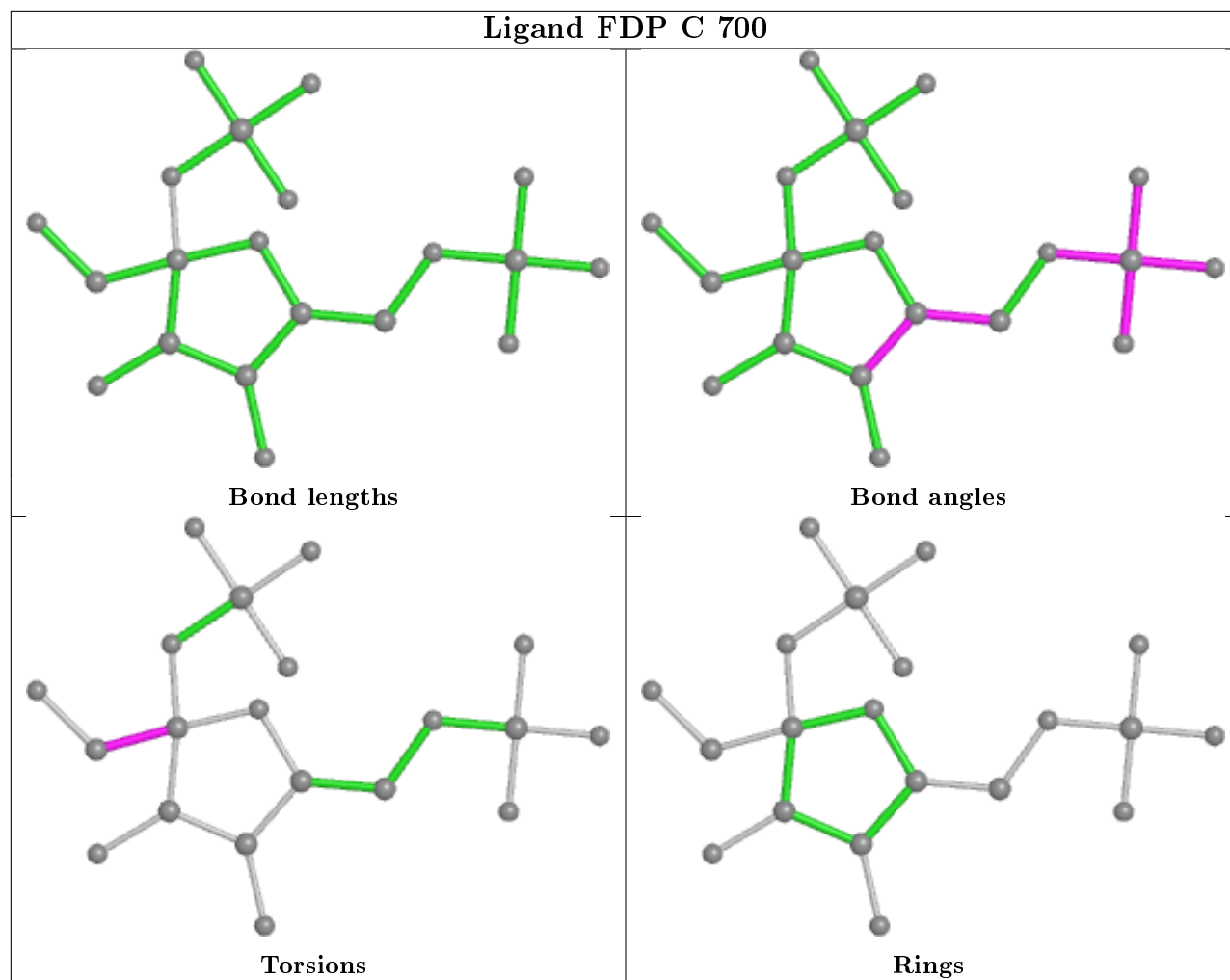


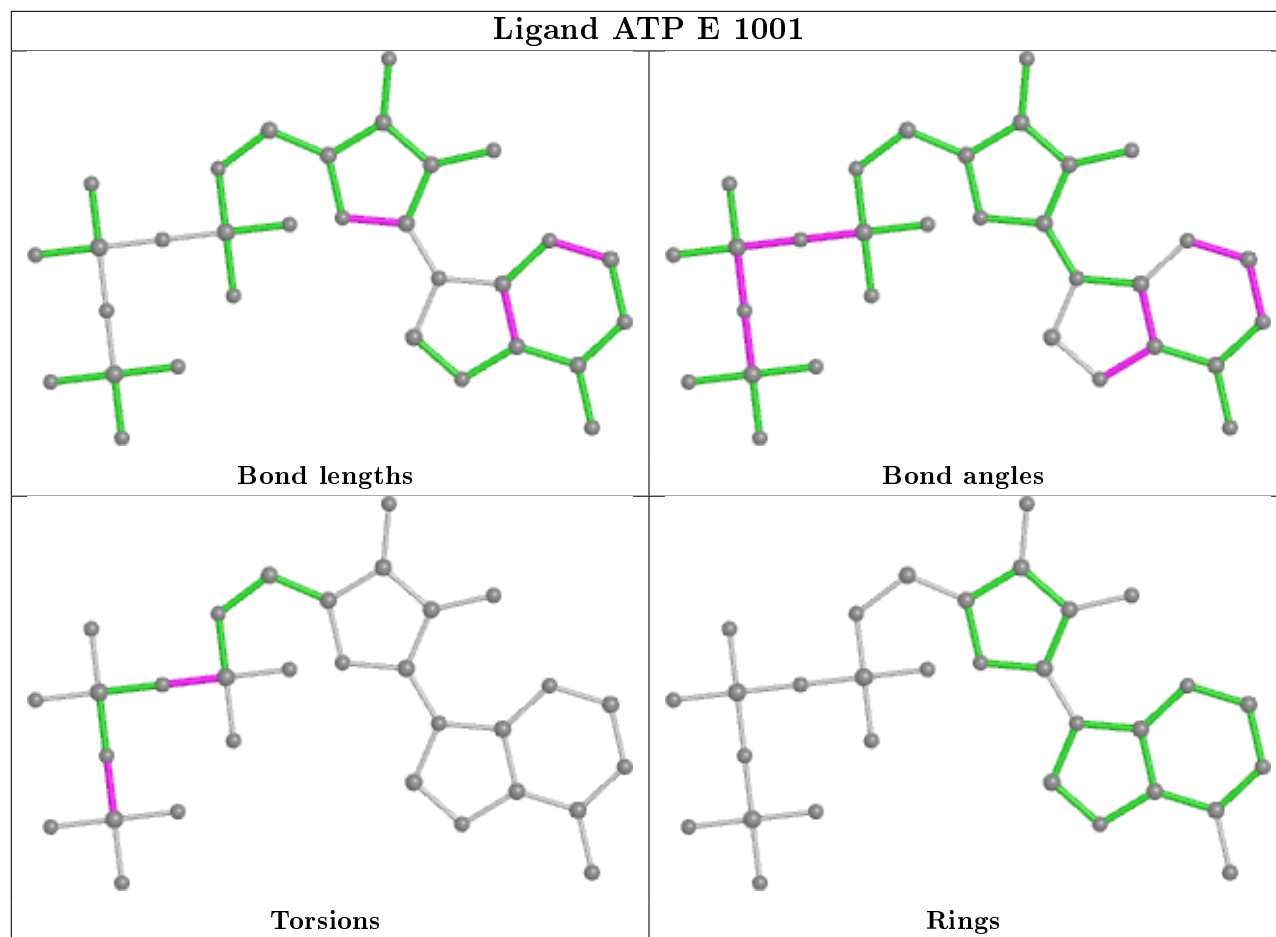


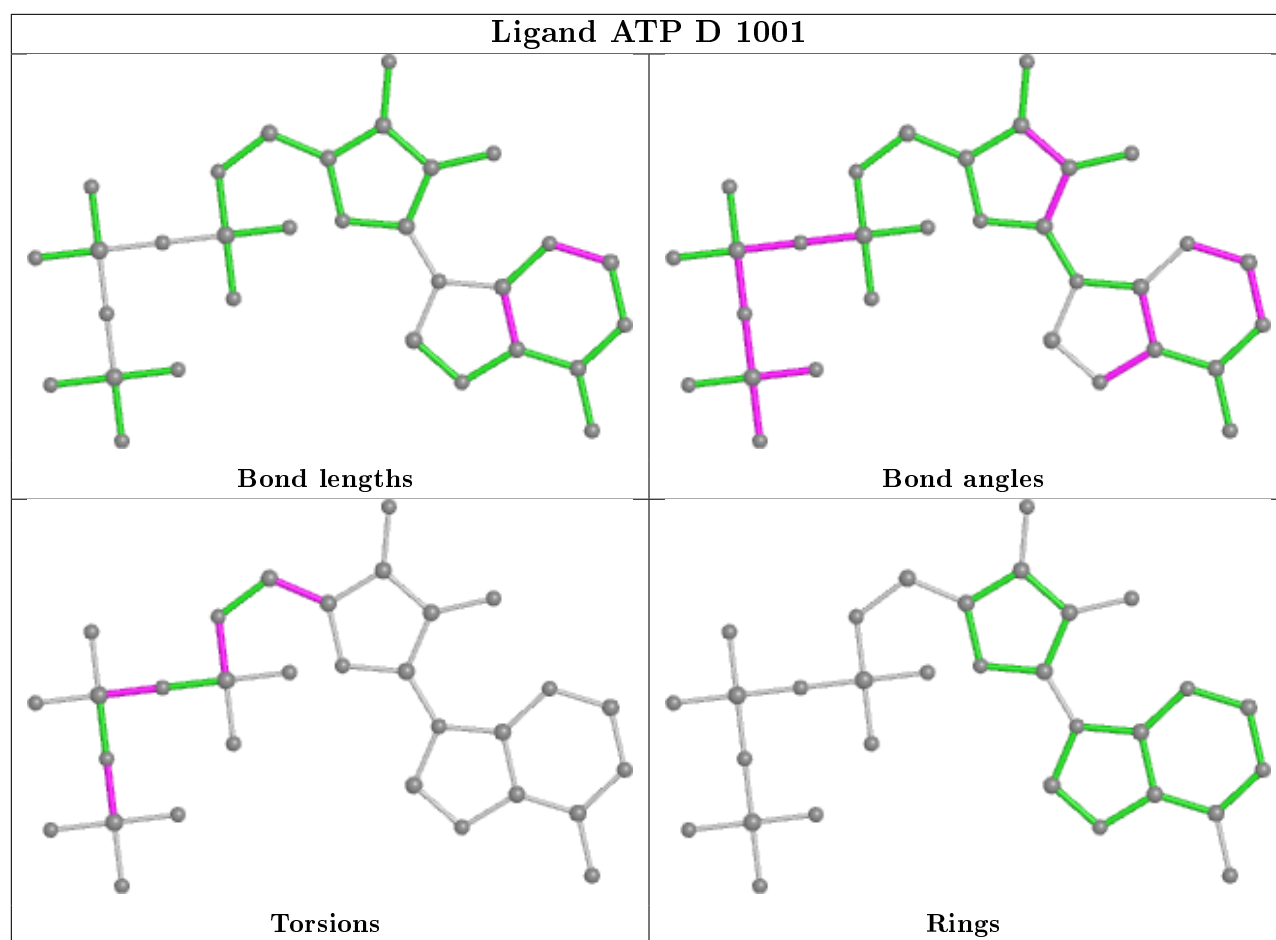


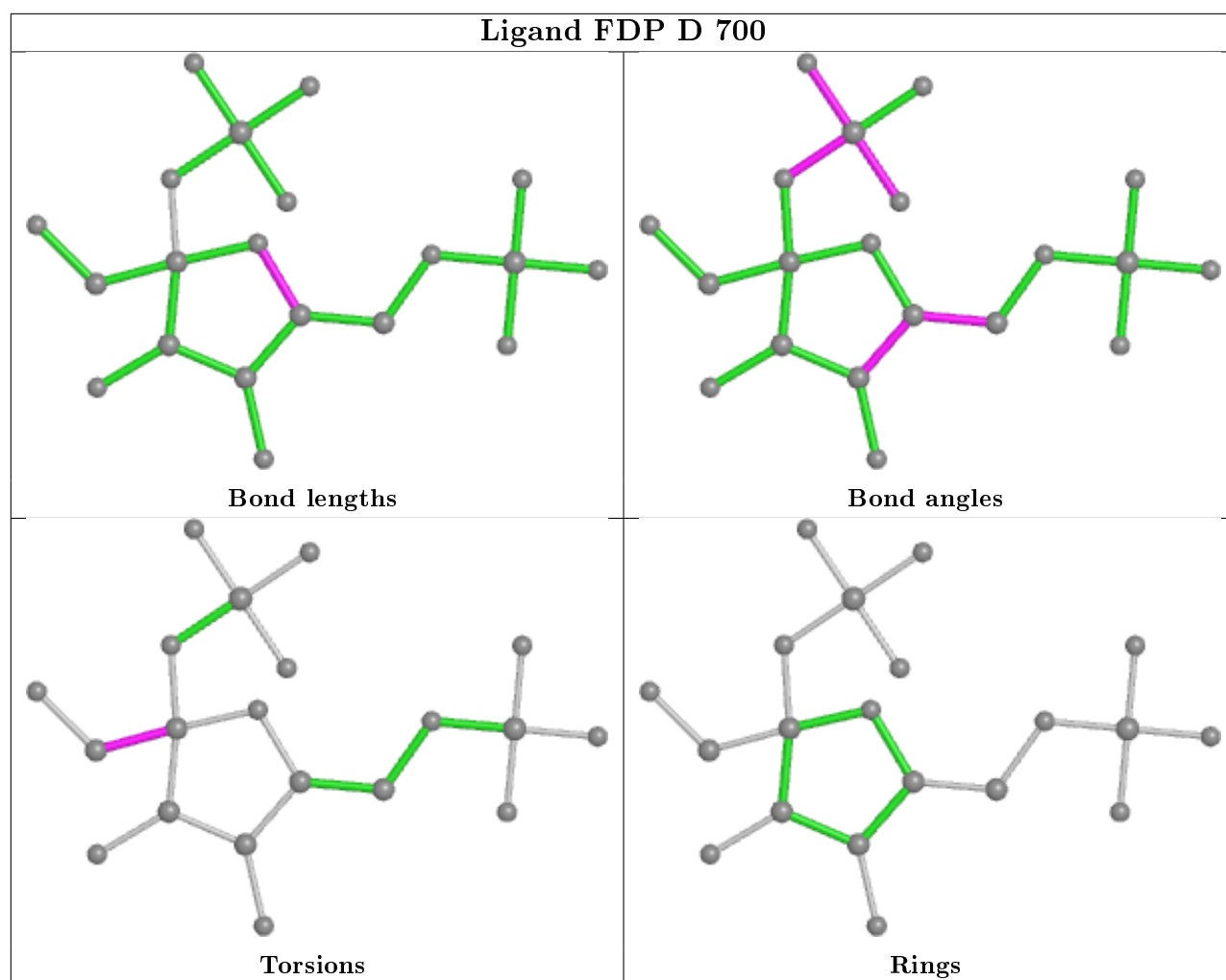




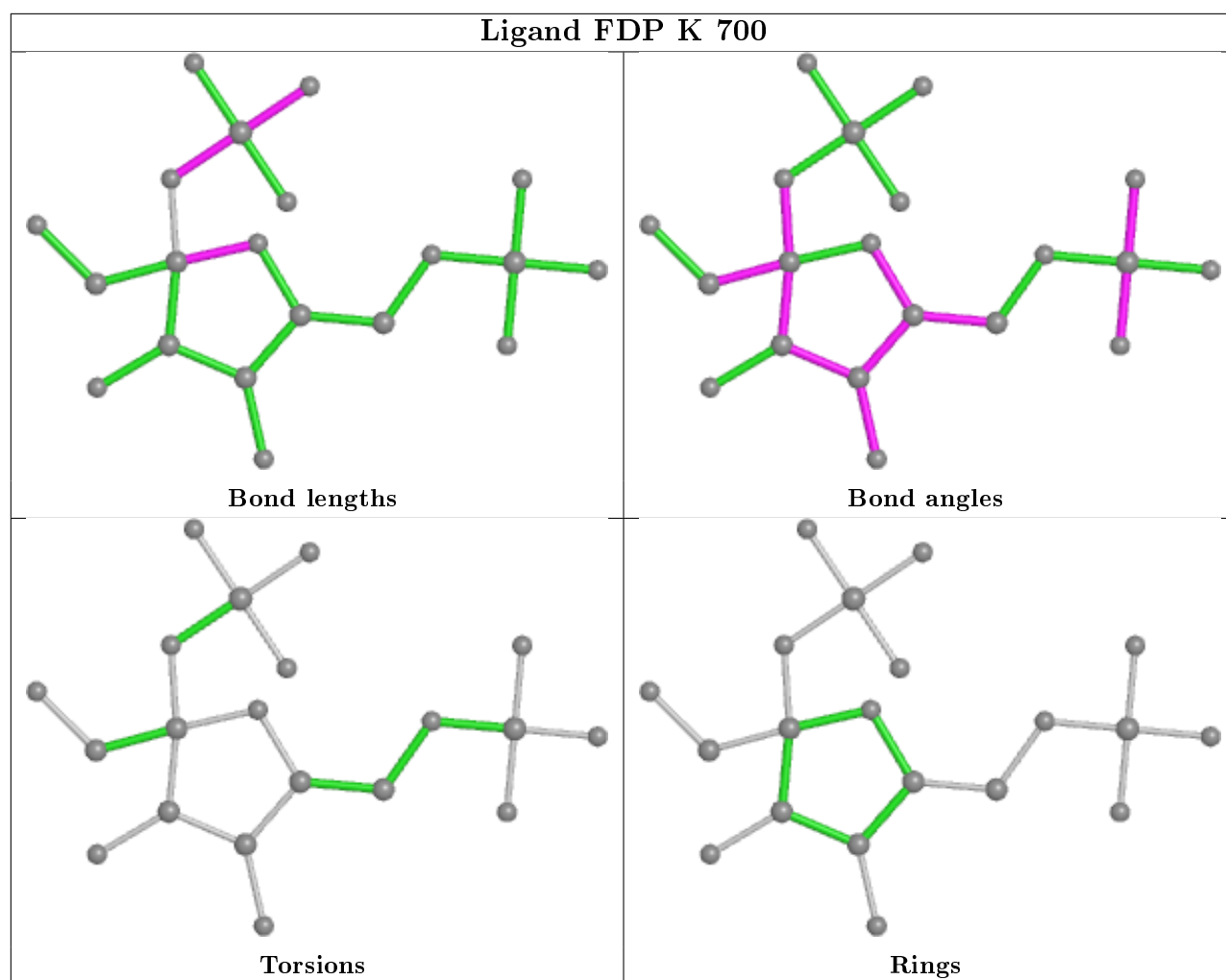


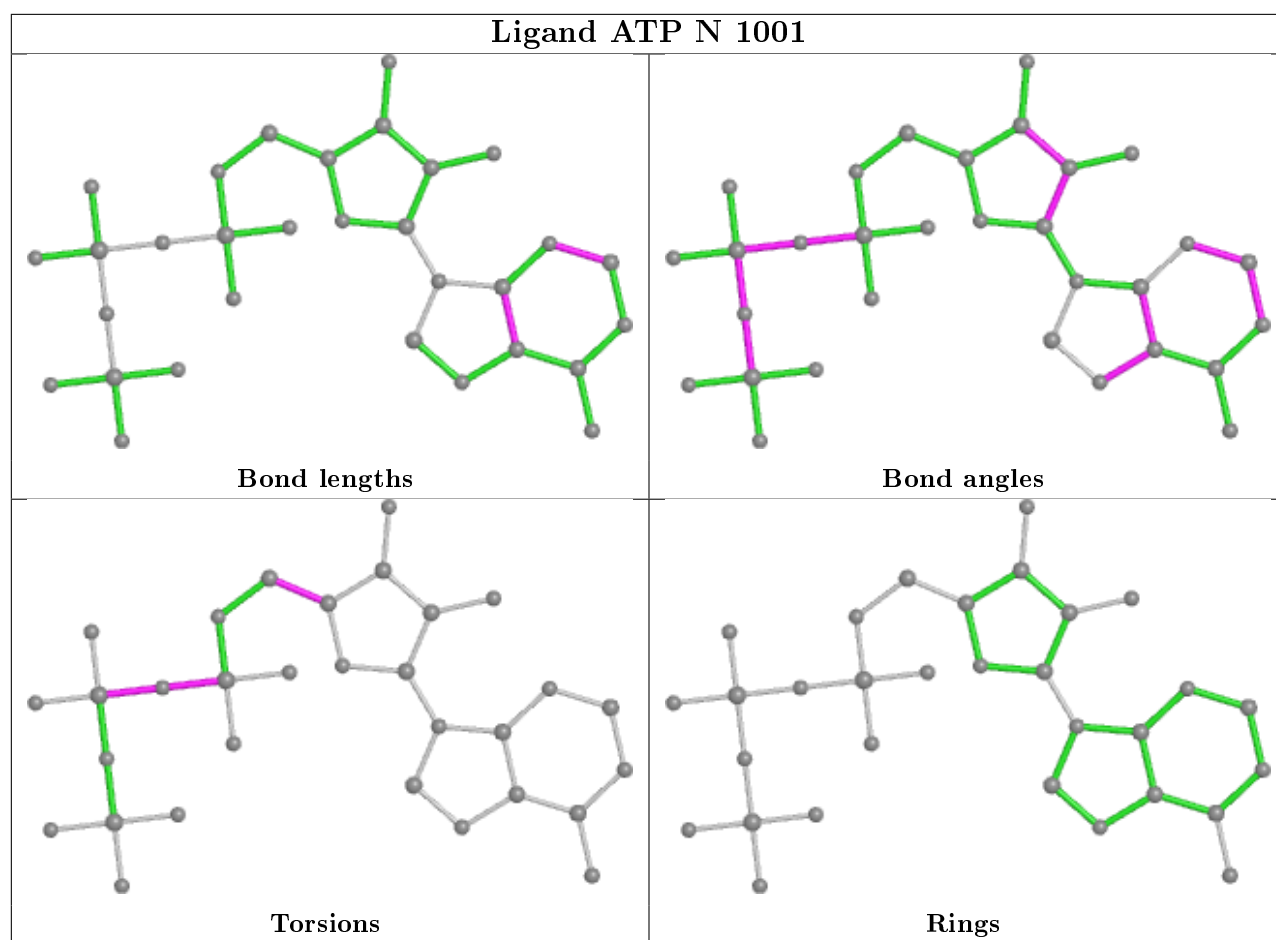


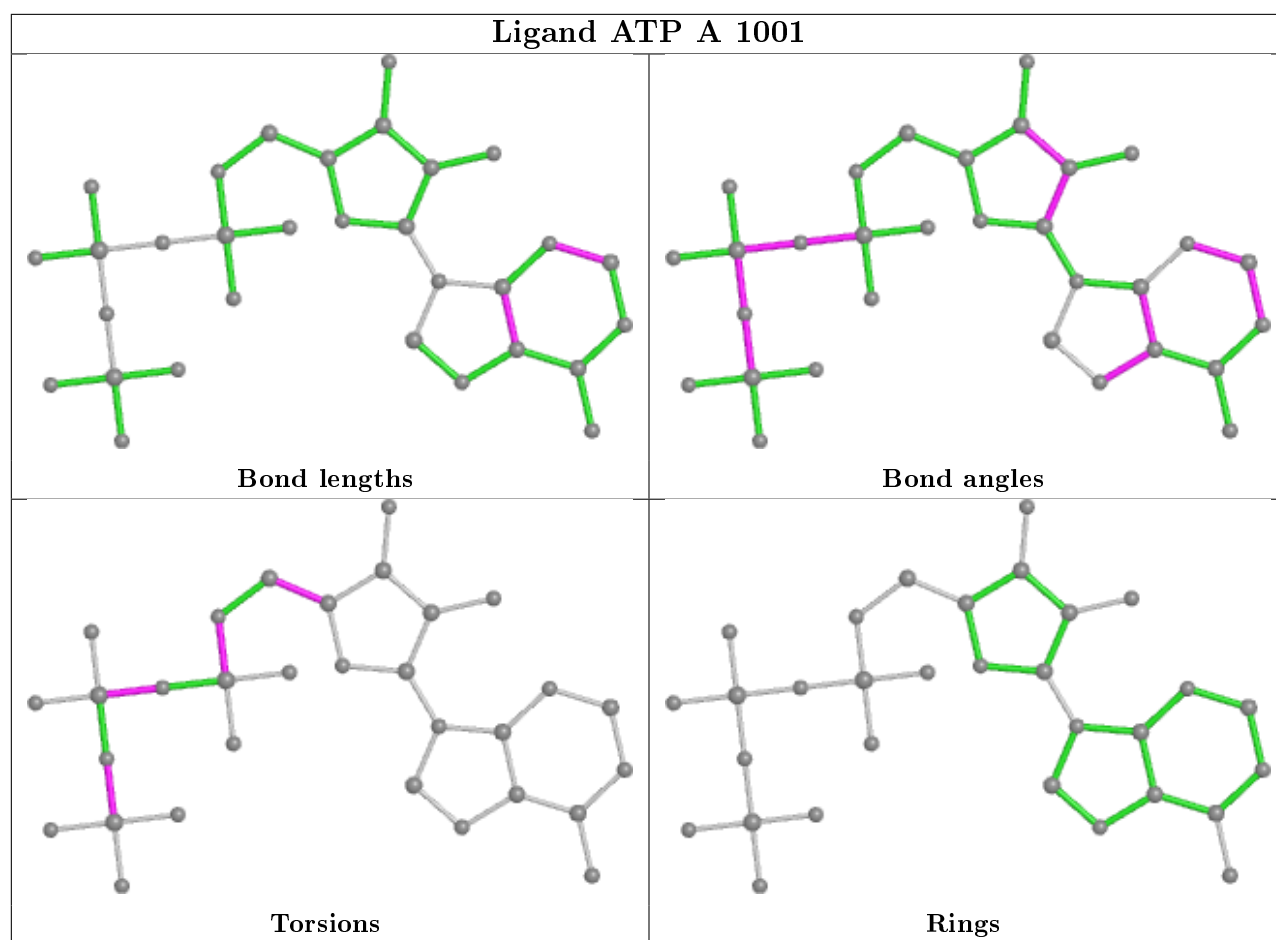


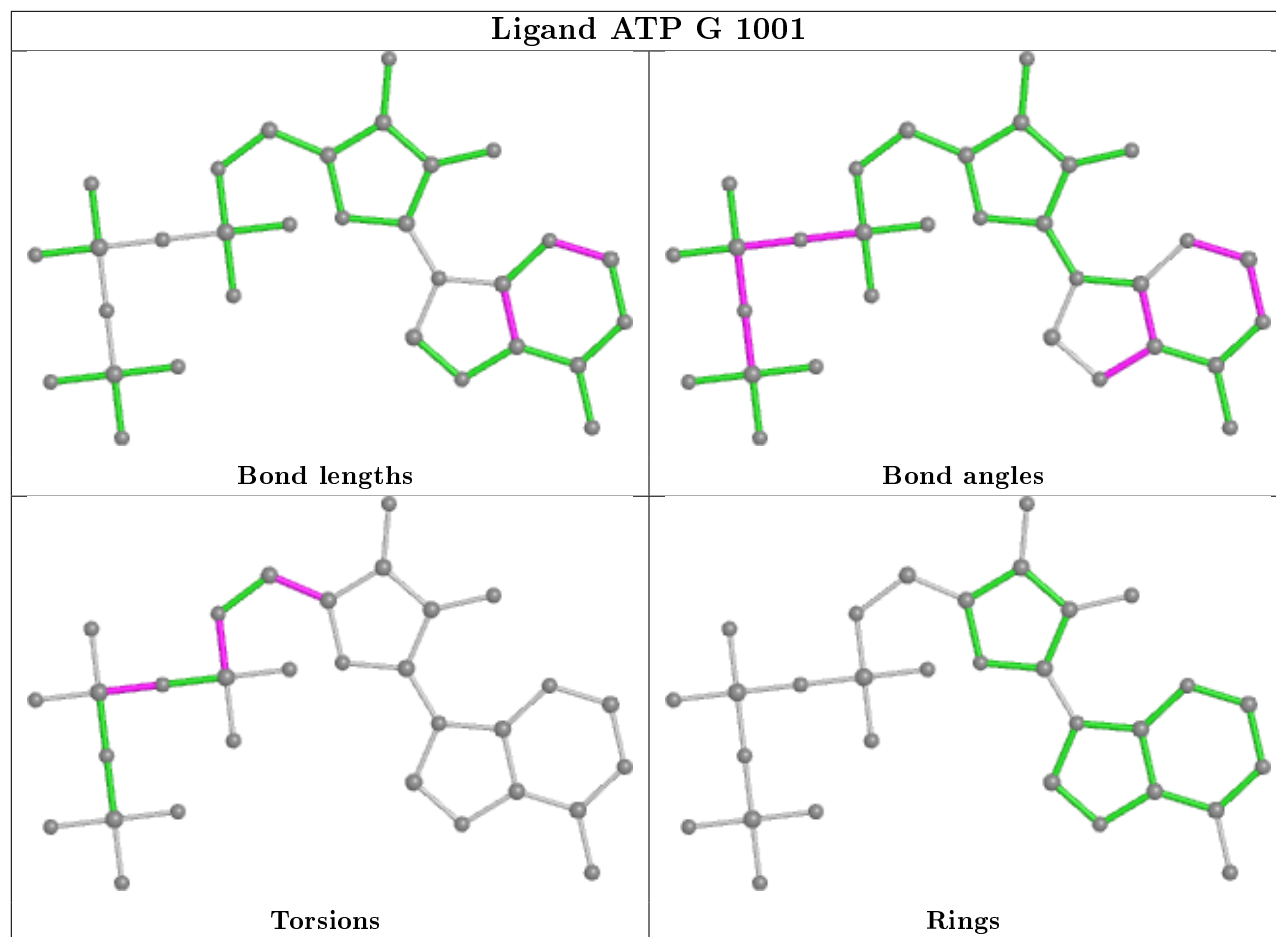




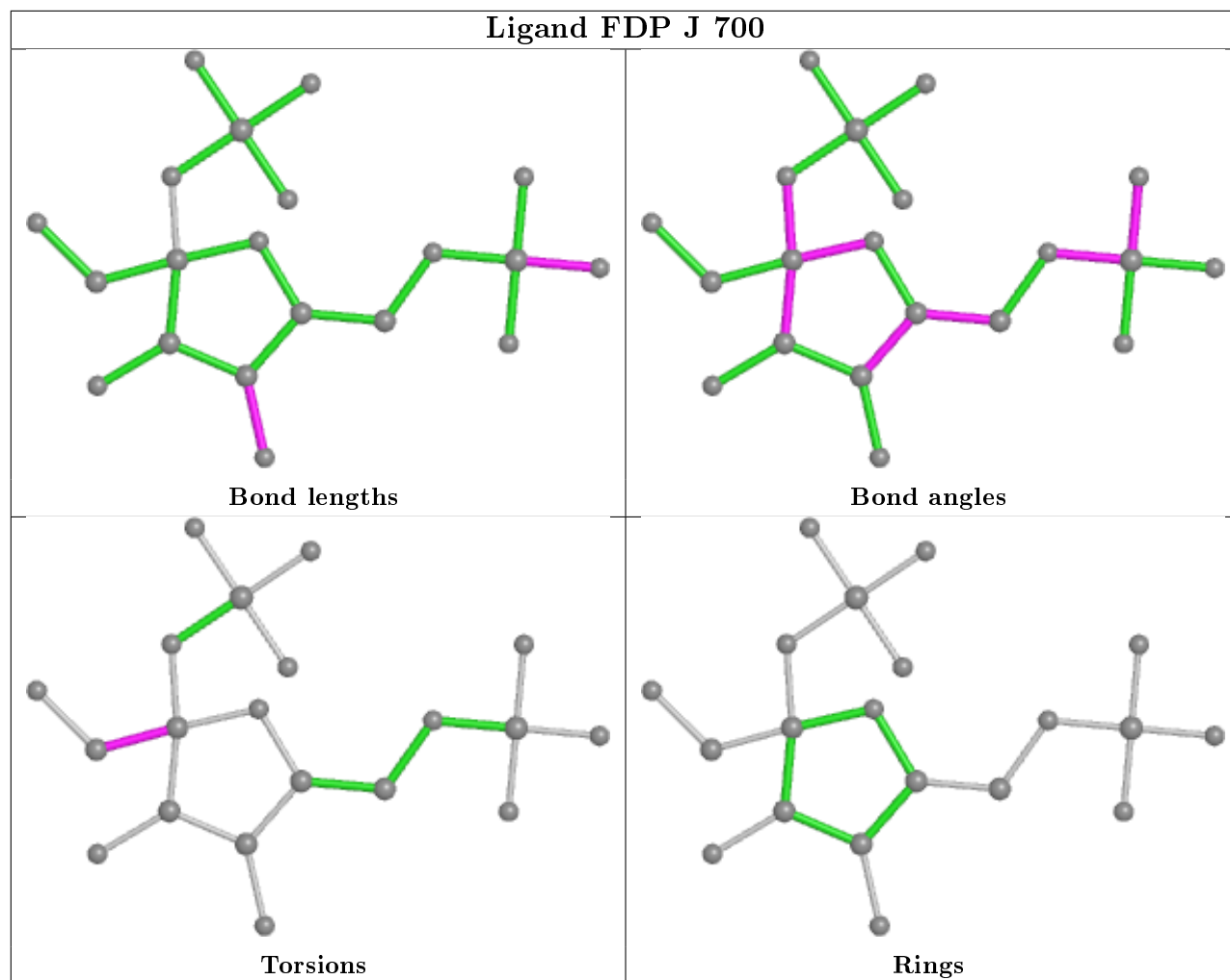


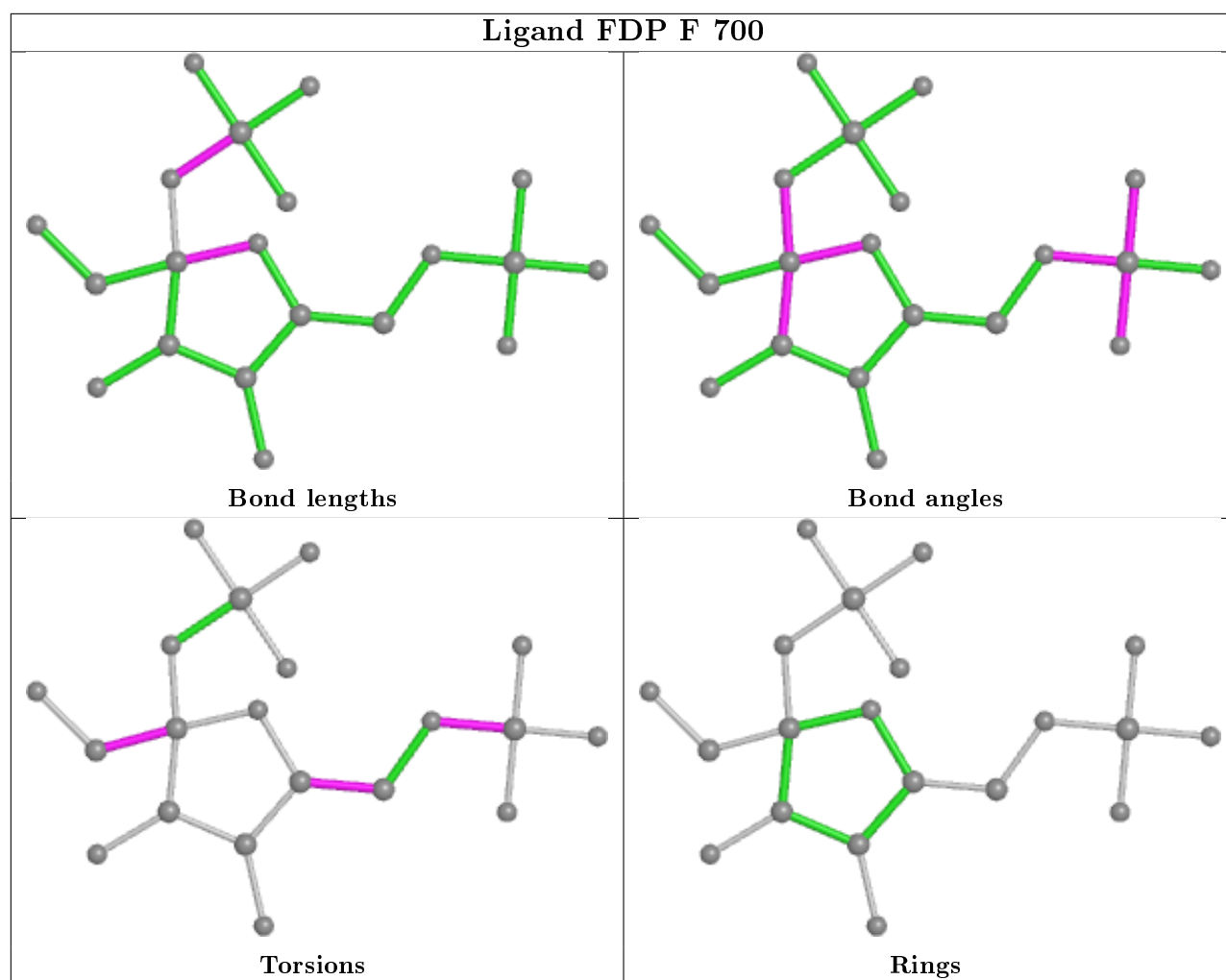




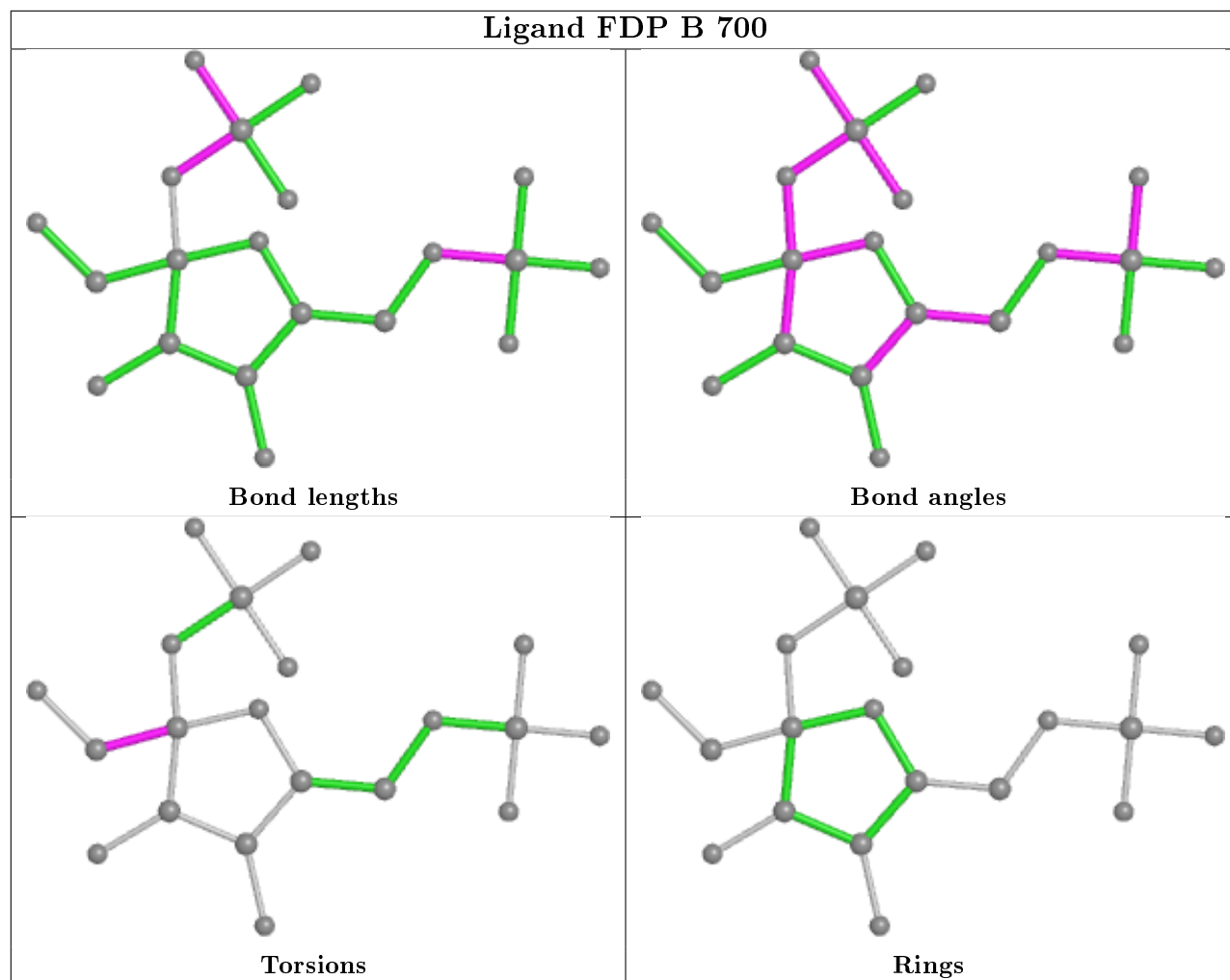


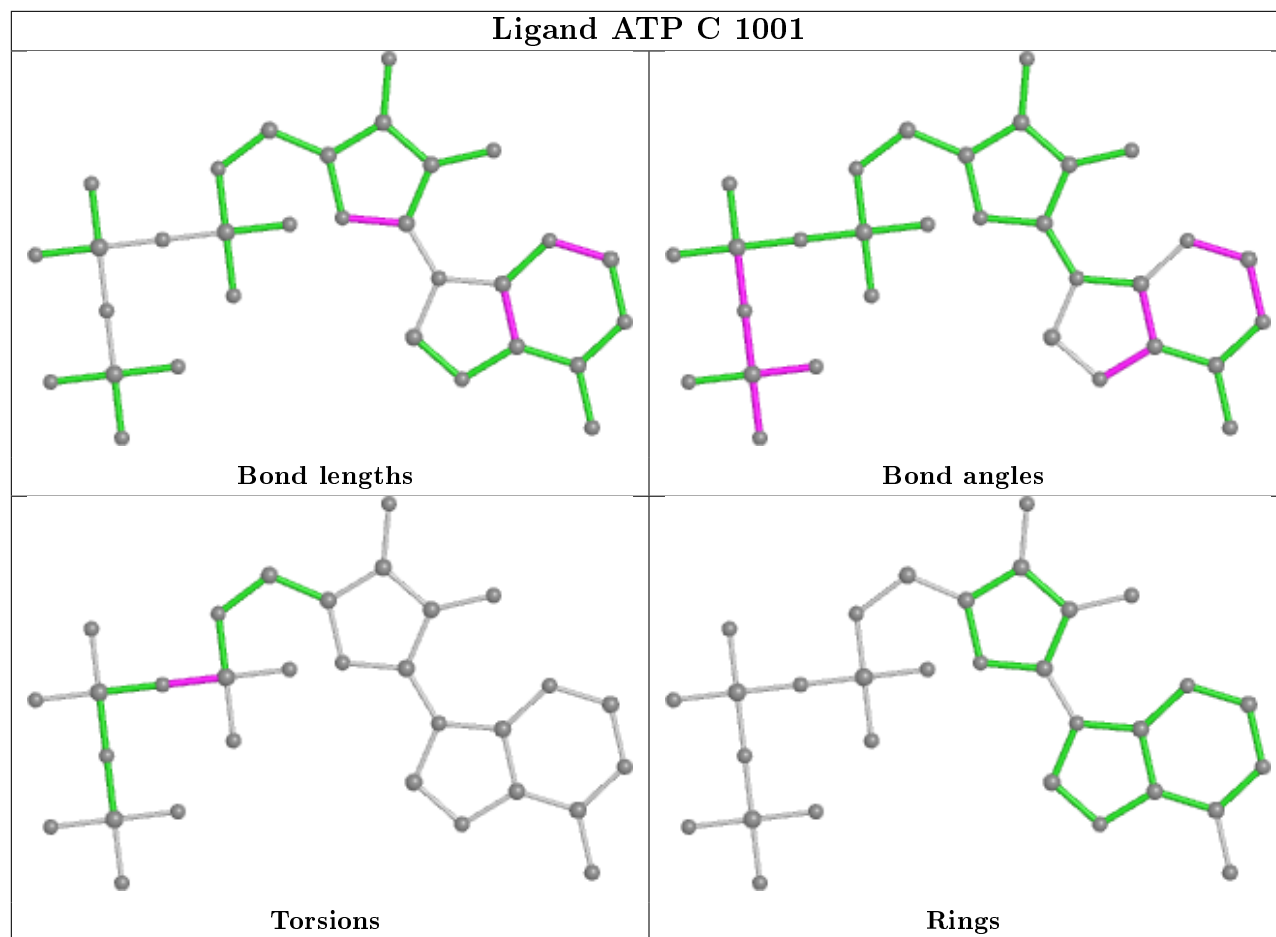
## Ligand FDP J 700





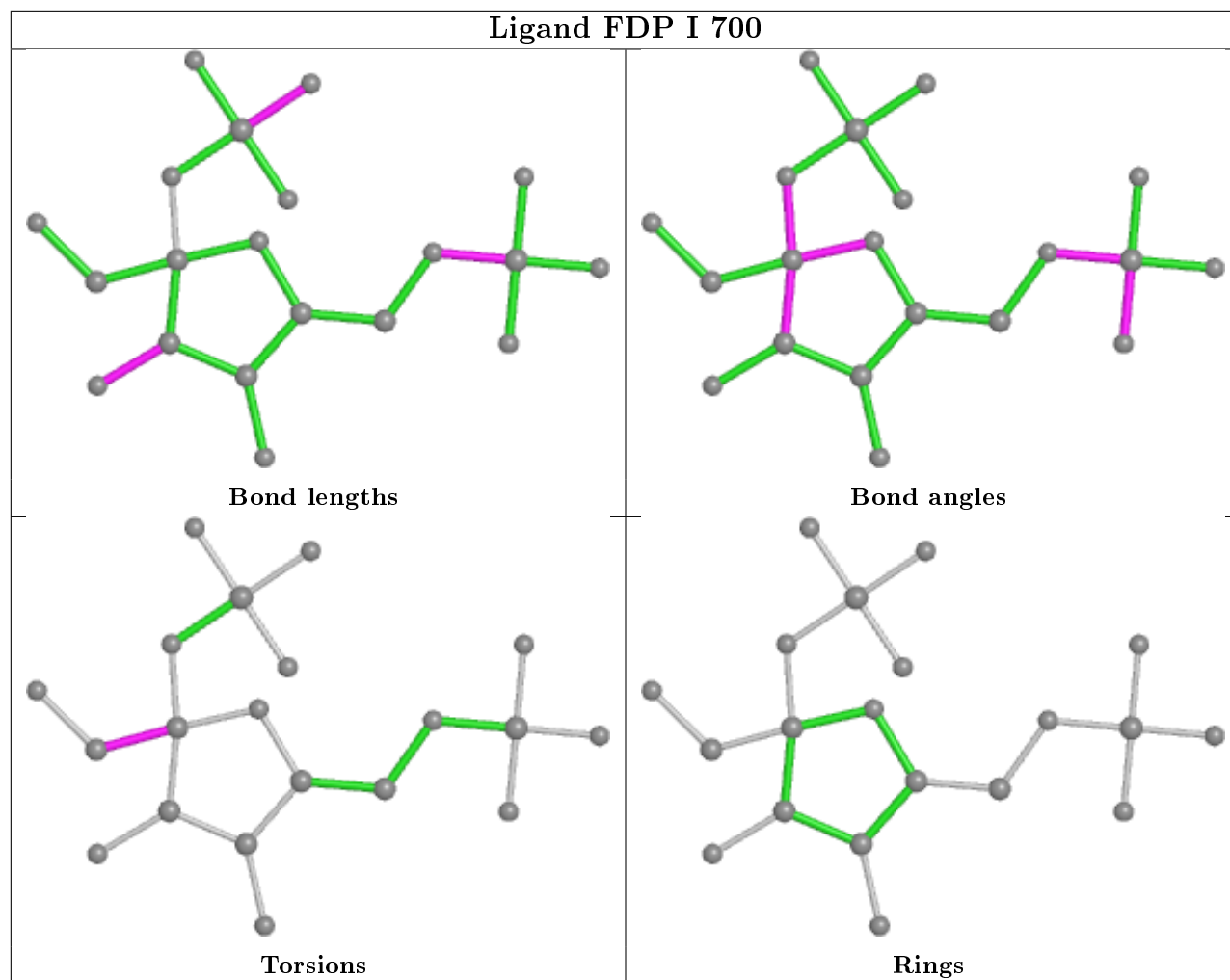
## Ligand FDP B 700

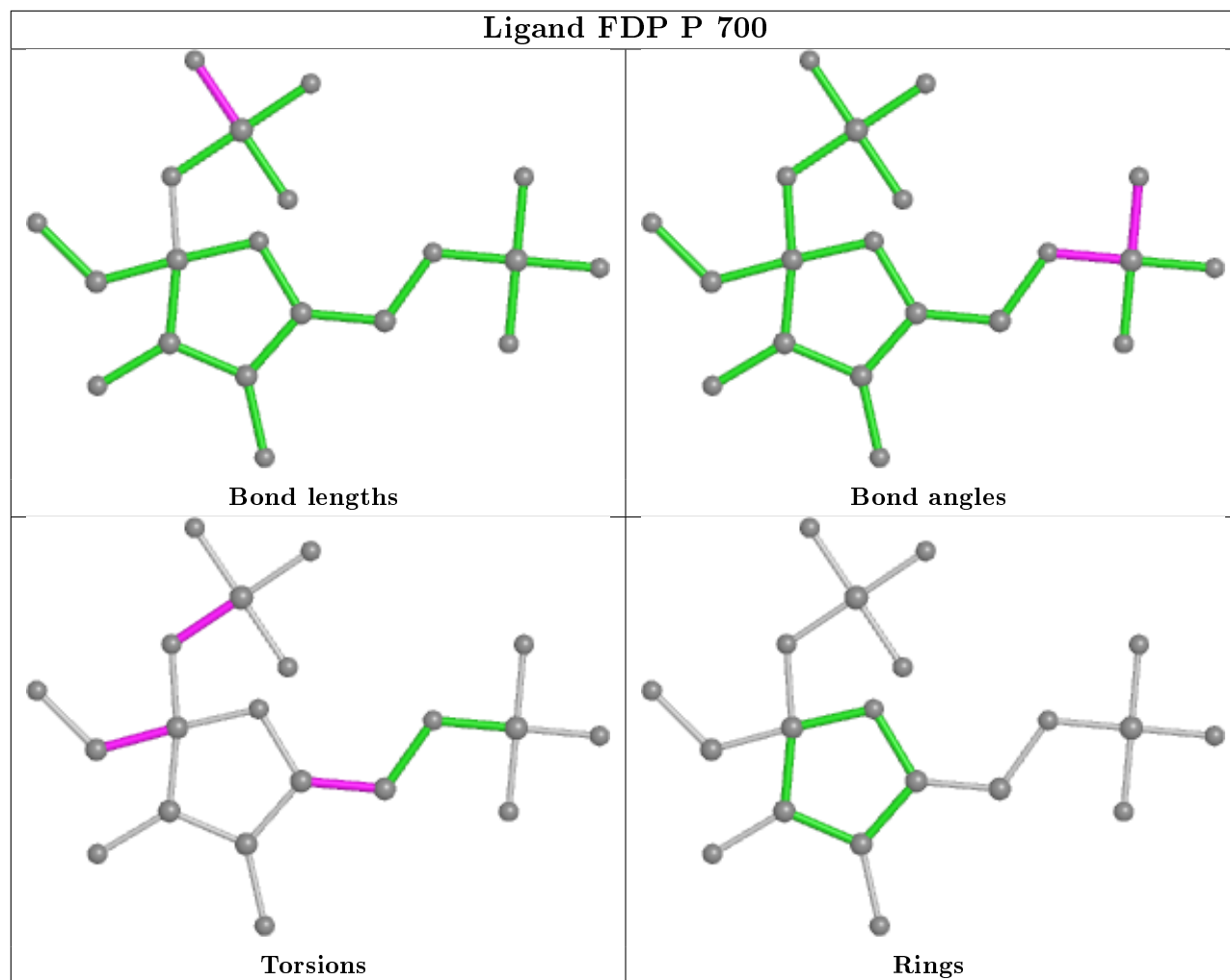


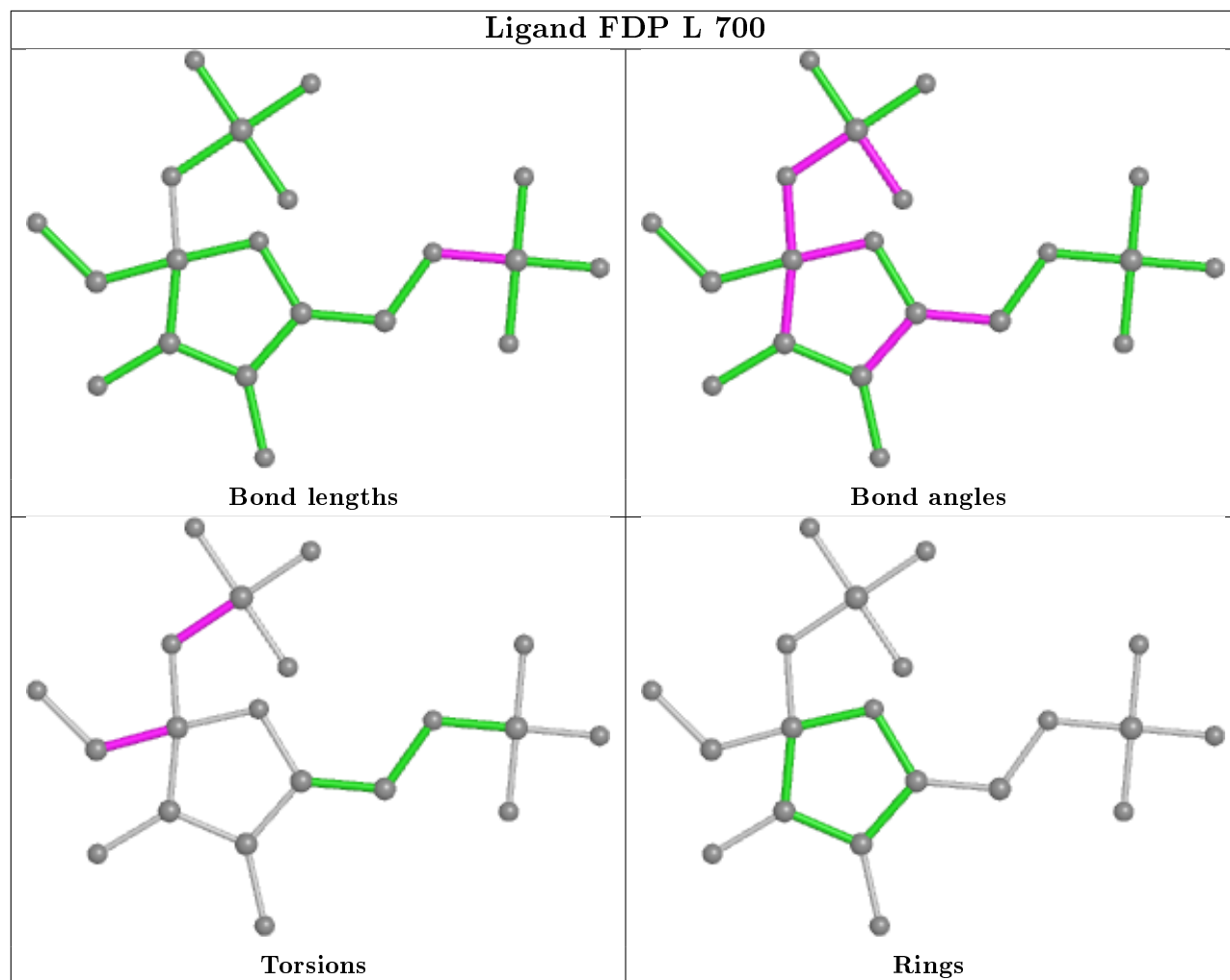


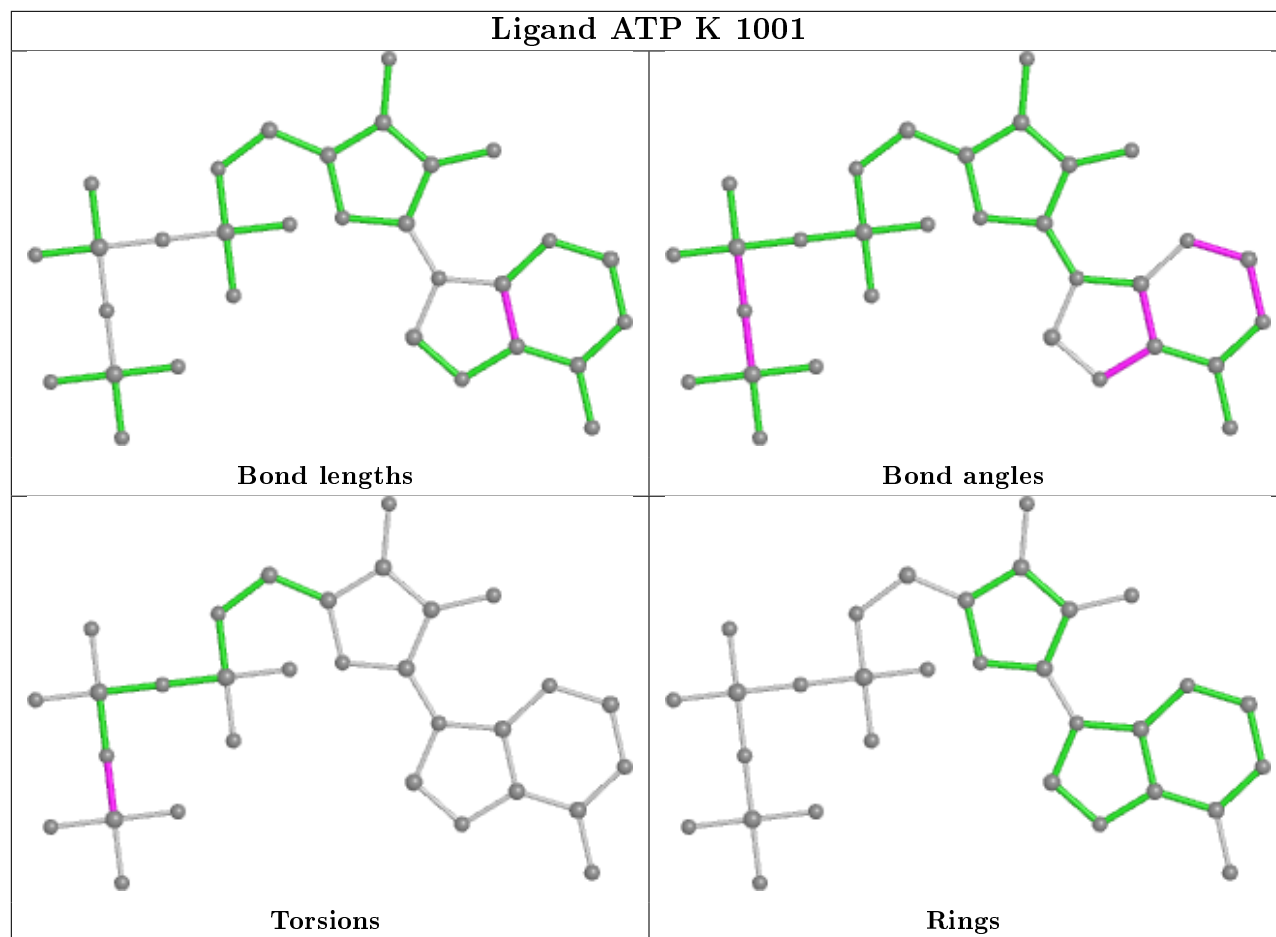


## Ligand FDP I 700









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	498/499 (99%)	1.11	118 (23%) 0 0	31, 42, 59, 61	0
1	B	498/499 (99%)	0.34	35 (7%) 16 21	15, 25, 34, 42	0
1	C	498/499 (99%)	0.56	47 (9%) 8 11	28, 39, 50, 59	0
1	D	498/499 (99%)	0.47	47 (9%) 8 11	17, 27, 43, 45	0
1	E	498/499 (99%)	0.64	61 (12%) 4 6	30, 42, 52, 56	0
1	F	498/499 (99%)	0.77	76 (15%) 2 3	36, 52, 66, 70	0
1	G	498/499 (99%)	1.39	136 (27%) 0 0	44, 52, 60, 63	0
1	H	498/499 (99%)	0.83	73 (14%) 2 3	38, 46, 52, 55	0
1	I	498/499 (99%)	0.46	45 (9%) 9 12	13, 22, 47, 53	0
1	J	498/499 (99%)	0.34	36 (7%) 15 20	15, 22, 30, 41	0
1	K	498/499 (99%)	0.26	31 (6%) 20 26	13, 22, 31, 40	0
1	L	498/499 (99%)	0.59	54 (10%) 5 8	19, 29, 60, 62	0
1	M	498/499 (99%)	1.15	126 (25%) 0 0	35, 47, 56, 59	0
1	N	498/499 (99%)	1.81	192 (38%) 0 0	45, 60, 69, 71	0
1	O	498/499 (99%)	2.39	248 (49%) 0 0	35, 55, 84, 86	0
1	P	498/499 (99%)	2.26	241 (48%) 0 0	48, 60, 83, 86	0
All	All	7968/7984 (99%)	0.96	1566 (19%) 1 1	13, 43, 65, 86	0

The worst 5 of 1566 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	155	HIS	9.8
1	O	444	ALA	9.6
1	O	100	VAL	9.5
1	O	95	VAL	9.3
1	N	447	LEU	9.2

## 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	K	O	500	1/1	0.66	0.30	122,122,122,122	0
7	GOL	J	499	6/6	0.66	0.37	69,71,71,72	0
3	K	A	504	1/1	0.68	0.28	106,106,106,106	0
3	K	G	501	1/1	0.71	0.37	137,137,137,137	0
3	K	N	499	1/1	0.71	0.27	107,107,107,107	0
3	K	P	504	1/1	0.79	0.19	98,98,98,98	0
3	K	M	499	1/1	0.79	0.15	106,106,106,106	0
3	K	P	499	1/1	0.80	0.22	119,119,119,119	0
7	GOL	I	499	6/6	0.82	0.44	91,91,91,92	0
4	OXL	P	510	6/6	0.83	0.19	85,85,85,86	0
3	K	G	504	1/1	0.84	0.16	82,82,82,82	0
7	GOL	O	499	6/6	0.84	0.41	74,75,75,75	0
7	GOL	I	501	6/6	0.85	0.47	85,85,85,85	0
6	ATP	P	1001	31/31	0.86	0.20	132,134,134,134	0
2	MG	P	500	1/1	0.86	0.39	94,94,94,94	0
7	GOL	G	499	6/6	0.88	0.16	97,97,97,97	0
2	MG	F	502	1/1	0.88	0.10	60,60,60,60	0
2	MG	P	502	1/1	0.89	0.07	64,64,64,64	0
5	FDP	P	700	20/20	0.89	0.15	110,115,119,119	0
3	K	F	499	1/1	0.89	0.09	85,85,85,85	0
2	MG	N	500	1/1	0.89	0.43	88,88,88,88	0
6	ATP	G	1001	31/31	0.90	0.18	77,97,101,101	0
3	K	N	504	1/1	0.90	0.20	84,84,84,84	0
4	OXL	M	510	6/6	0.90	0.16	64,66,67,67	0
4	OXL	N	510	6/6	0.90	0.15	77,79,80,80	0
2	MG	I	502	1/1	0.91	0.12	30,30,30,30	0
2	MG	N	502	1/1	0.91	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OXL	A	510	6/6	0.91	0.14	63,65,66,66	0
4	OXL	F	510	6/6	0.91	0.26	83,83,83,83	0
2	MG	I	500	1/1	0.91	0.12	36,36,36,36	0
4	OXL	G	510	6/6	0.91	0.15	71,74,75,75	0
7	GOL	E	499	6/6	0.91	0.16	78,79,80,80	0
5	FDP	O	700	20/20	0.92	0.13	118,119,121,121	0
6	ATP	N	1001	31/31	0.92	0.12	83,94,95,95	0
2	MG	E	500	1/1	0.93	0.08	55,55,55,55	0
2	MG	H	500	1/1	0.93	0.14	63,63,63,63	0
3	K	C	504	1/1	0.94	0.13	56,56,56,56	0
6	ATP	A	1001	31/31	0.94	0.15	70,85,87,87	0
6	ATP	H	1001	31/31	0.94	0.12	62,69,72,72	0
3	K	F	504	1/1	0.94	0.07	69,69,69,69	0
6	ATP	M	1001	31/31	0.95	0.10	66,73,76,76	0
6	ATP	C	1001	31/31	0.95	0.11	43,52,54,54	0
2	MG	G	500	1/1	0.95	0.36	81,81,81,81	0
4	OXL	H	510	6/6	0.95	0.10	54,54,55,55	0
2	MG	L	500	1/1	0.95	0.07	46,46,46,46	0
6	ATP	F	1001	31/31	0.95	0.12	64,73,76,76	0
3	K	E	501	1/1	0.95	0.10	75,75,75,75	0
3	K	C	499	1/1	0.95	0.08	68,68,68,68	0
5	FDP	A	700	20/20	0.96	0.11	53,58,61,64	0
6	ATP	E	1001	31/31	0.96	0.10	52,58,63,63	0
2	MG	E	502	1/1	0.96	0.13	48,48,48,48	0
3	K	H	499	1/1	0.96	0.06	76,76,76,76	0
2	MG	M	500	1/1	0.96	0.14	69,69,69,69	0
3	K	O	501	1/1	0.96	0.42	30,30,30,30	0
2	MG	M	502	1/1	0.96	0.14	60,60,60,60	0
2	MG	H	502	1/1	0.96	0.31	61,61,61,61	0
6	ATP	L	1001	31/31	0.96	0.11	44,55,59,59	0
3	K	L	504	1/1	0.96	0.06	52,52,52,52	0
4	OXL	C	510	6/6	0.96	0.17	39,40,41,41	0
2	MG	J	502	1/1	0.97	0.07	26,26,26,26	0
6	ATP	I	1001	31/31	0.97	0.10	36,37,39,40	0
5	FDP	N	700	20/20	0.97	0.12	76,78,81,82	0
3	K	B	499	1/1	0.97	0.04	60,60,60,60	0
2	MG	G	502	1/1	0.97	0.20	66,66,66,66	0
4	OXL	L	510	6/6	0.97	0.10	37,38,38,39	0
3	K	H	504	1/1	0.97	0.07	59,59,59,59	0
2	MG	A	502	1/1	0.97	0.15	58,58,58,58	0
2	MG	C	500	1/1	0.97	0.18	45,45,45,45	0
2	MG	B	502	1/1	0.97	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	502	1/1	0.97	0.14	38,38,38,38	0
5	FDP	G	700	20/20	0.97	0.09	69,74,75,75	0
2	MG	D	500	1/1	0.97	0.10	37,37,37,37	0
3	K	D	499	1/1	0.98	0.07	53,53,53,53	0
6	ATP	J	1001	31/31	0.98	0.11	26,34,36,36	0
5	FDP	H	700	20/20	0.98	0.10	54,57,59,60	0
5	FDP	C	700	20/20	0.98	0.09	36,45,48,50	0
5	FDP	F	700	20/20	0.98	0.07	48,53,55,56	0
5	FDP	L	700	20/20	0.98	0.08	37,41,43,43	0
3	K	M	504	1/1	0.98	0.04	61,61,61,61	0
2	MG	D	502	1/1	0.98	0.11	34,34,34,34	0
6	ATP	B	1001	31/31	0.98	0.10	31,35,39,40	0
5	FDP	D	700	20/20	0.98	0.07	32,40,43,45	0
6	ATP	D	1001	31/31	0.98	0.10	35,42,44,44	0
4	OXL	K	510	6/6	0.98	0.12	25,27,28,28	0
6	ATP	K	1001	31/31	0.98	0.14	28,31,37,38	0
2	MG	K	502	1/1	0.98	0.10	28,28,28,28	0
2	MG	K	500	1/1	0.98	0.11	29,29,29,29	0
2	MG	F	500	1/1	0.98	0.24	67,67,67,67	0
5	FDP	B	700	20/20	0.98	0.08	37,40,45,46	0
5	FDP	M	700	20/20	0.98	0.07	55,59,62,64	0
5	FDP	K	700	20/20	0.98	0.07	36,38,42,43	0
2	MG	A	500	1/1	0.98	0.19	77,77,77,77	0
4	OXL	E	510	6/6	0.98	0.15	48,49,49,50	0
3	K	A	499	1/1	0.98	0.12	60,60,60,60	0
3	K	K	499	1/1	0.98	0.13	52,52,52,52	0
2	MG	L	502	1/1	0.98	0.12	37,37,37,37	0
4	OXL	I	510	6/6	0.99	0.14	32,33,34,35	0
3	K	I	504	1/1	0.99	0.05	36,36,36,36	0
3	K	B	504	1/1	0.99	0.05	38,38,38,38	0
4	OXL	J	510	6/6	0.99	0.11	30,31,32,33	0
5	FDP	E	700	20/20	0.99	0.07	38,41,46,47	0
5	FDP	J	700	20/20	0.99	0.05	25,32,34,35	0
3	K	D	504	1/1	0.99	0.08	33,33,33,33	0
3	K	E	504	1/1	0.99	0.07	48,48,48,48	0
3	K	J	501	1/1	0.99	0.09	50,50,50,50	0
4	OXL	B	510	6/6	0.99	0.06	30,32,33,33	0
2	MG	J	500	1/1	0.99	0.12	27,27,27,27	0
4	OXL	D	510	6/6	0.99	0.10	37,38,39,39	0
3	K	I	503	1/1	0.99	0.12	47,47,47,47	0
3	K	L	499	1/1	0.99	0.04	47,47,47,47	0
5	FDP	I	700	20/20	0.99	0.07	29,32,34,35	0

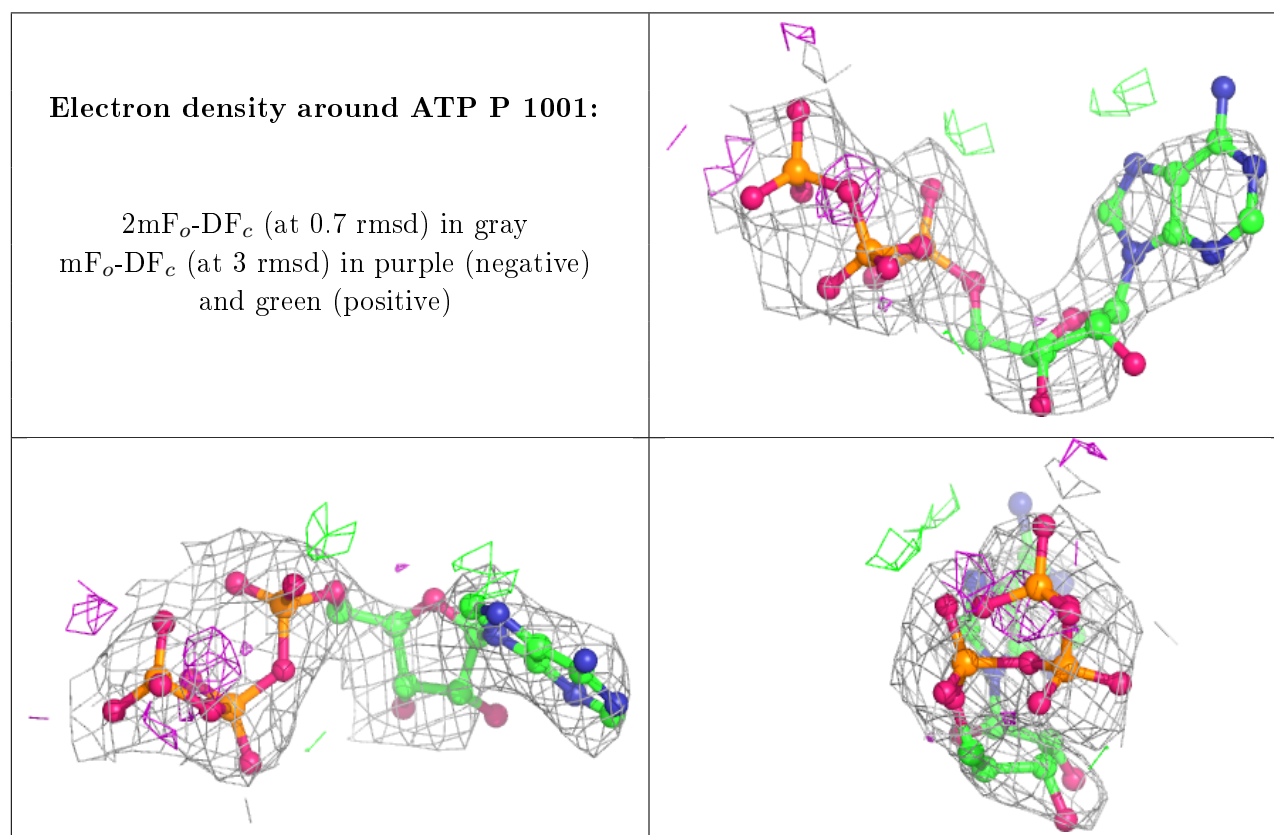
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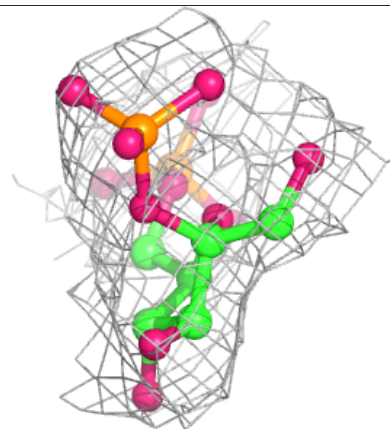
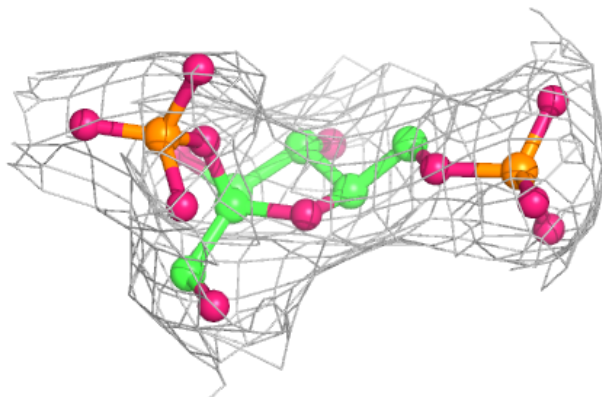
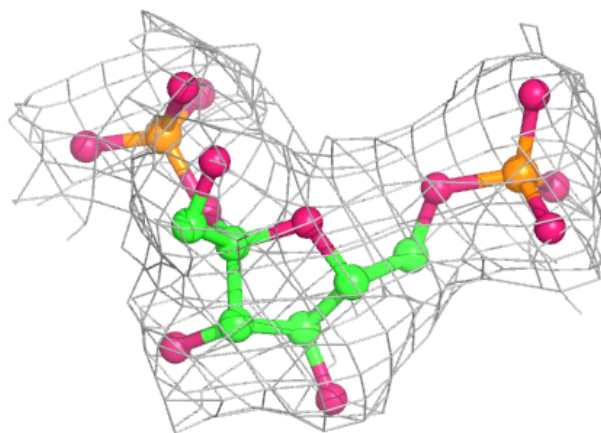
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	J	504	1/1	0.99	0.07	35,35,35,35	0
2	MG	B	500	1/1	0.99	0.08	35,35,35,35	0
3	K	K	504	1/1	1.00	0.10	29,29,29,29	0

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.

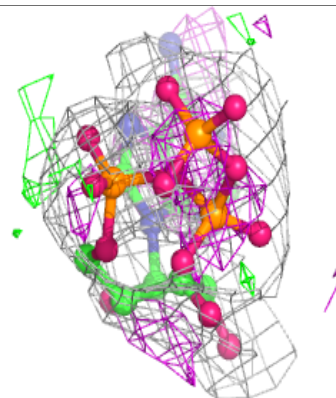
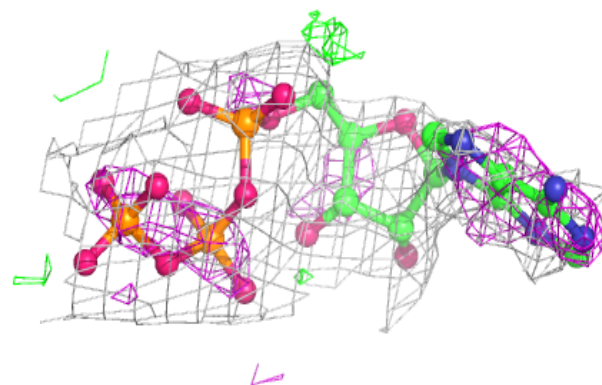
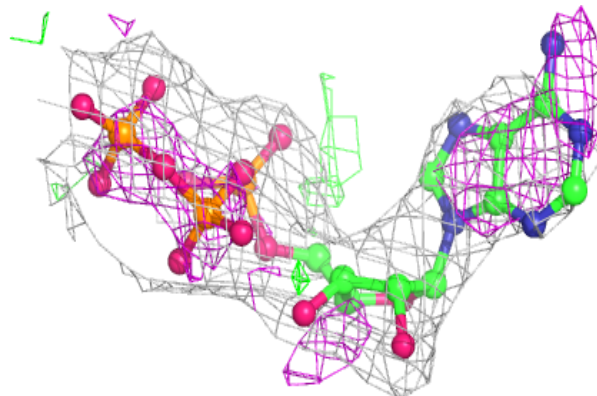


**Electron density around FDP P 700:**

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

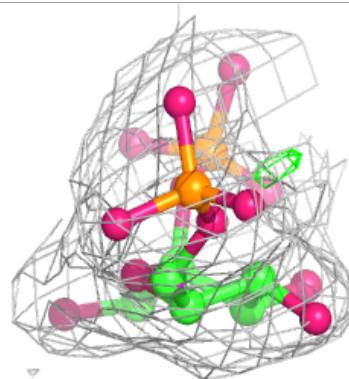
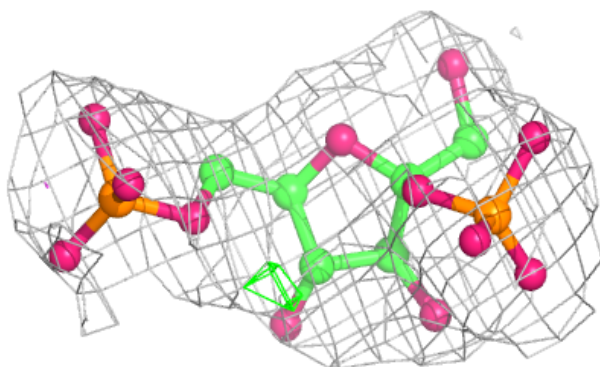
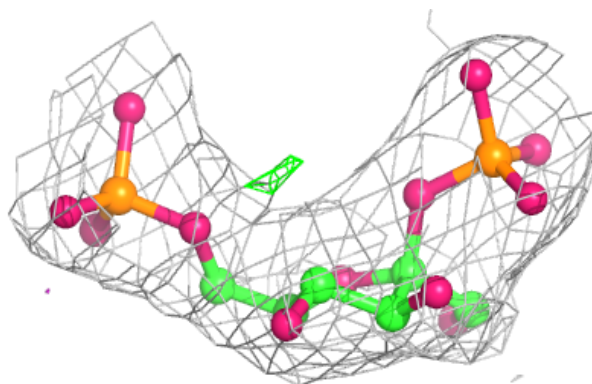
**Electron density around ATP G 1001:**

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

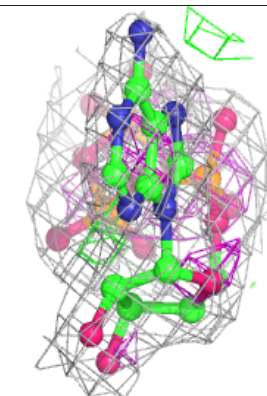
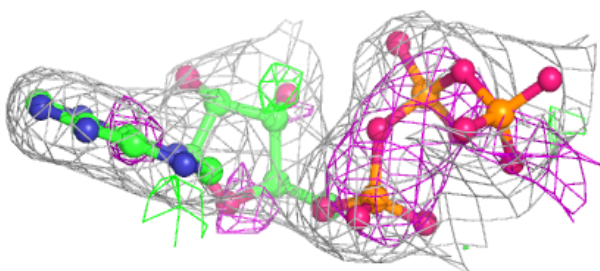
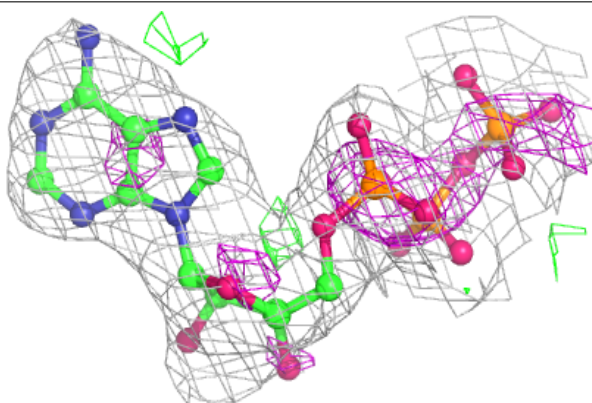


**Electron density around FDP O 700:**

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

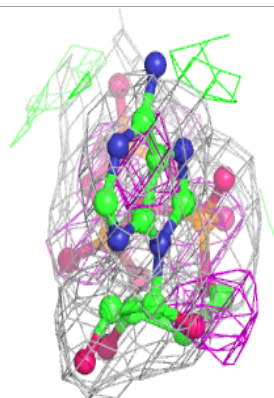
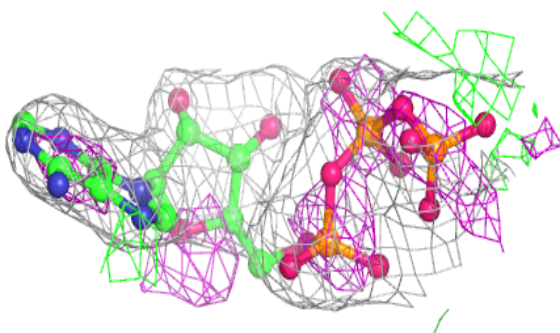
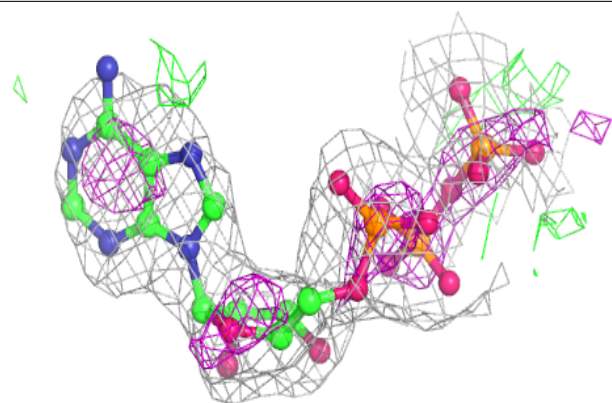
**Electron density around ATP N 1001:**

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

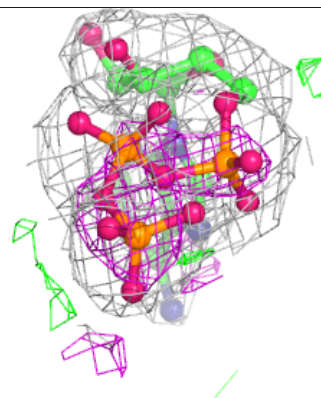
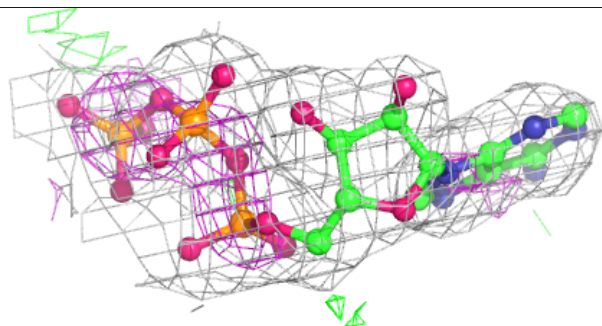
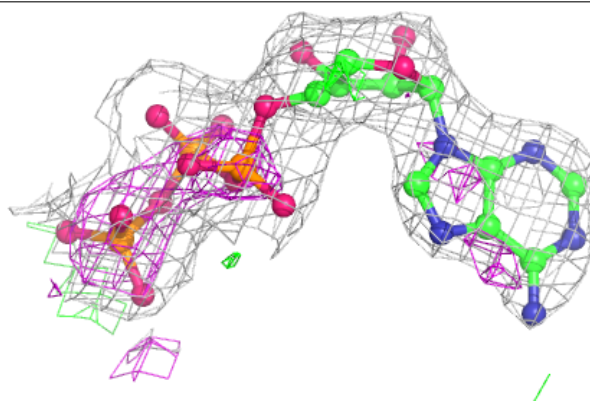


**Electron density around ATP A 1001:**

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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP H 1001:**

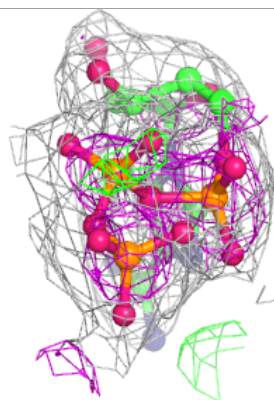
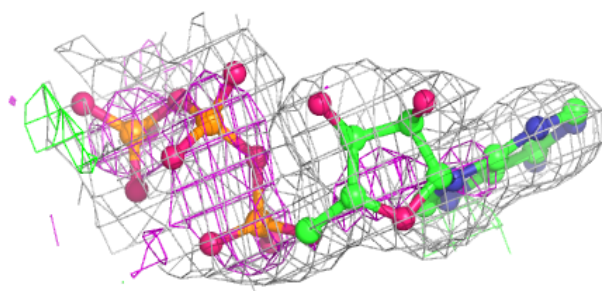
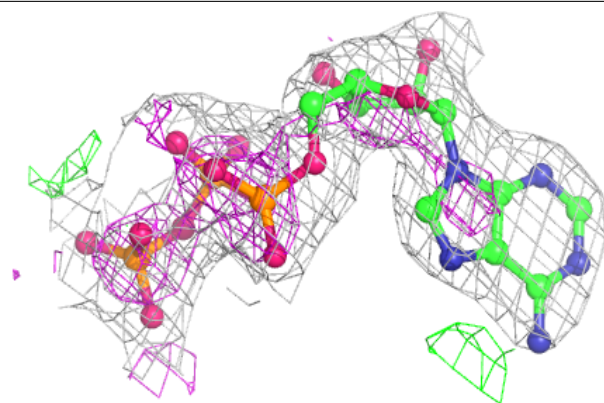
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



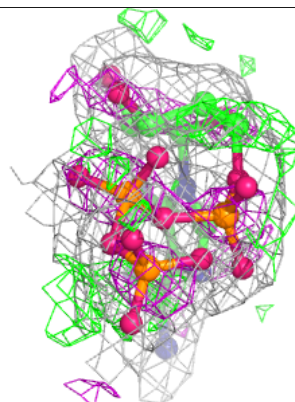
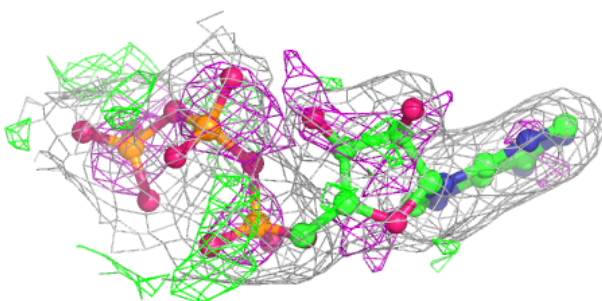
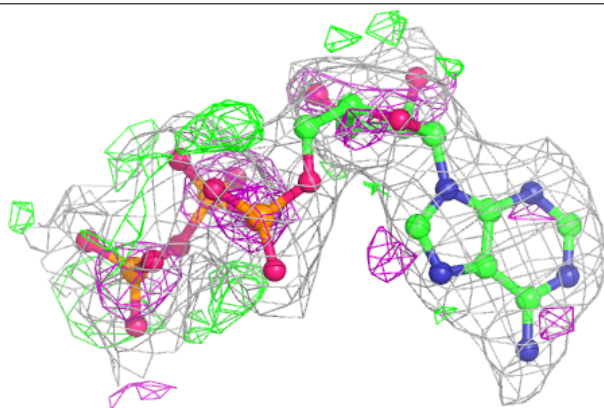


**Electron density around ATP M 1001:**

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

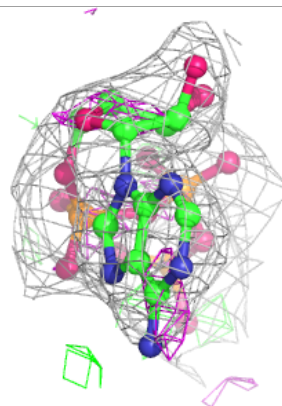
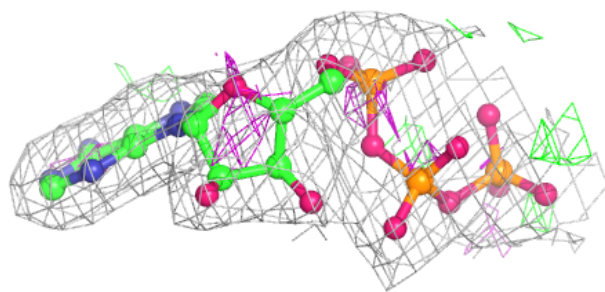
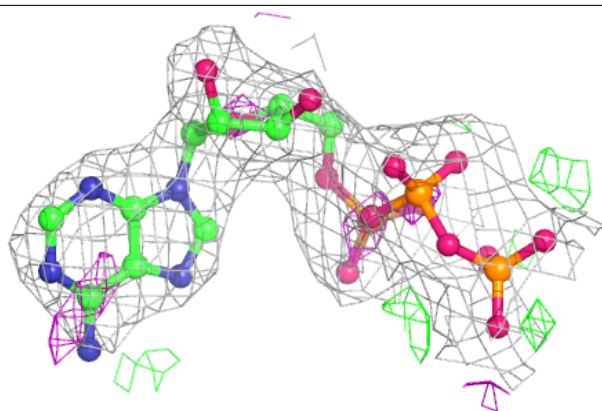
**Electron density around ATP C 1001:**

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

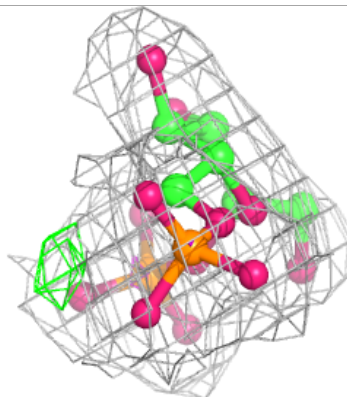
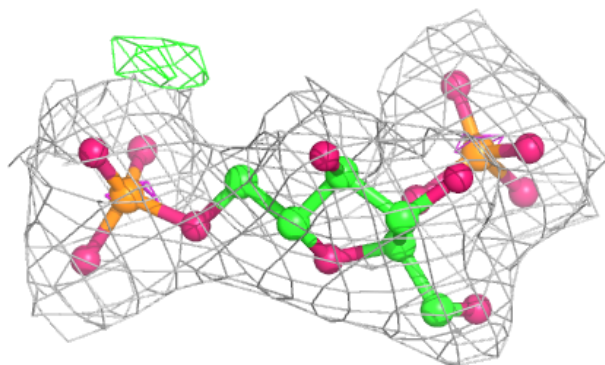
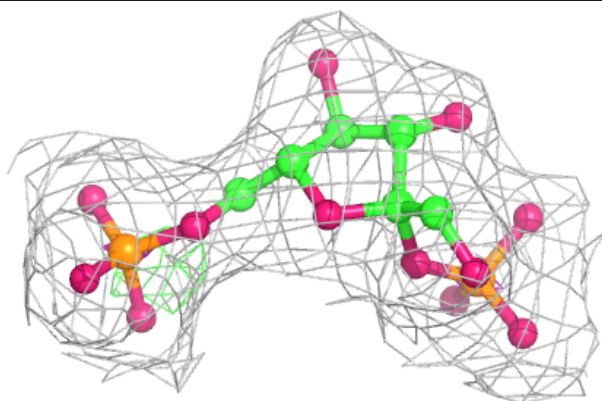


**Electron density around ATP F 1001:**

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

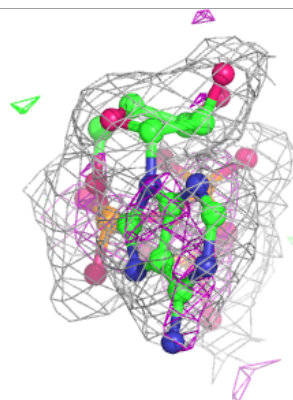
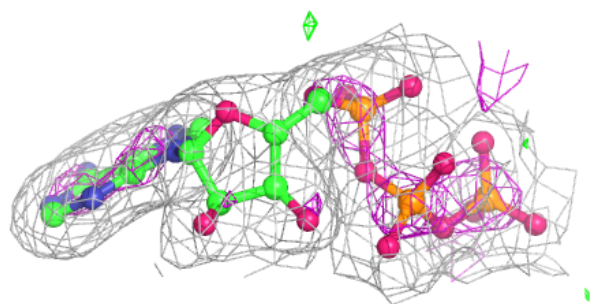
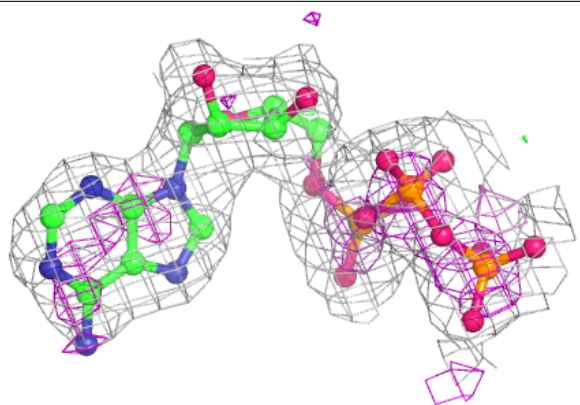
**Electron density around FDP A 700:**

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

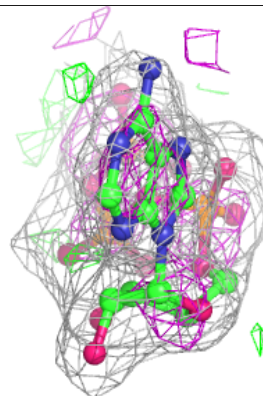
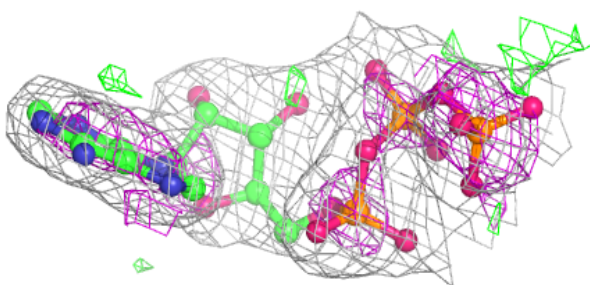
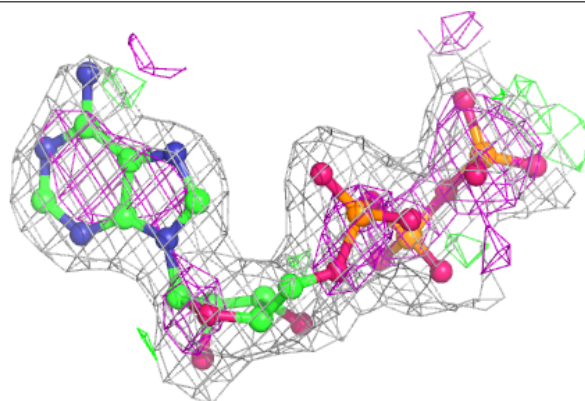


**Electron density around ATP E 1001:**

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

**Electron density around ATP L 1001:**

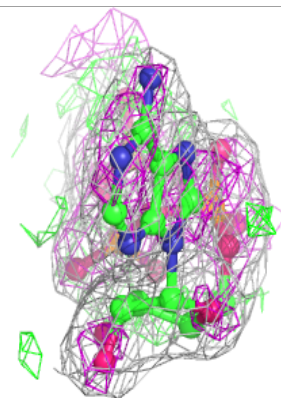
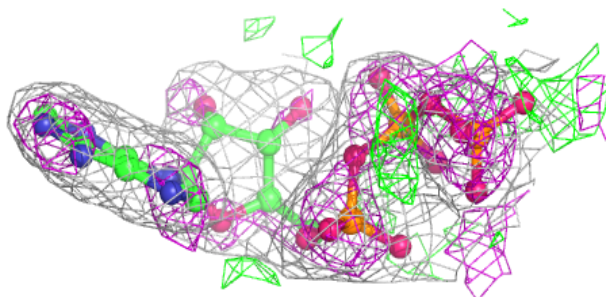
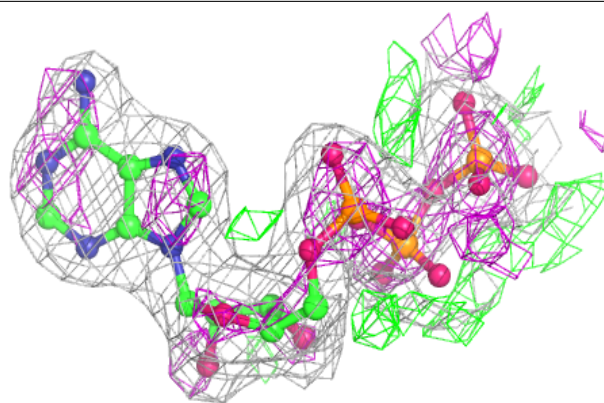
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



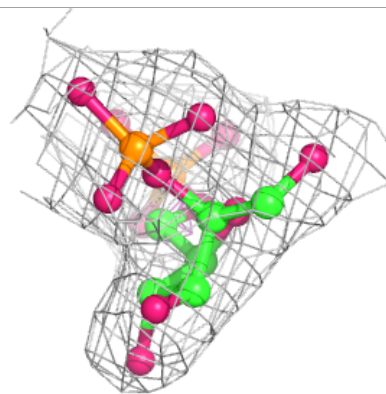
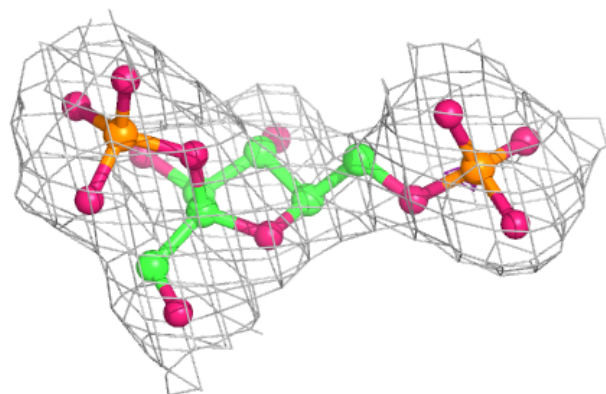
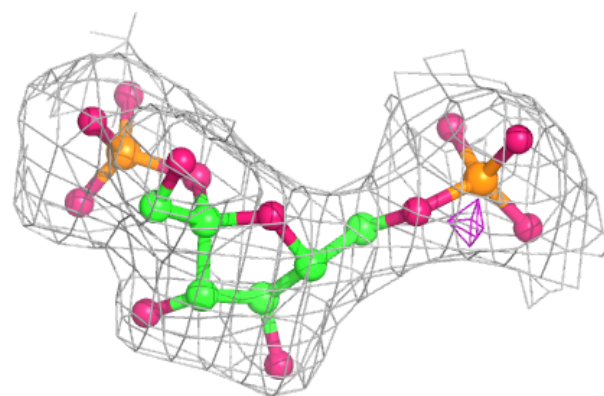


**Electron density around ATP I 1001:**

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

**Electron density around FDP N 700:**

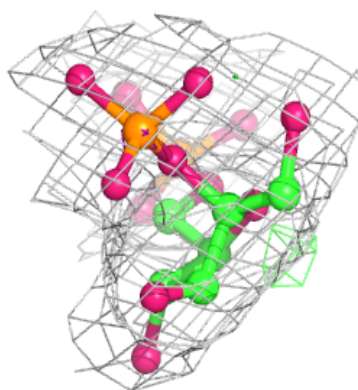
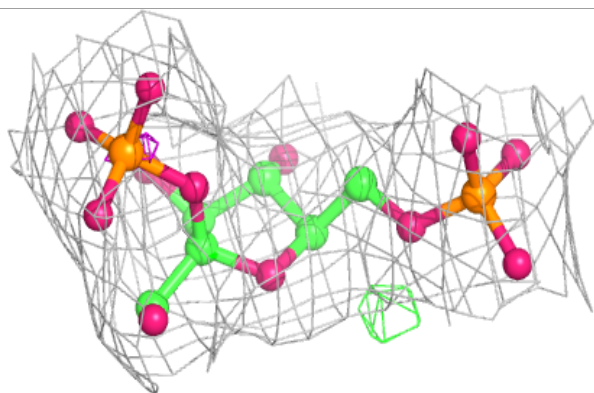
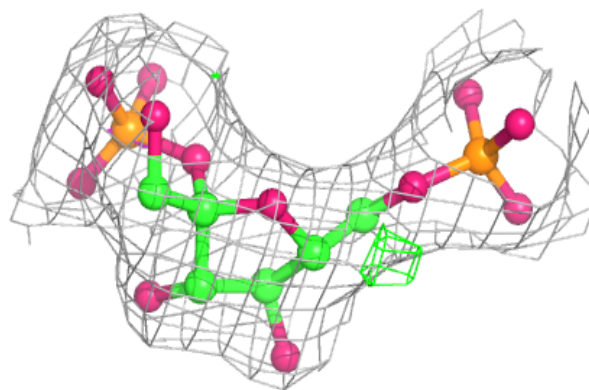
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



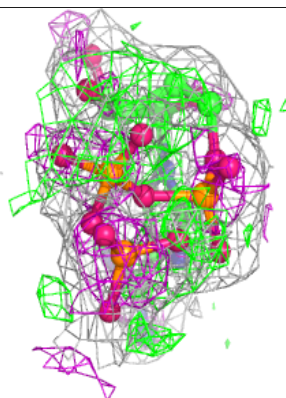
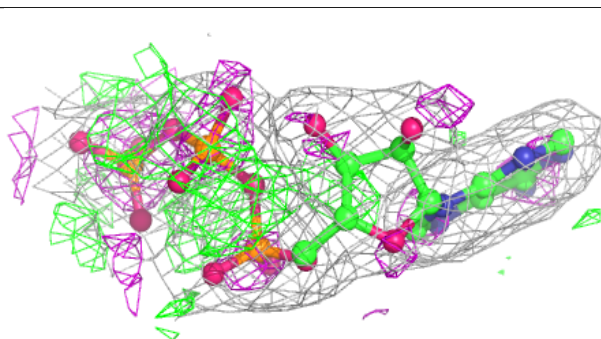
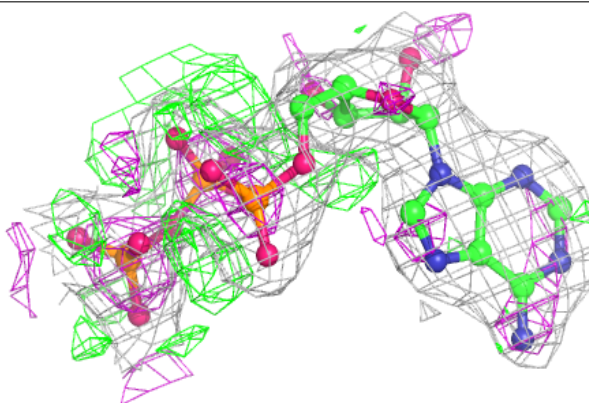


**Electron density around FDP G 700:**

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

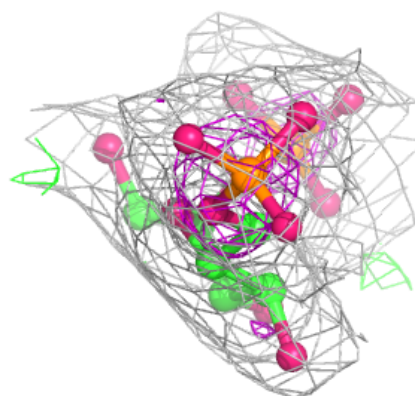
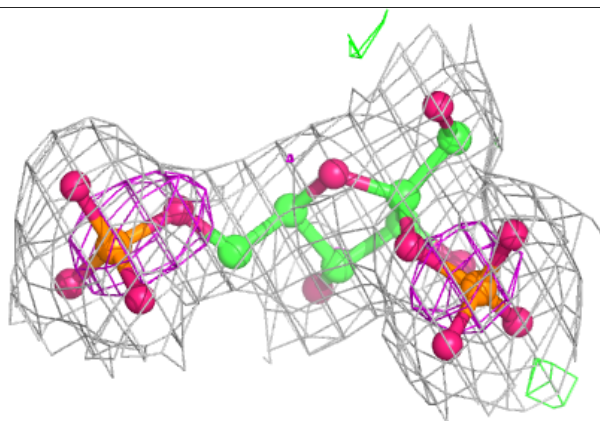
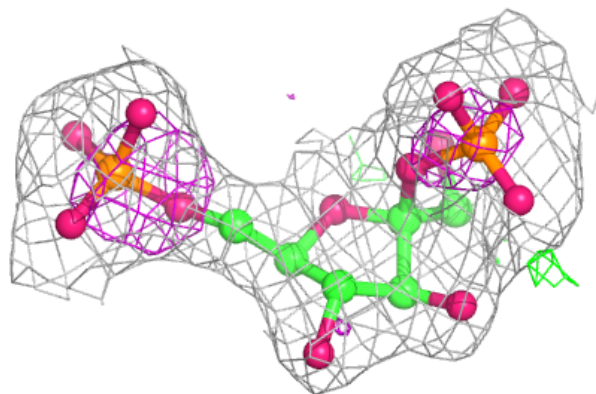
**Electron density around ATP J 1001:**

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

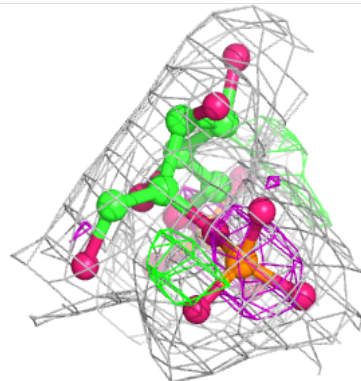
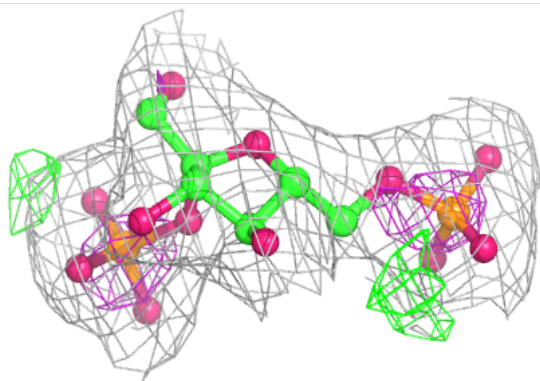
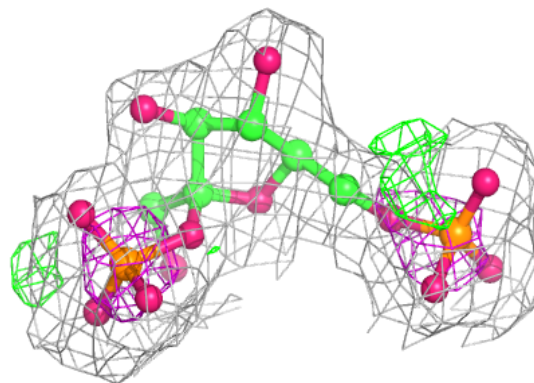


**Electron density around FDP H 700:**

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

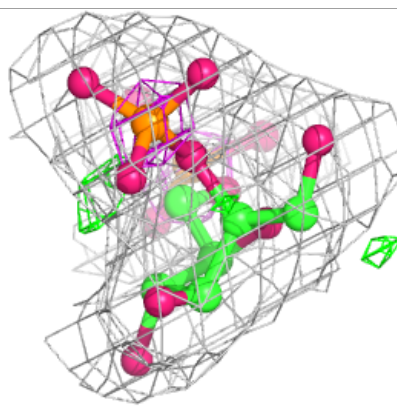
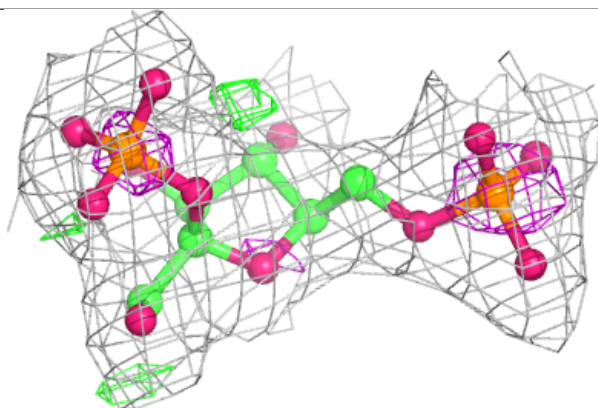
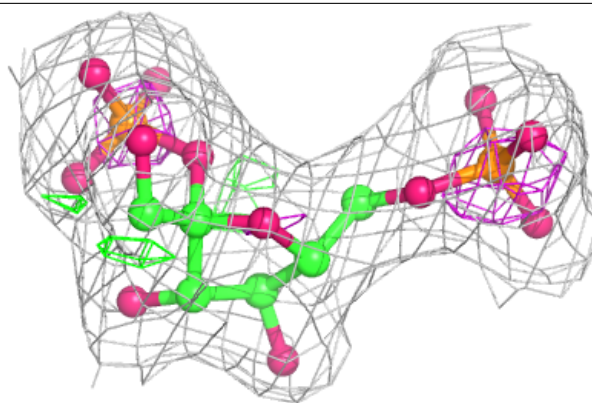
**Electron density around FDP C 700:**

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

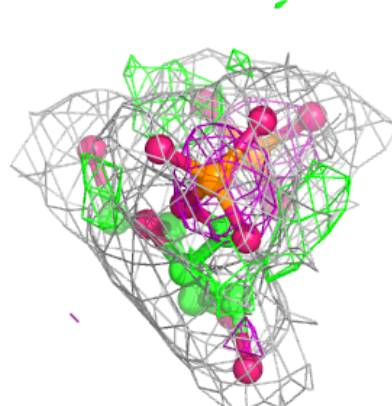
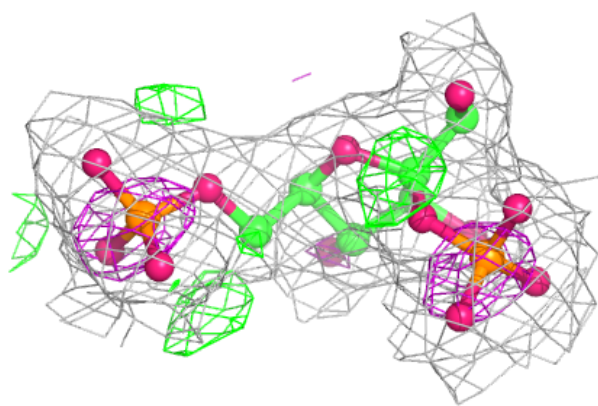
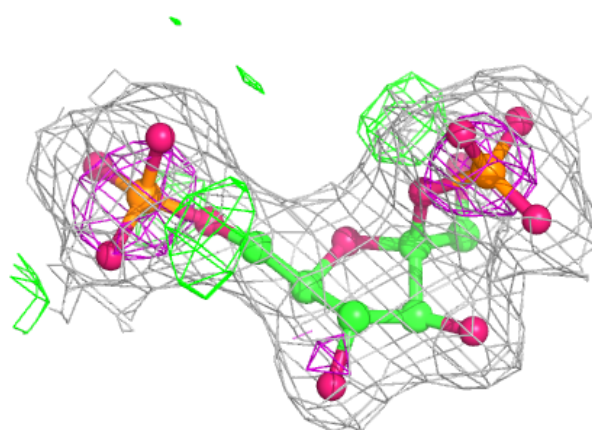


**Electron density around FDP F 700:**

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

**Electron density around FDP L 700:**

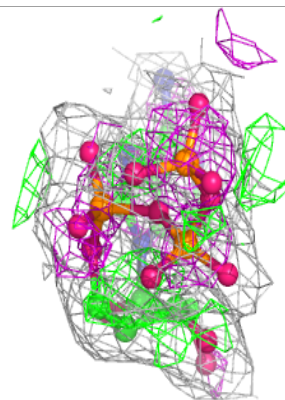
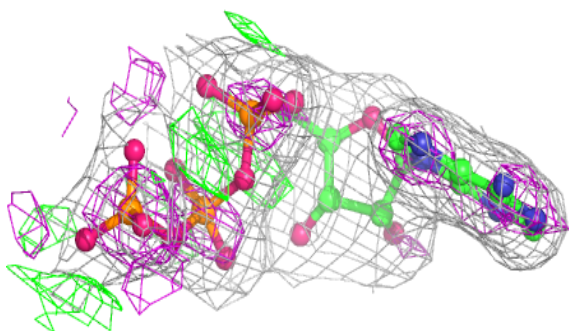
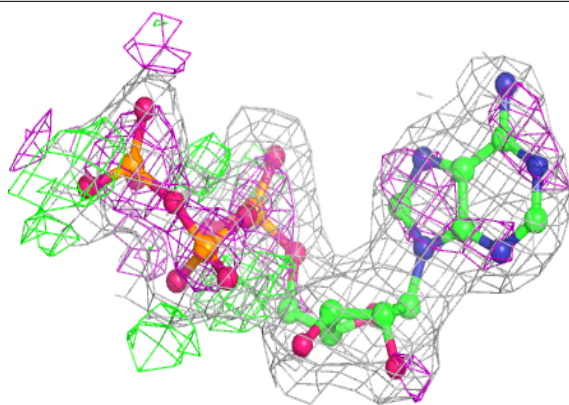
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



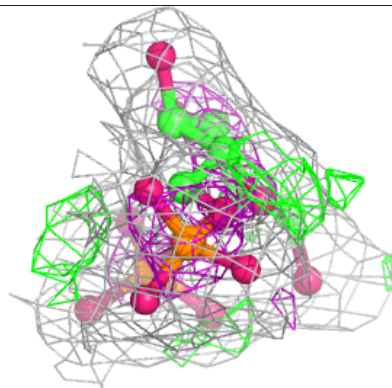
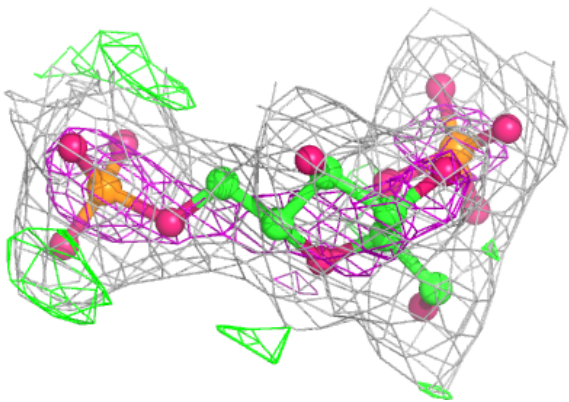
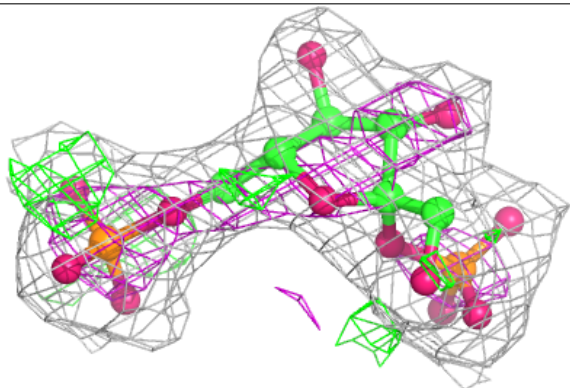


**Electron density around ATP B 1001:**

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

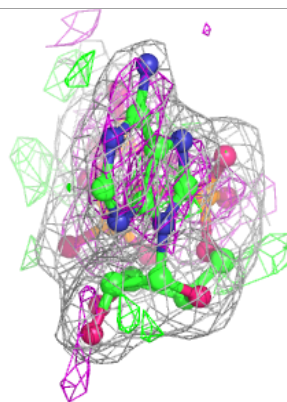
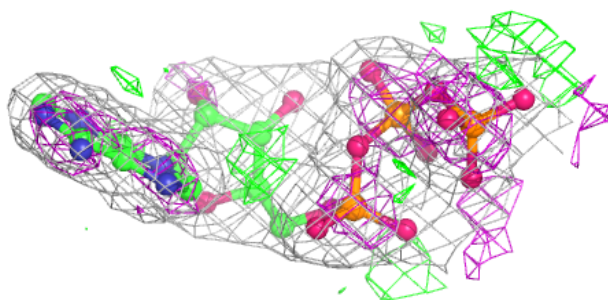
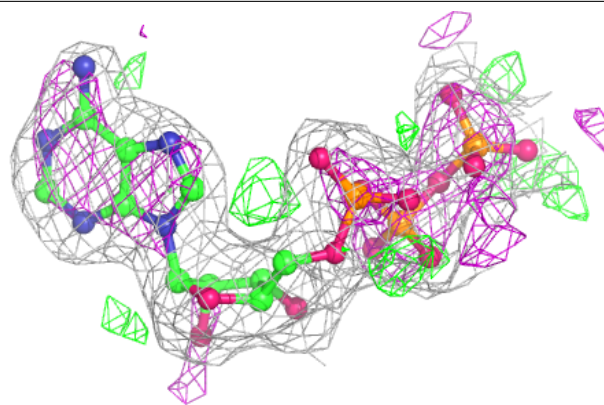
**Electron density around FDP D 700:**

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

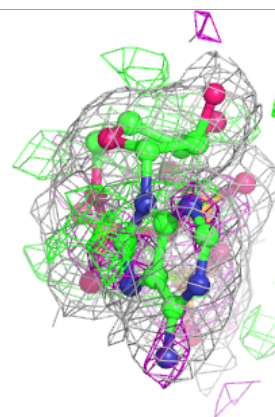
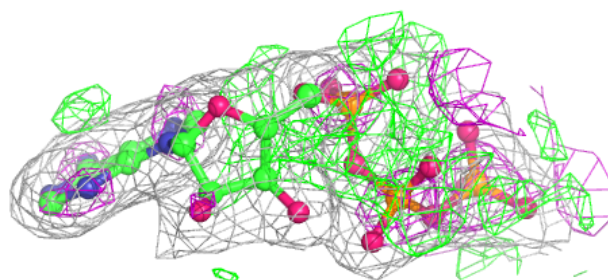
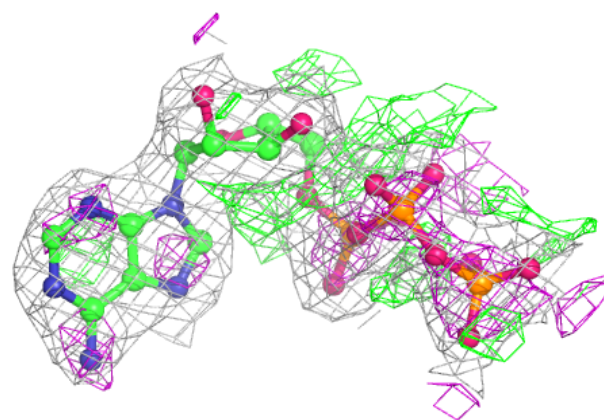


**Electron density around ATP D 1001:**

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

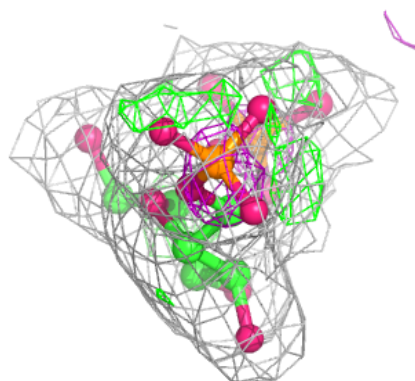
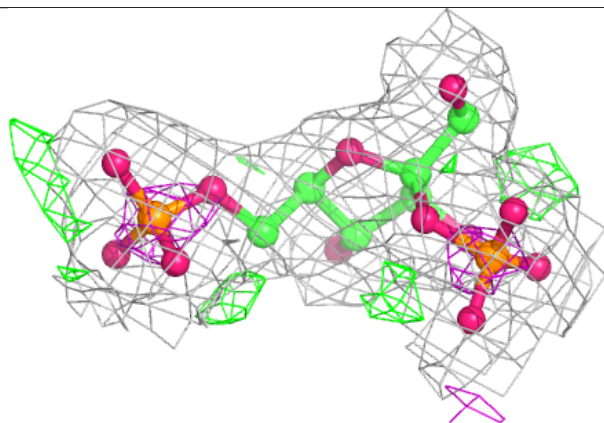
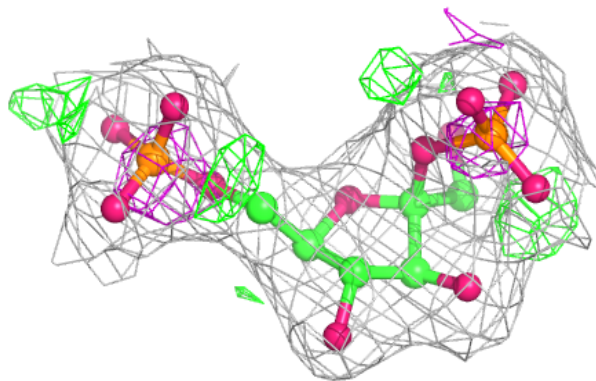
**Electron density around ATP K 1001:**

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

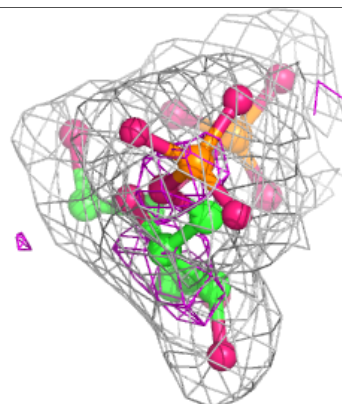
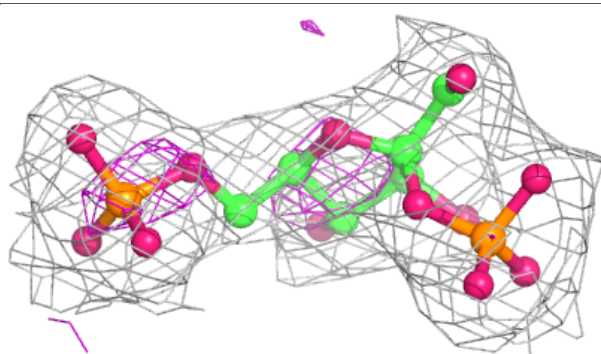
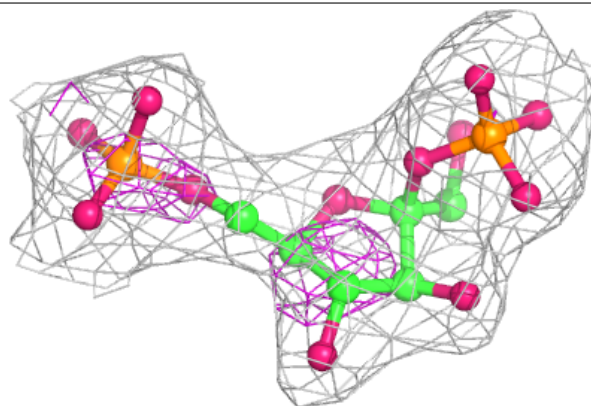


**Electron density around FDP B 700:**

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

**Electron density around FDP M 700:**

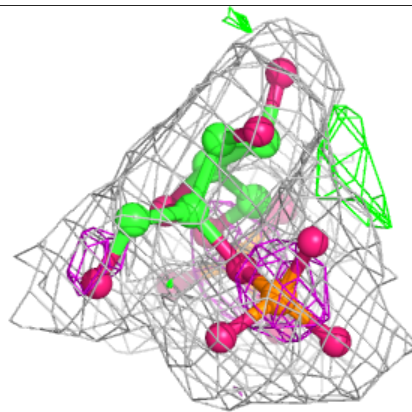
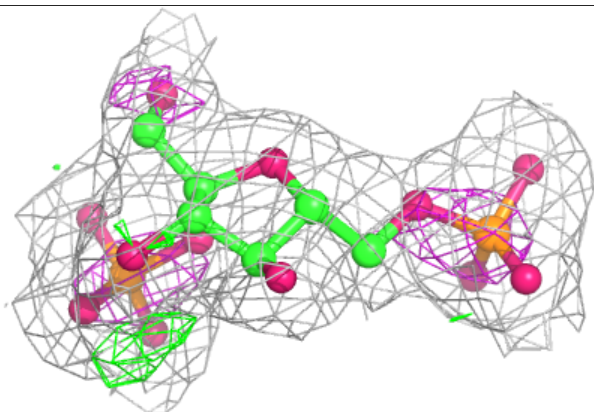
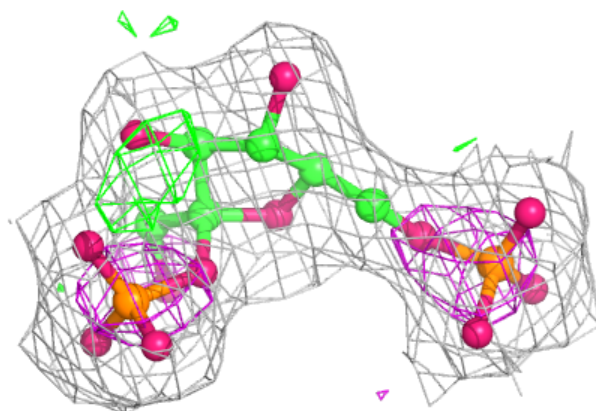
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



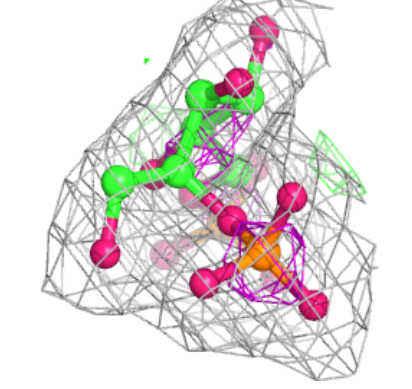
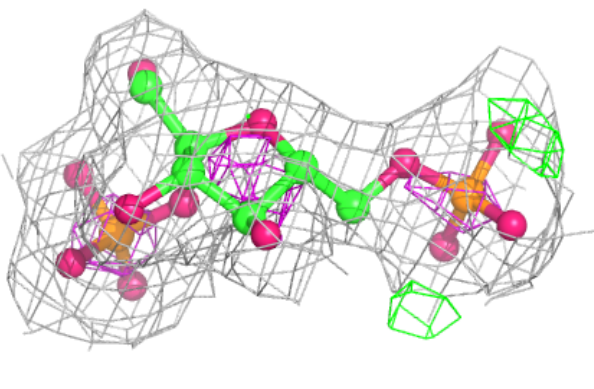
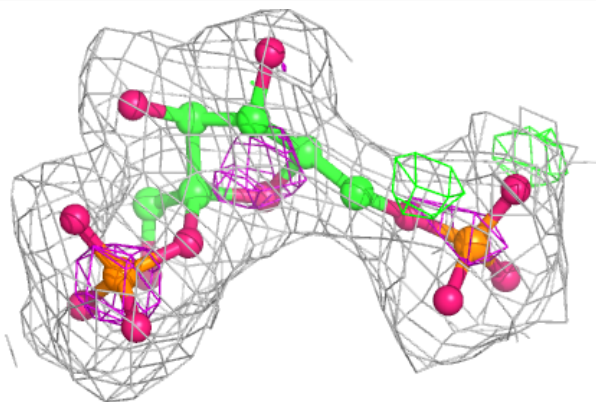


**Electron density around FDP K 700:**

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

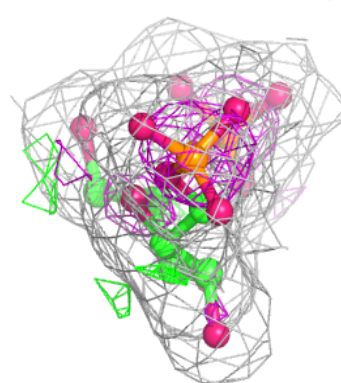
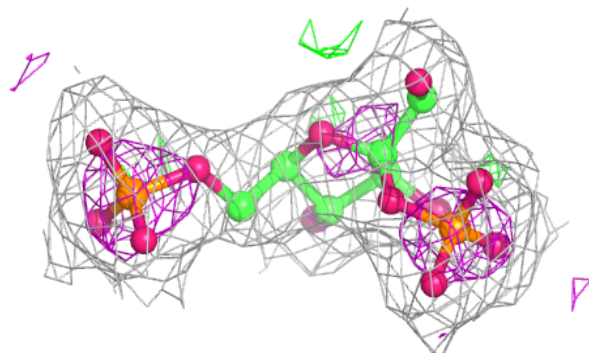
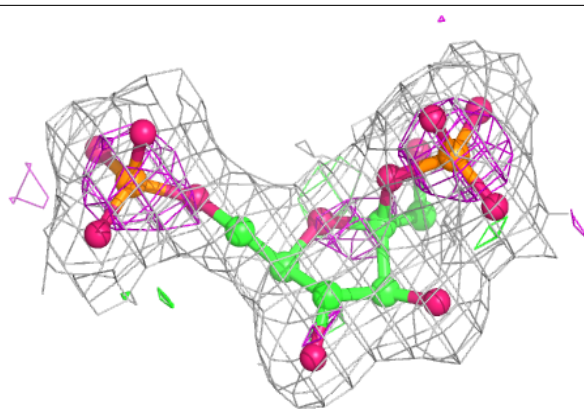
**Electron density around FDP E 700:**

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

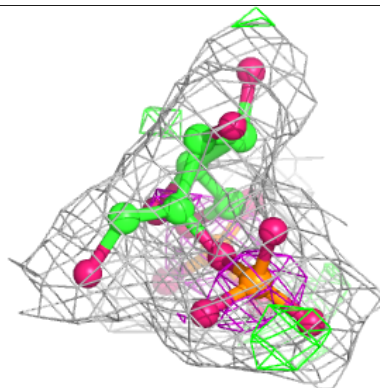
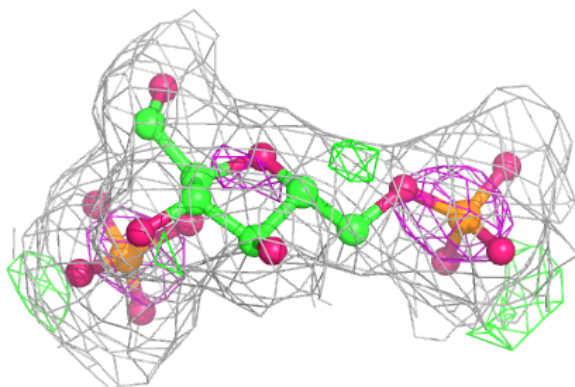
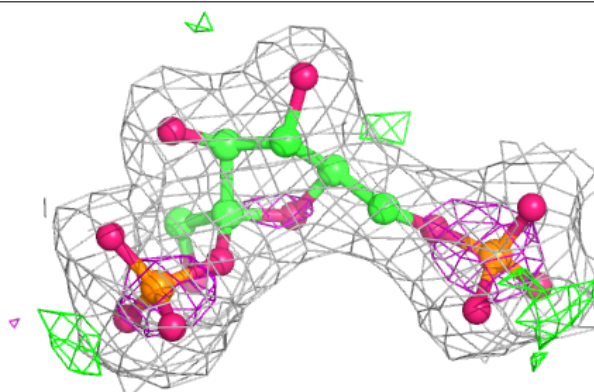


**Electron density around FDP J 700:**

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

**Electron density around FDP I 700:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.