



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:46 AM UTC

PDB ID : 3HQQ / pdb_00003hqq
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with Fructose 2,6 biphosphate
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-06-08
Resolution : 5.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

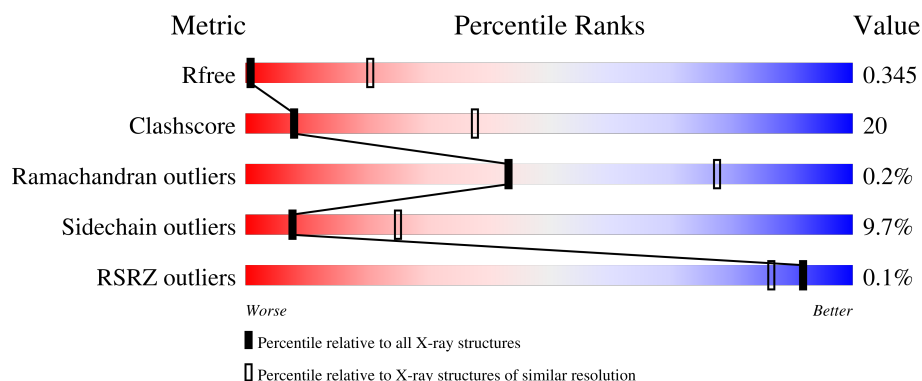
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.07 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.



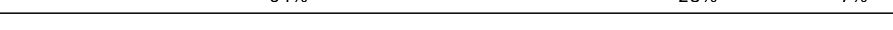
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1020 (6.16-3.98)
Clashscore	190562	1053 (6.16-4.00)
Ramachandran outliers	187476	1022 (6.22-3.92)
Sidechain outliers	187428	1139 (6.22-3.90)
RSRZ outliers	180081	1015 (6.16-3.98)

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	499	64% 28% 7%
1	B	499	65% 27% 7%
1	C	499	63% 30% 7%
1	D	499	64% 29% 6%
1	E	499	64% 29% 6%

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Mol	Chain	Length	Quality of chain
1	F	499	 65% 29% 6%
1	G	499	 65% 28% 7%
1	H	499	 63% 30% 7%
1	I	499	 64% 28% 7%
1	J	499	 65% 28% 7%
1	K	499	 64% 29% 6%
1	L	499	 64% 28% 7%
1	M	499	 63% 29% 7%
1	N	499	 64% 28% 7%
1	O	499	 63% 29% 7%
1	P	499	 64% 28% 7%
1	Q	499	 63% 29% 7%
1	R	499	 65% 28% 7%
1	S	499	 64% 28% 7%
1	T	499	 64% 28% 7%
1	U	499	 63% 30% 7%
1	V	499	 64% 28% 7%
1	W	499	 64% 29% 6%
1	X	499	 65% 29% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 91656 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	0	0
			3799	2368	670	735	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	0	0
			3799	2368	670	735	26			
1	D	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	E	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	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	0	0
			3799	2368	670	735	26			
1	I	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	J	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	K	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	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	0	0
			3799	2368	670	735	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	R	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	S	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	T	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	U	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	V	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	W	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	X	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			

There are 96 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

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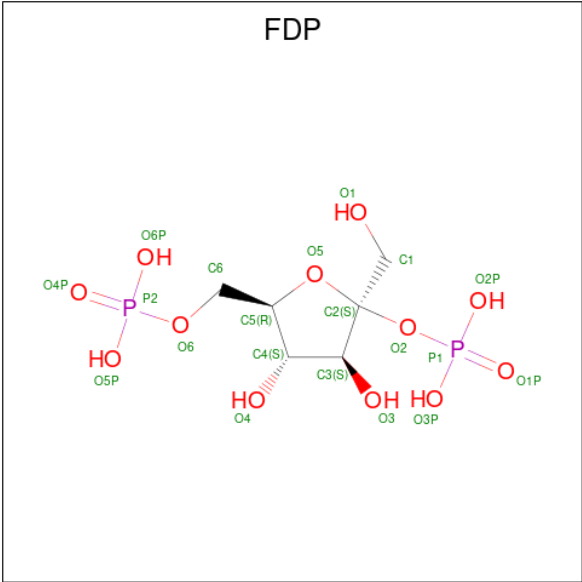
Chain	Residue	Modelled	Actual	Comment	Reference
F	405	SER	GLY	SEE REMARK 999	UNP Q27686
G	382	SER	GLY	SEE REMARK 999	UNP Q27686
G	389	TYR	SER	SEE REMARK 999	UNP Q27686
G	404	ARG	ALA	SEE REMARK 999	UNP Q27686
G	405	SER	GLY	SEE REMARK 999	UNP Q27686
H	382	SER	GLY	SEE REMARK 999	UNP Q27686
H	389	TYR	SER	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
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
Q	382	SER	GLY	SEE REMARK 999	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	389	TYR	SER	SEE REMARK 999	UNP Q27686
Q	404	ARG	ALA	SEE REMARK 999	UNP Q27686
Q	405	SER	GLY	SEE REMARK 999	UNP Q27686
R	382	SER	GLY	SEE REMARK 999	UNP Q27686
R	389	TYR	SER	SEE REMARK 999	UNP Q27686
R	404	ARG	ALA	SEE REMARK 999	UNP Q27686
R	405	SER	GLY	SEE REMARK 999	UNP Q27686
S	382	SER	GLY	SEE REMARK 999	UNP Q27686
S	389	TYR	SER	SEE REMARK 999	UNP Q27686
S	404	ARG	ALA	SEE REMARK 999	UNP Q27686
S	405	SER	GLY	SEE REMARK 999	UNP Q27686
T	382	SER	GLY	SEE REMARK 999	UNP Q27686
T	389	TYR	SER	SEE REMARK 999	UNP Q27686
T	404	ARG	ALA	SEE REMARK 999	UNP Q27686
T	405	SER	GLY	SEE REMARK 999	UNP Q27686
U	382	SER	GLY	SEE REMARK 999	UNP Q27686
U	389	TYR	SER	SEE REMARK 999	UNP Q27686
U	404	ARG	ALA	SEE REMARK 999	UNP Q27686
U	405	SER	GLY	SEE REMARK 999	UNP Q27686
V	382	SER	GLY	SEE REMARK 999	UNP Q27686
V	389	TYR	SER	SEE REMARK 999	UNP Q27686
V	404	ARG	ALA	SEE REMARK 999	UNP Q27686
V	405	SER	GLY	SEE REMARK 999	UNP Q27686
W	382	SER	GLY	SEE REMARK 999	UNP Q27686
W	389	TYR	SER	SEE REMARK 999	UNP Q27686
W	404	ARG	ALA	SEE REMARK 999	UNP Q27686
W	405	SER	GLY	SEE REMARK 999	UNP Q27686
X	382	SER	GLY	SEE REMARK 999	UNP Q27686
X	389	TYR	SER	SEE REMARK 999	UNP Q27686
X	404	ARG	ALA	SEE REMARK 999	UNP Q27686
X	405	SER	GLY	SEE REMARK 999	UNP Q27686

- Molecule 2 is 2,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FDP) (formula: $C_6H_{14}O_{12}P_2$).



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

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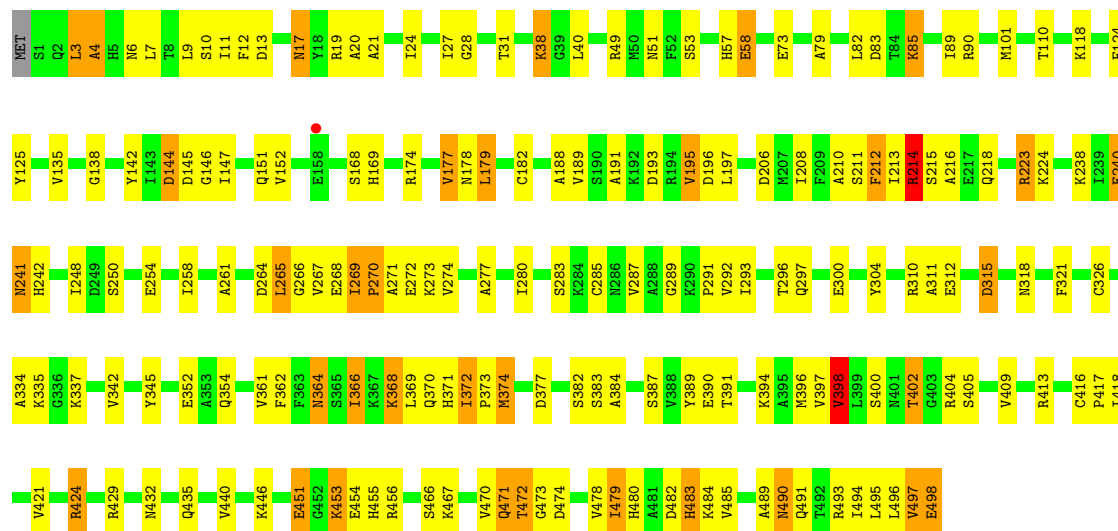
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	O	P	0	0
			20	6	12	2		
2	P	1	Total	C	O	P	0	0
			20	6	12	2		
2	Q	1	Total	C	O	P	0	0
			20	6	12	2		
2	R	1	Total	C	O	P	0	0
			20	6	12	2		
2	S	1	Total	C	O	P	0	0
			20	6	12	2		
2	T	1	Total	C	O	P	0	0
			20	6	12	2		
2	U	1	Total	C	O	P	0	0
			20	6	12	2		
2	V	1	Total	C	O	P	0	0
			20	6	12	2		
2	W	1	Total	C	O	P	0	0
			20	6	12	2		
2	X	1	Total	C	O	P	0	0
			20	6	12	2		



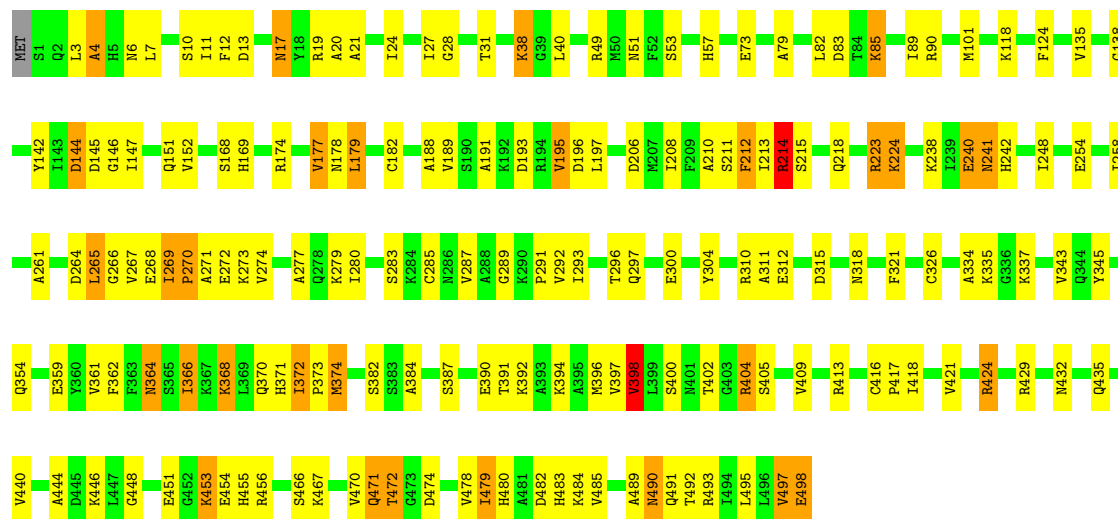
• Molecule 1: Pyruvate kinase

Chain C: 63% 30% 7%



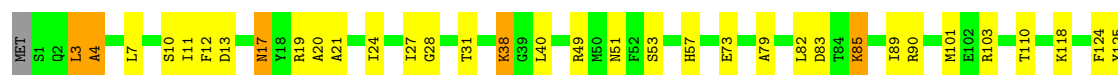
• Molecule 1: Pyruvate kinase

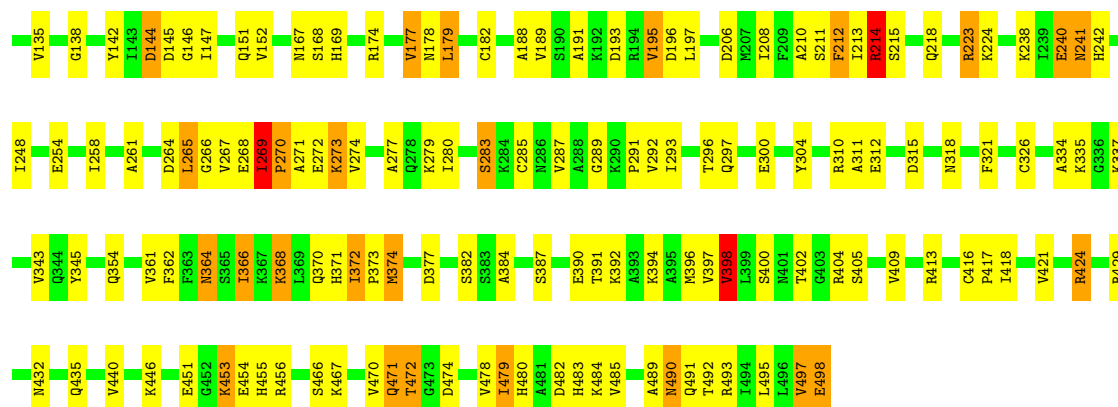
Chain D: 64% 29% 6%



• Molecule 1: Pyruvate kinase

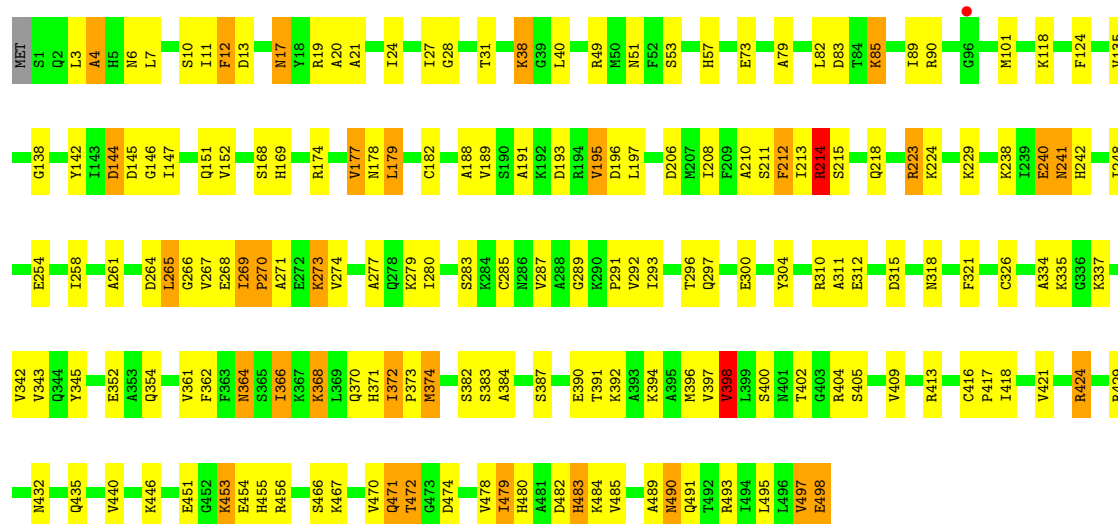
Chain E: 64% 29% 6%





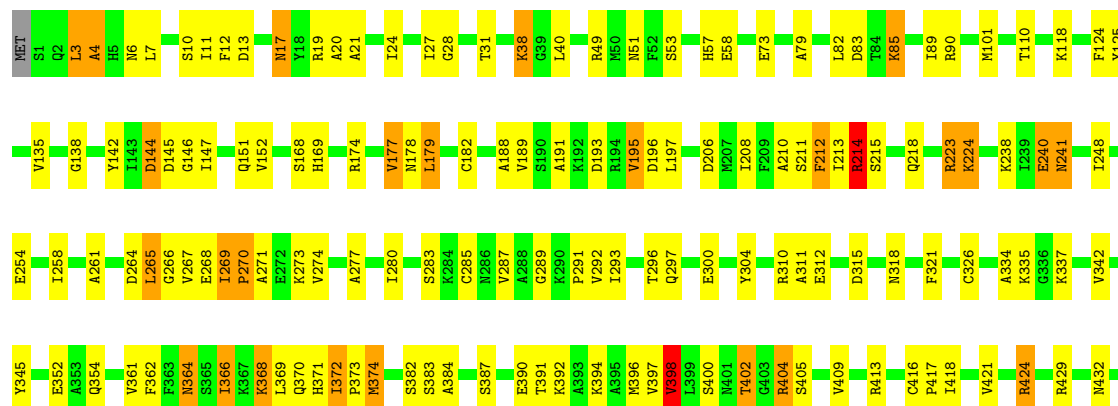
• Molecule 1: Pyruvate kinase

Chain F: 65% 29% 6%



• Molecule 1: Pyruvate kinase

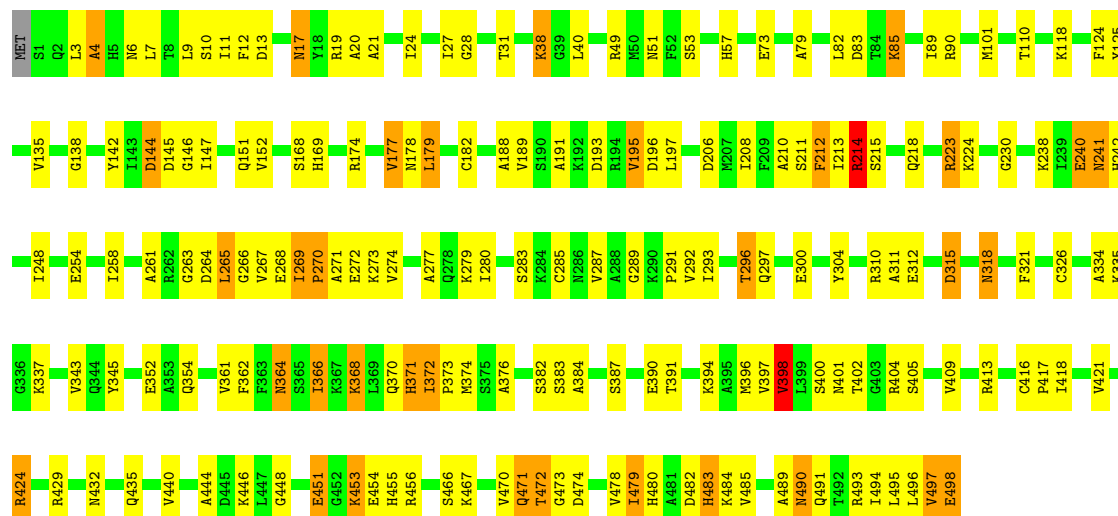
Chain G: 65% 28% 7%





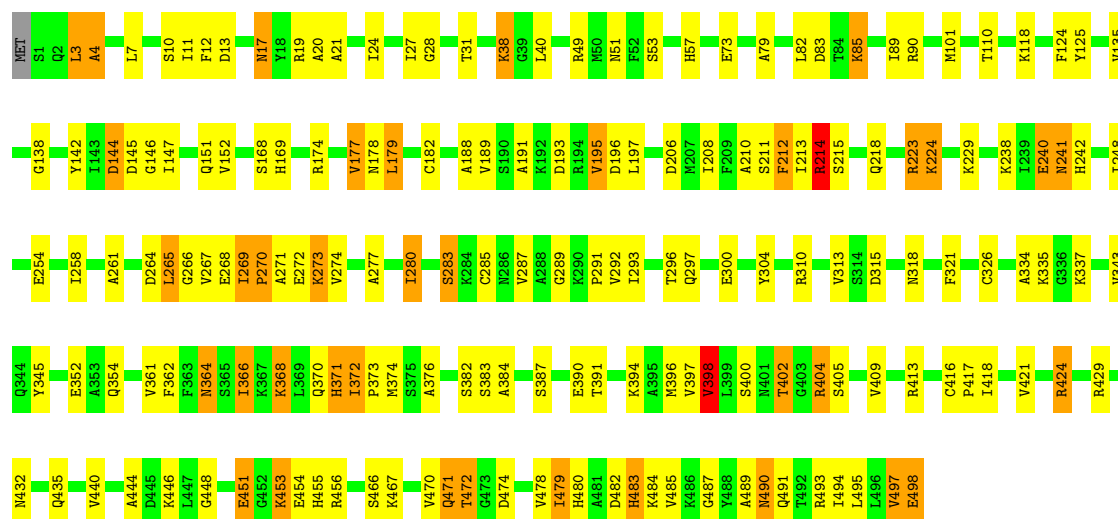
• Molecule 1: Pyruvate kinase

Chain H: 63% 30% 7%



• Molecule 1: Pyruvate kinase

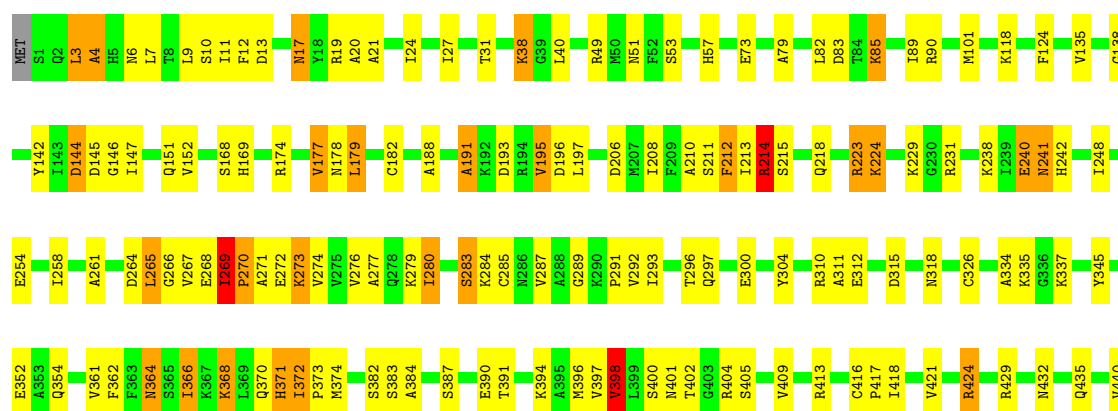
Chain I: 64% 28% 7%

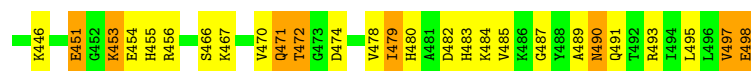


• Molecule 1: Pyruvate kinase

Chain J: 65% 28% 7%

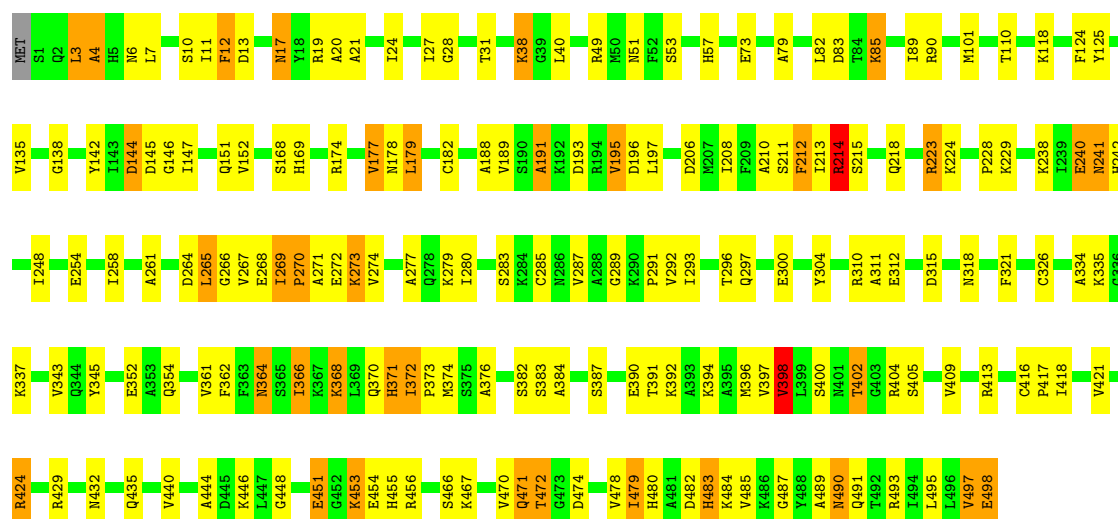






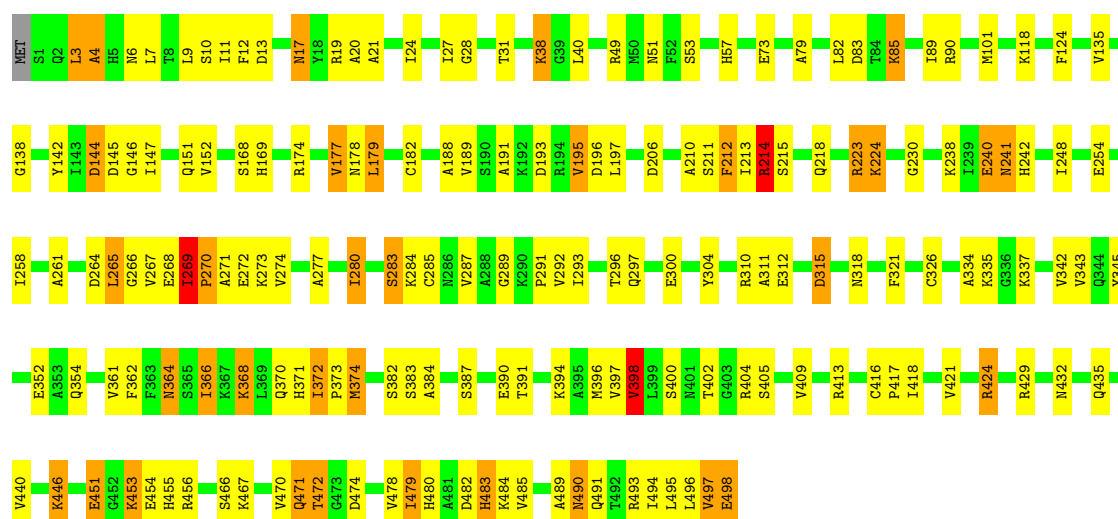
• Molecule 1: Pyruvate kinase

Chain M: 63% 29% 7%



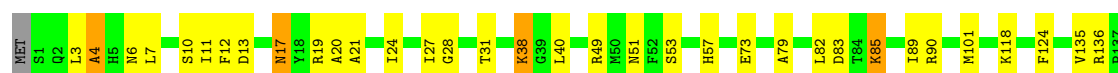
• Molecule 1: Pyruvate kinase

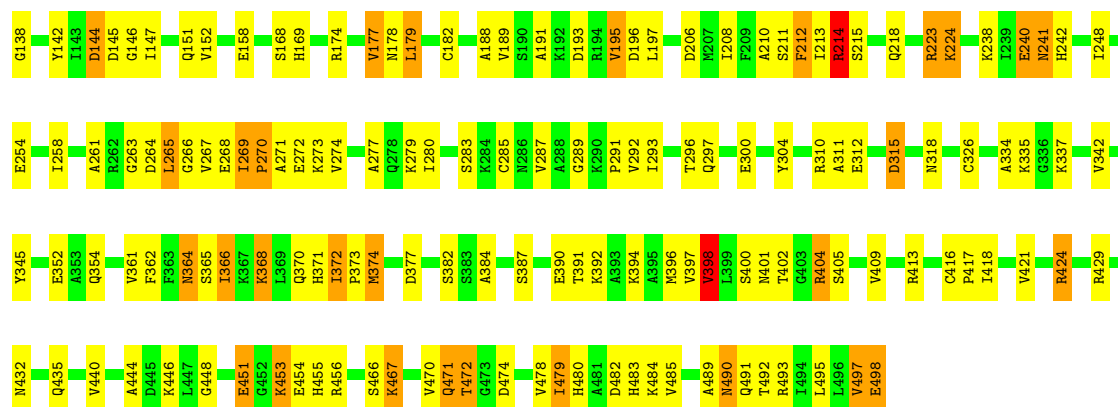
Chain N: 64% 28% 7%



• Molecule 1: Pyruvate kinase

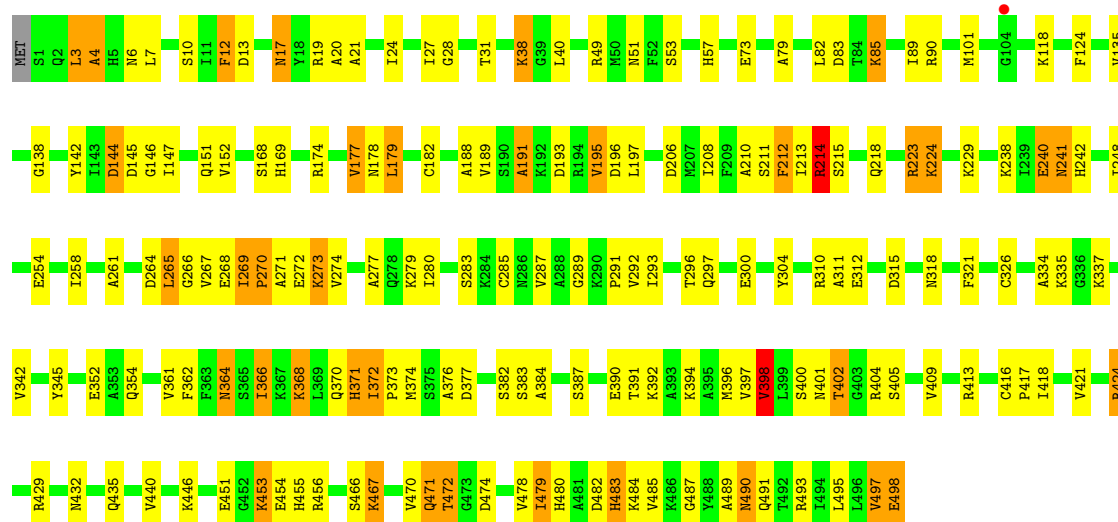
Chain O: 63% 29% 7%





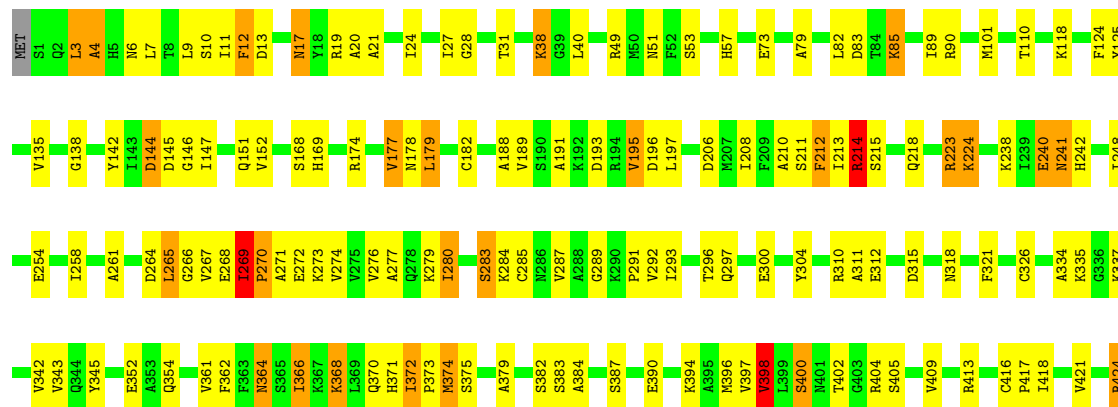
• Molecule 1: Pyruvate kinase

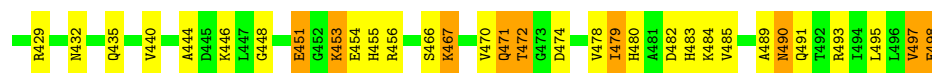
Chain P: 64% 28% 7%



• Molecule 1: Pyruvate kinase

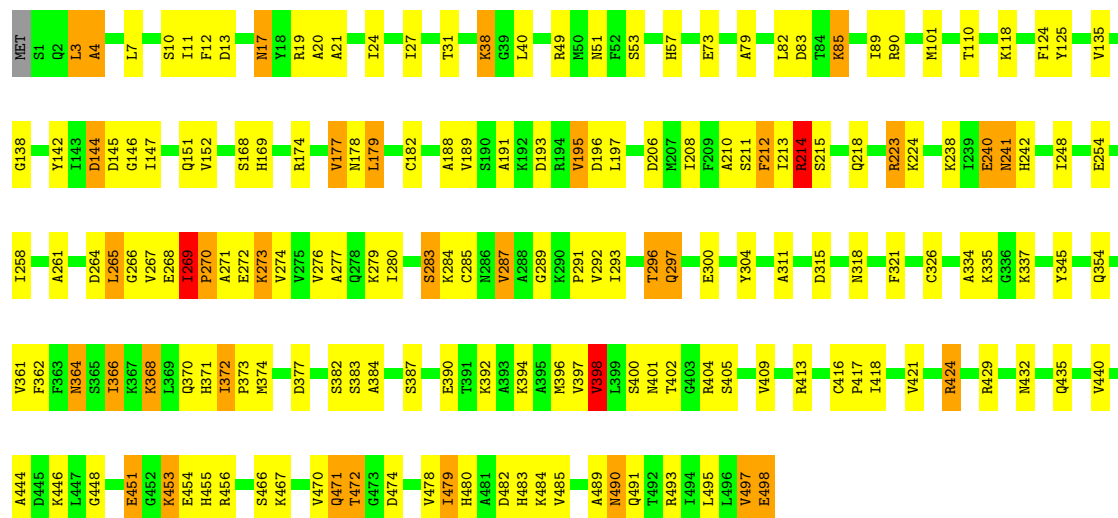
Chain Q: 63% 29% 7%





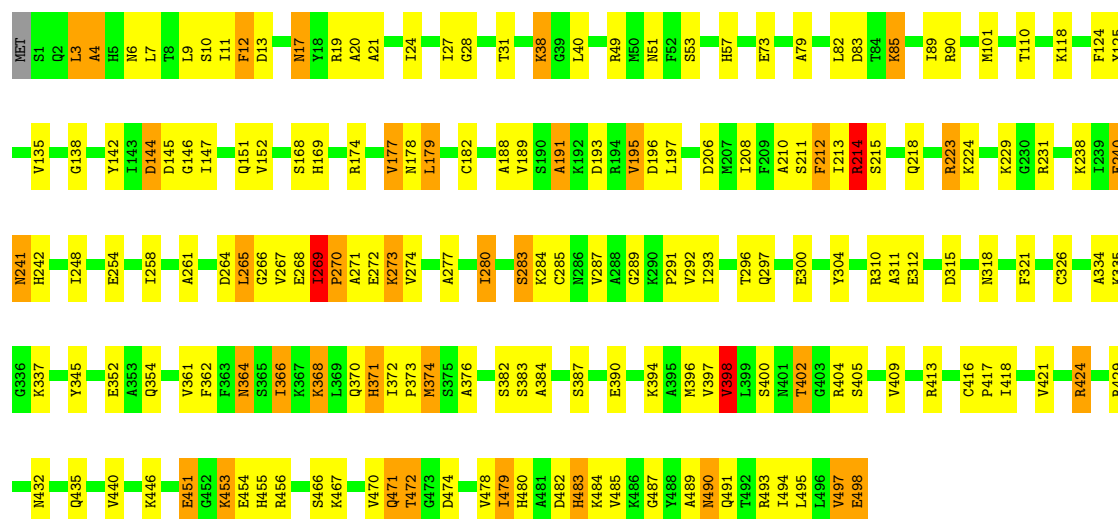
• Molecule 1: Pyruvate kinase

Chain R: 65% 28% 7%



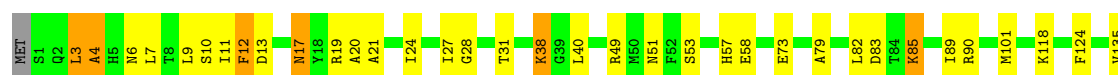
• Molecule 1: Pyruvate kinase

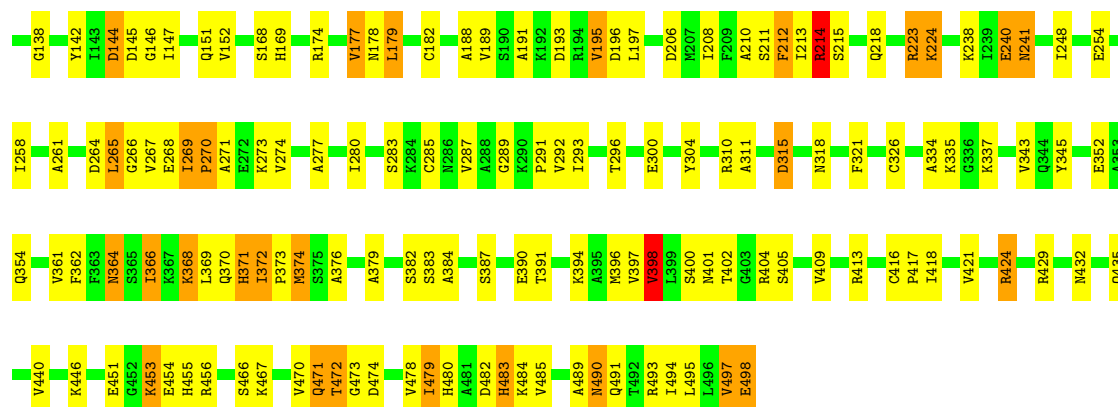
Chain S: 64% 28% 7%



• Molecule 1: Pyruvate kinase

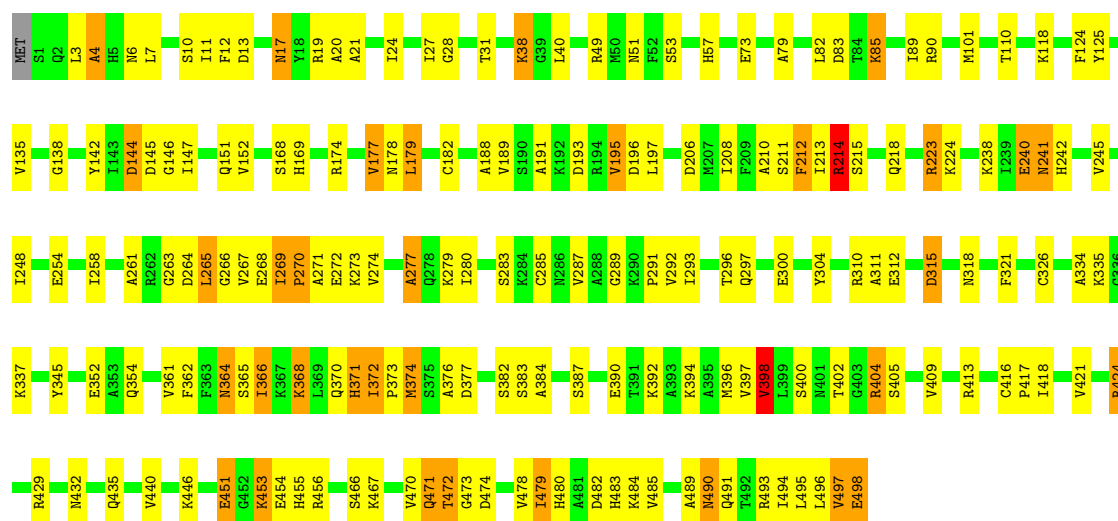
Chain T: 64% 28% 7%





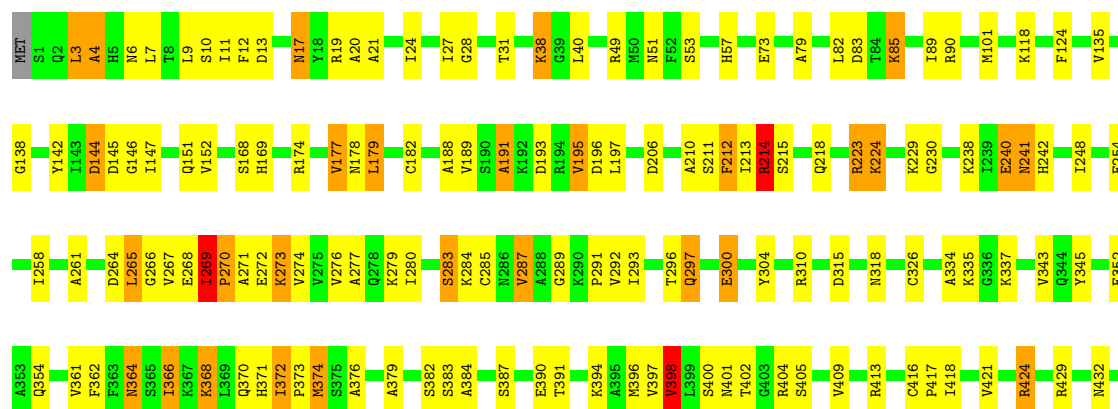
• Molecule 1: Pyruvate kinase

Chain U: 63% 30% 7%



• Molecule 1: Pyruvate kinase

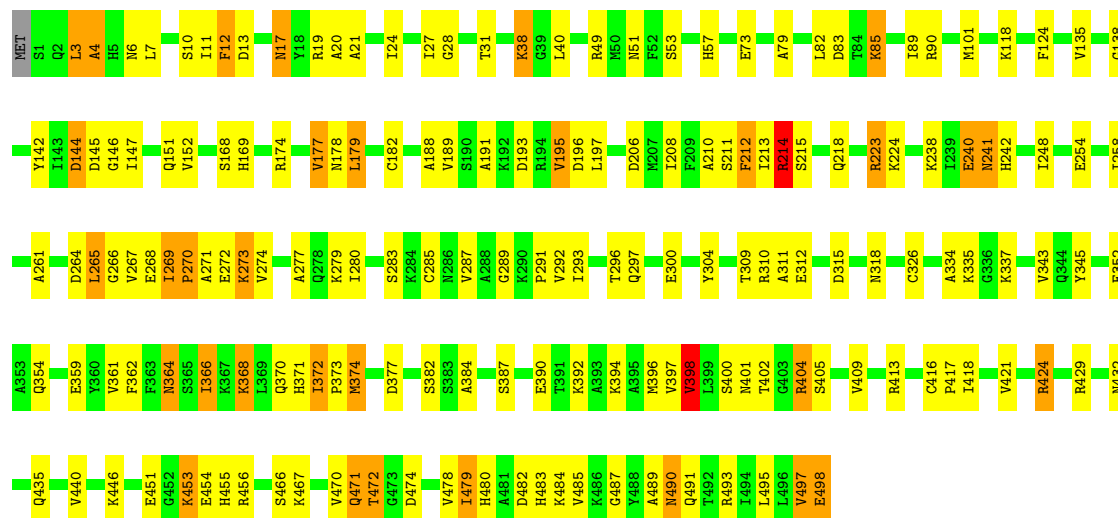
Chain V: 64% 28% 7%





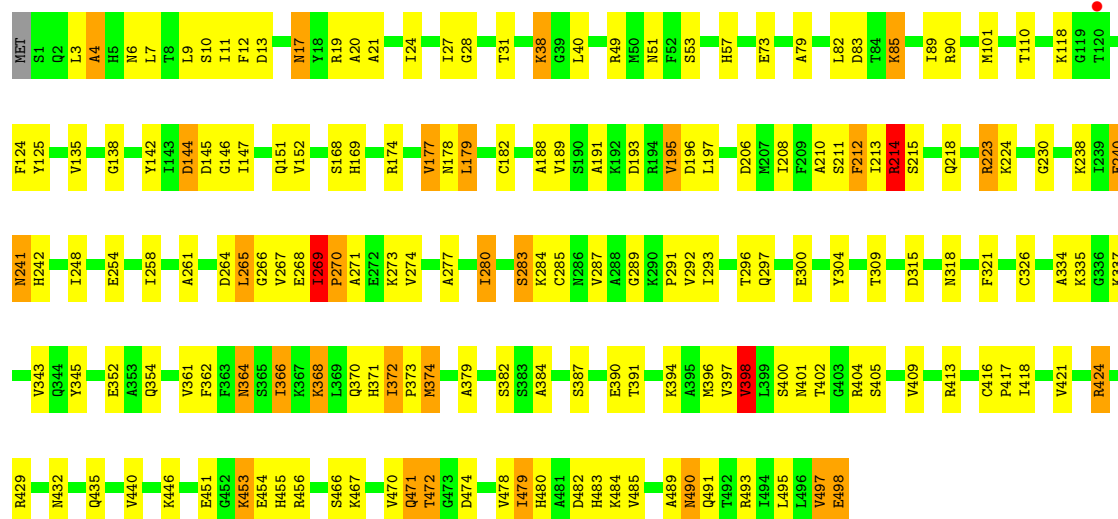
• Molecule 1: Pyruvate kinase

Chain W: 64% 29% 6%



• Molecule 1: Pyruvate kinase

Chain X: 65% 29% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	243.84Å 254.69Å 892.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 5.07 39.81 – 5.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.81-5.07) 86.3 (39.81-5.07)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 5.09Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.353 , 0.357 0.343 , 0.345	Depositor DCC
R_{free} test set	5652 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.118 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	91656	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: FDP

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	1.87	47/3856 (1.2%)	1.26	33/5220 (0.6%)
1	B	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	C	1.87	46/3856 (1.2%)	1.26	32/5220 (0.6%)
1	D	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	E	1.88	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	F	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	G	1.88	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	H	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	I	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	J	1.87	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	K	1.87	45/3856 (1.2%)	1.26	31/5220 (0.6%)
1	L	1.87	43/3856 (1.1%)	1.26	30/5220 (0.6%)
1	M	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	N	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	O	1.87	44/3856 (1.1%)	1.26	33/5220 (0.6%)
1	P	1.87	46/3856 (1.2%)	1.26	33/5220 (0.6%)
1	Q	1.87	47/3856 (1.2%)	1.26	33/5220 (0.6%)
1	R	1.87	43/3856 (1.1%)	1.26	30/5220 (0.6%)
1	S	1.87	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	T	1.87	45/3856 (1.2%)	1.26	34/5220 (0.7%)
1	U	1.87	44/3856 (1.1%)	1.26	33/5220 (0.6%)
1	V	1.87	43/3856 (1.1%)	1.26	32/5220 (0.6%)
1	W	1.88	45/3856 (1.2%)	1.26	33/5220 (0.6%)
1	X	1.87	46/3856 (1.2%)	1.26	34/5220 (0.7%)
All	All	1.87	1087/92544 (1.2%)	1.26	784/125280 (0.6%)

The worst 5 of 1087 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	413	ARG	C-O	-7.01	1.20	1.23
1	L	413	ARG	C-O	-6.87	1.20	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	413	ARG	C-O	-6.86	1.20	1.23
1	S	413	ARG	C-O	-6.86	1.20	1.23
1	E	413	ARG	C-O	-6.85	1.20	1.23

The worst 5 of 784 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	270	PRO	O-C-N	9.28	134.24	123.10
1	K	270	PRO	O-C-N	9.26	134.21	123.10
1	P	270	PRO	O-C-N	9.23	134.18	123.10
1	I	270	PRO	O-C-N	9.22	134.17	123.10
1	C	270	PRO	O-C-N	9.21	134.16	123.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3799	0	3802	144	0
1	B	3799	0	3802	168	0
1	C	3799	0	3802	213	0
1	D	3799	0	3802	136	0
1	E	3799	0	3802	156	0
1	F	3799	0	3802	146	3
1	G	3799	0	3802	158	0
1	H	3799	0	3802	242	0
1	I	3799	0	3802	184	0
1	J	3799	0	3802	199	1
1	K	3799	0	3802	174	0
1	L	3799	0	3802	231	0
1	M	3799	0	3802	197	0
1	N	3799	0	3802	238	0
1	O	3799	0	3802	169	0
1	P	3799	0	3802	204	0
1	Q	3799	0	3802	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	3799	0	3802	202	0
1	S	3799	0	3802	233	0
1	T	3799	0	3802	216	1
1	U	3799	0	3802	220	0
1	V	3799	0	3802	259	0
1	W	3799	0	3802	192	3
1	X	3799	0	3802	188	0
2	A	20	0	10	4	0
2	B	20	0	10	4	0
2	C	20	0	10	4	0
2	D	20	0	10	4	0
2	E	20	0	10	4	0
2	F	20	0	10	4	0
2	G	20	0	10	4	0
2	H	20	0	10	5	0
2	I	20	0	10	5	0
2	J	20	0	10	4	0
2	K	20	0	10	5	0
2	L	20	0	10	5	0
2	M	20	0	10	4	0
2	N	20	0	10	4	0
2	O	20	0	10	5	0
2	P	20	0	10	5	0
2	Q	20	0	10	4	0
2	R	20	0	10	5	0
2	S	20	0	10	4	0
2	T	20	0	10	5	0
2	U	20	0	10	4	0
2	V	20	0	10	5	0
2	W	20	0	10	5	0
2	X	20	0	10	5	0
All	All	91656	0	91488	3592	4

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 20.

The worst 5 of 3592 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:C:216:ALA:CB	1:N:446:LYS:HD3	1.49	1.42
1:C:250:SER:CB	1:N:446:LYS:HG2	1.49	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:242:HIS:HE1	1:W:12:PHE:CZ	1.42	1.38
1:H:12:PHE:CZ	1:J:242:HIS:HE1	1.41	1.37
1:P:487:GLY:HA2	1:V:229:LYS:CE	1.56	1.33

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:ARG:CD	1:T:58:GLU:OE1[5_545]	1.91	0.29
1:F:229:LYS:CE	1:W:487:GLY:CA[5_545]	2.08	0.12
1:F:229:LYS:CD	1:W:487:GLY:CA[5_545]	2.15	0.05
1:F:229:LYS:CG	1:W:487:GLY:CA[5_545]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	B	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	C	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	D	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	E	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	F	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	G	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	H	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	I	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	43	77
1	J	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	K	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	M	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	N	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	O	496/499 (99%)	485 (98%)	10 (2%)	1 (0%)	43	77
1	P	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	Q	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	R	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	S	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	T	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	U	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	V	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	W	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
1	X	496/499 (99%)	486 (98%)	9 (2%)	1 (0%)	43	77
All	All	11904/11976 (99%)	11662 (98%)	218 (2%)	24 (0%)	43	77

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
1	B	296	THR
1	C	296	THR
1	D	296	THR
1	E	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	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	B	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	C	416/417 (100%)	375 (90%)	41 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	E	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	F	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	G	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	H	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	I	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	J	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	K	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	L	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	M	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	N	416/417 (100%)	377 (91%)	39 (9%)	8	26
1	O	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	P	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	Q	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	R	416/417 (100%)	376 (90%)	40 (10%)	8	25
1	S	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	T	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	U	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	V	416/417 (100%)	375 (90%)	41 (10%)	7	24
1	W	416/417 (100%)	374 (90%)	42 (10%)	7	23
1	X	416/417 (100%)	378 (91%)	38 (9%)	9	28
All	All	9984/10008 (100%)	9017 (90%)	967 (10%)	8	25

5 of 967 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	382	SER
1	V	498	GLU
1	O	240	GLU
1	V	453	LYS
1	X	366	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 431 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	483	HIS
1	P	483	HIS
1	W	151	GLN
1	N	151	GLN
1	O	246	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](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FDP	N	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	R	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	Q	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	G	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	K	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	I	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	H	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	V	700	-	19,20,20	1.09	2 (10%)	29,32,32	1.40	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDP	D	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	X	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	J	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	P	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	B	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	A	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	O	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	E	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	L	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	C	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	S	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	W	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	T	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	M	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	F	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
2	FDP	U	700	-	19,20,20	1.07	2 (10%)	29,32,32	1.40	5 (17%)

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	FDP	N	700	-	-	1/12/34/34	0/1/1/1
2	FDP	R	700	-	-	1/12/34/34	0/1/1/1
2	FDP	Q	700	-	-	1/12/34/34	0/1/1/1
2	FDP	G	700	-	-	1/12/34/34	0/1/1/1
2	FDP	K	700	-	-	1/12/34/34	0/1/1/1
2	FDP	I	700	-	-	1/12/34/34	0/1/1/1
2	FDP	H	700	-	-	1/12/34/34	0/1/1/1
2	FDP	V	700	-	-	1/12/34/34	0/1/1/1
2	FDP	D	700	-	-	1/12/34/34	0/1/1/1
2	FDP	X	700	-	-	1/12/34/34	0/1/1/1
2	FDP	J	700	-	-	1/12/34/34	0/1/1/1
2	FDP	P	700	-	-	1/12/34/34	0/1/1/1
2	FDP	B	700	-	-	1/12/34/34	0/1/1/1
2	FDP	A	700	-	-	1/12/34/34	0/1/1/1
2	FDP	O	700	-	-	1/12/34/34	0/1/1/1
2	FDP	E	700	-	-	1/12/34/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDP	L	700	-	-	1/12/34/34	0/1/1/1
2	FDP	C	700	-	-	1/12/34/34	0/1/1/1
2	FDP	S	700	-	-	1/12/34/34	0/1/1/1
2	FDP	W	700	-	-	1/12/34/34	0/1/1/1
2	FDP	T	700	-	-	1/12/34/34	0/1/1/1
2	FDP	M	700	-	-	1/12/34/34	0/1/1/1
2	FDP	F	700	-	-	1/12/34/34	0/1/1/1
2	FDP	U	700	-	-	1/12/34/34	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	700	FDP	O4-C4	-2.35	1.37	1.43
2	X	700	FDP	O4-C4	-2.34	1.37	1.43
2	A	700	FDP	O4-C4	-2.34	1.37	1.43
2	W	700	FDP	O4-C4	-2.34	1.37	1.43
2	E	700	FDP	O4-C4	-2.34	1.37	1.43

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	700	FDP	O2-C2-C3	3.29	118.53	108.28
2	E	700	FDP	O2-C2-C3	3.29	118.52	108.28
2	R	700	FDP	O2-C2-C3	3.29	118.52	108.28
2	F	700	FDP	O2-C2-C3	3.29	118.52	108.28
2	I	700	FDP	O2-C2-C3	3.28	118.51	108.28

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

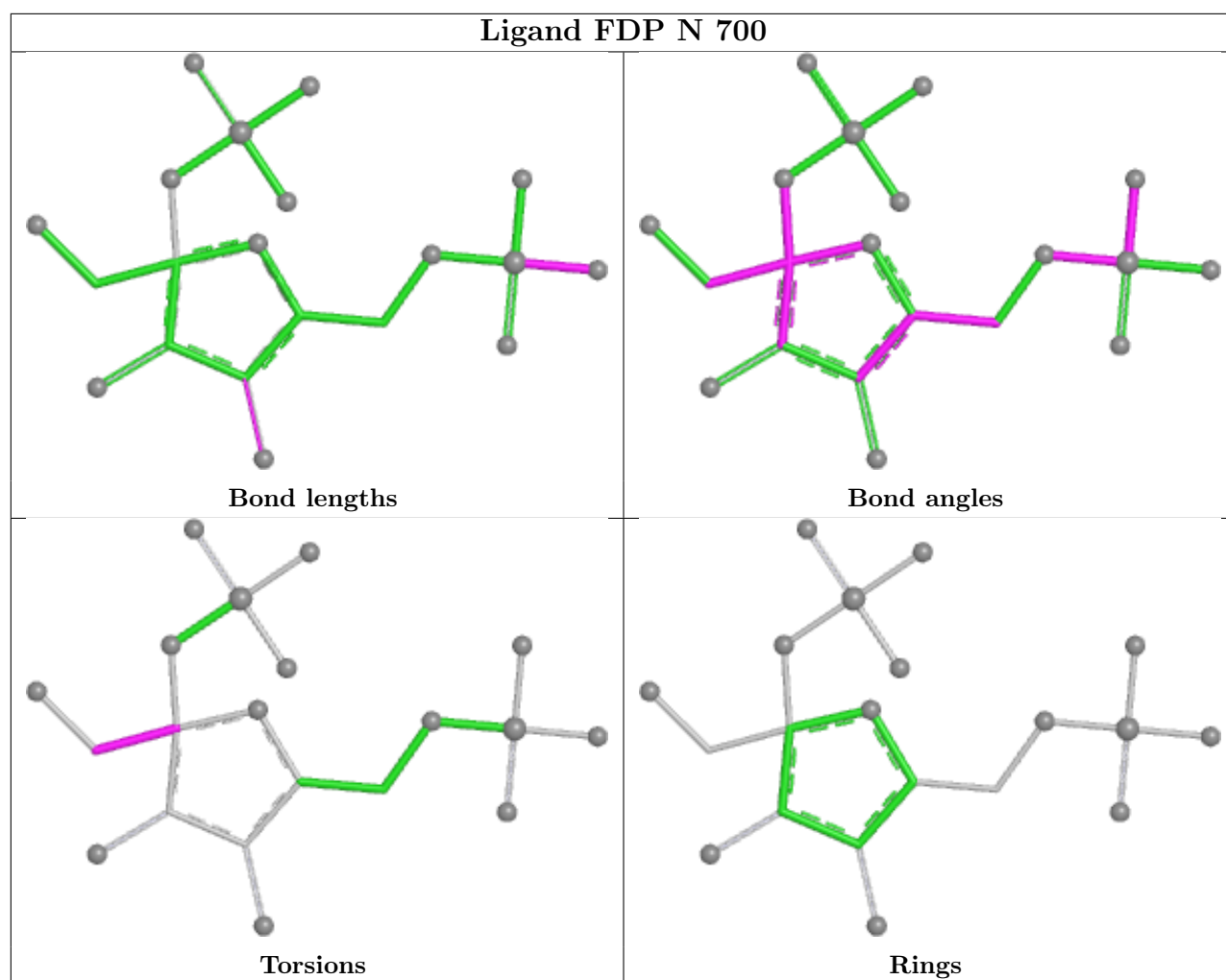
Mol	Chain	Res	Type	Atoms
2	A	700	FDP	O1-C1-C2-C3
2	B	700	FDP	O1-C1-C2-C3
2	C	700	FDP	O1-C1-C2-C3
2	D	700	FDP	O1-C1-C2-C3
2	E	700	FDP	O1-C1-C2-C3

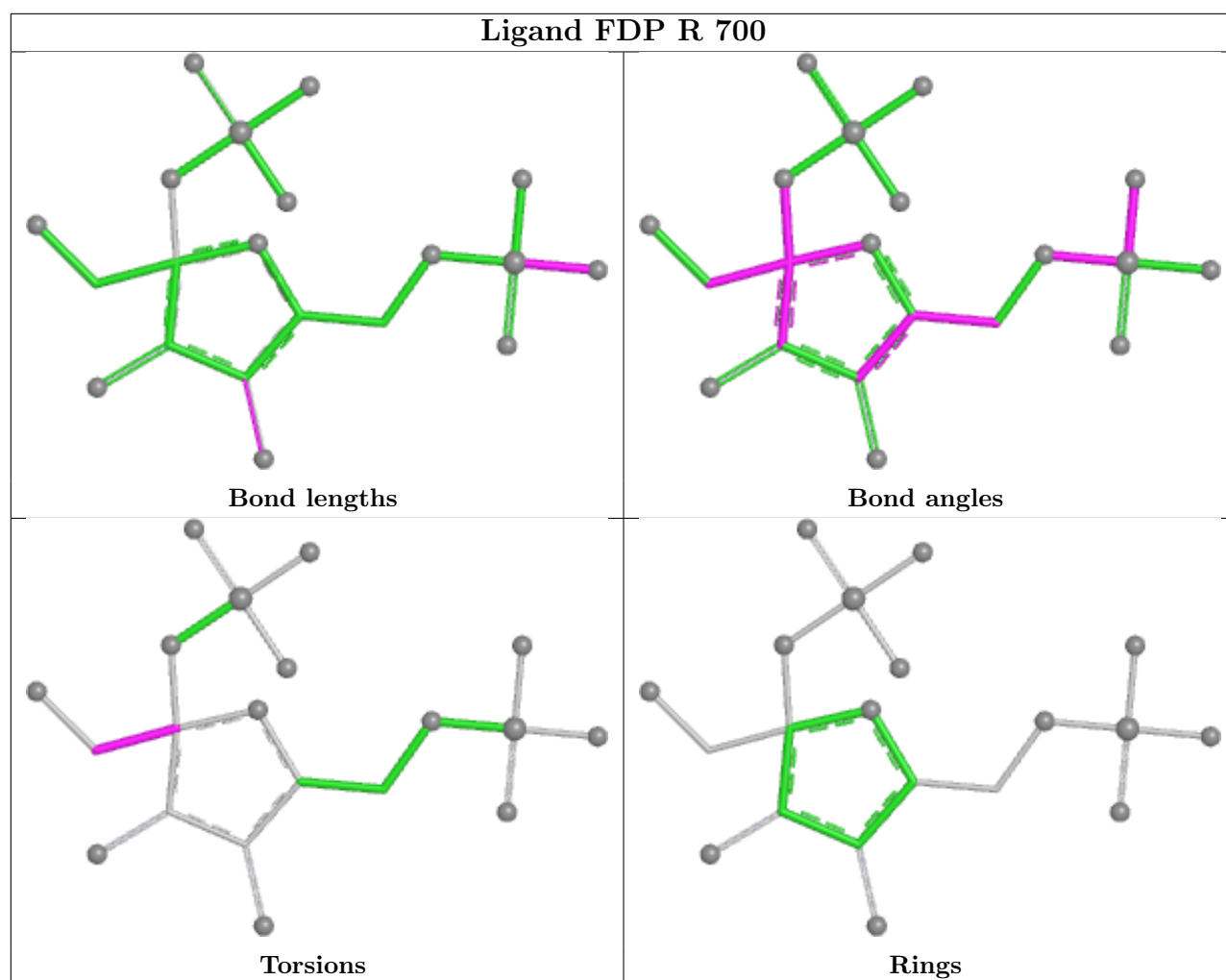
There are no ring outliers.

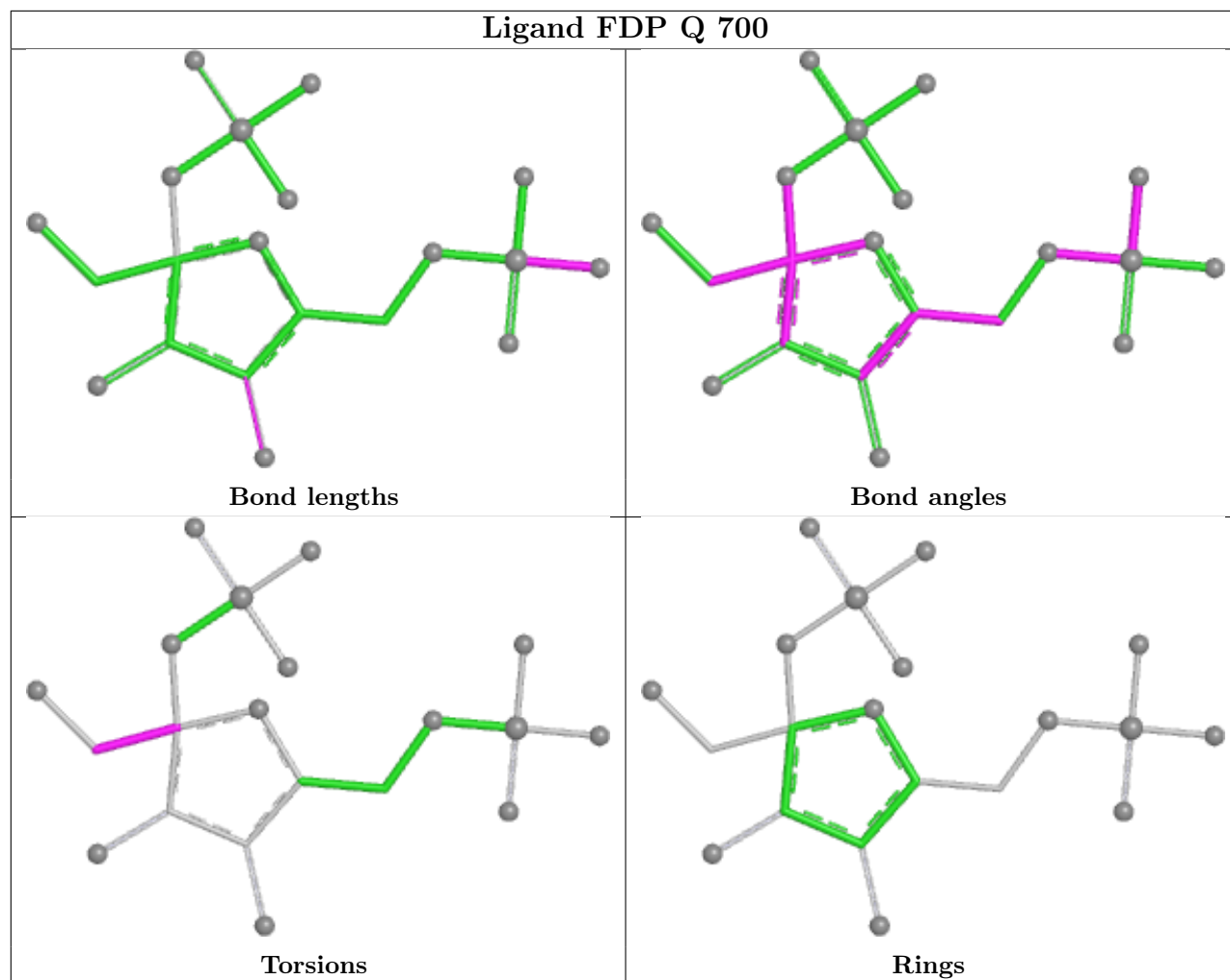
24 monomers are involved in 107 short contacts:

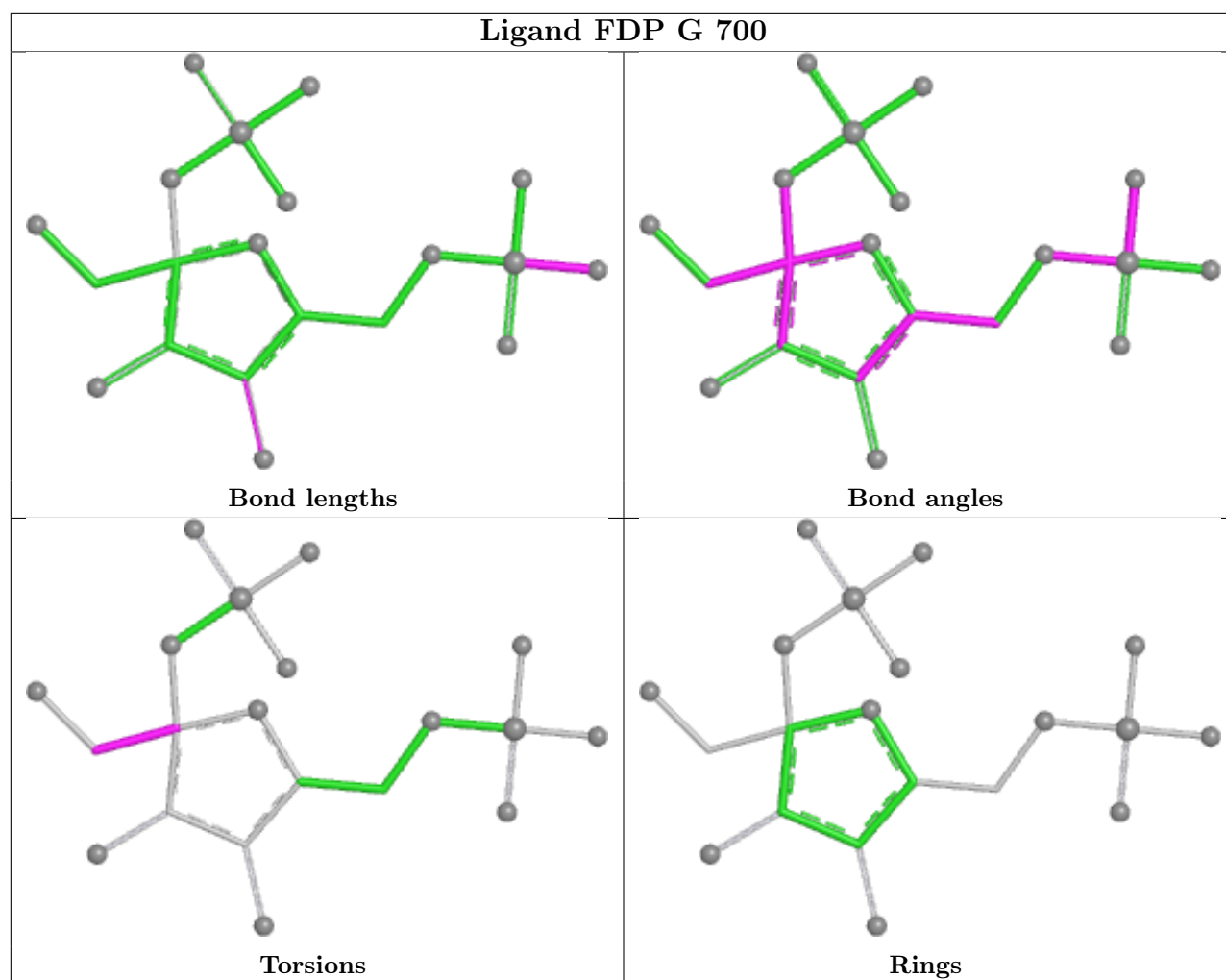
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	700	FDP	4	0
2	R	700	FDP	5	0
2	Q	700	FDP	4	0
2	G	700	FDP	4	0
2	K	700	FDP	5	0
2	I	700	FDP	5	0
2	H	700	FDP	5	0
2	V	700	FDP	5	0
2	D	700	FDP	4	0
2	X	700	FDP	5	0
2	J	700	FDP	4	0
2	P	700	FDP	5	0
2	B	700	FDP	4	0
2	A	700	FDP	4	0
2	O	700	FDP	5	0
2	E	700	FDP	4	0
2	L	700	FDP	5	0
2	C	700	FDP	4	0
2	S	700	FDP	4	0
2	W	700	FDP	5	0
2	T	700	FDP	5	0
2	M	700	FDP	4	0
2	F	700	FDP	4	0
2	U	700	FDP	4	0

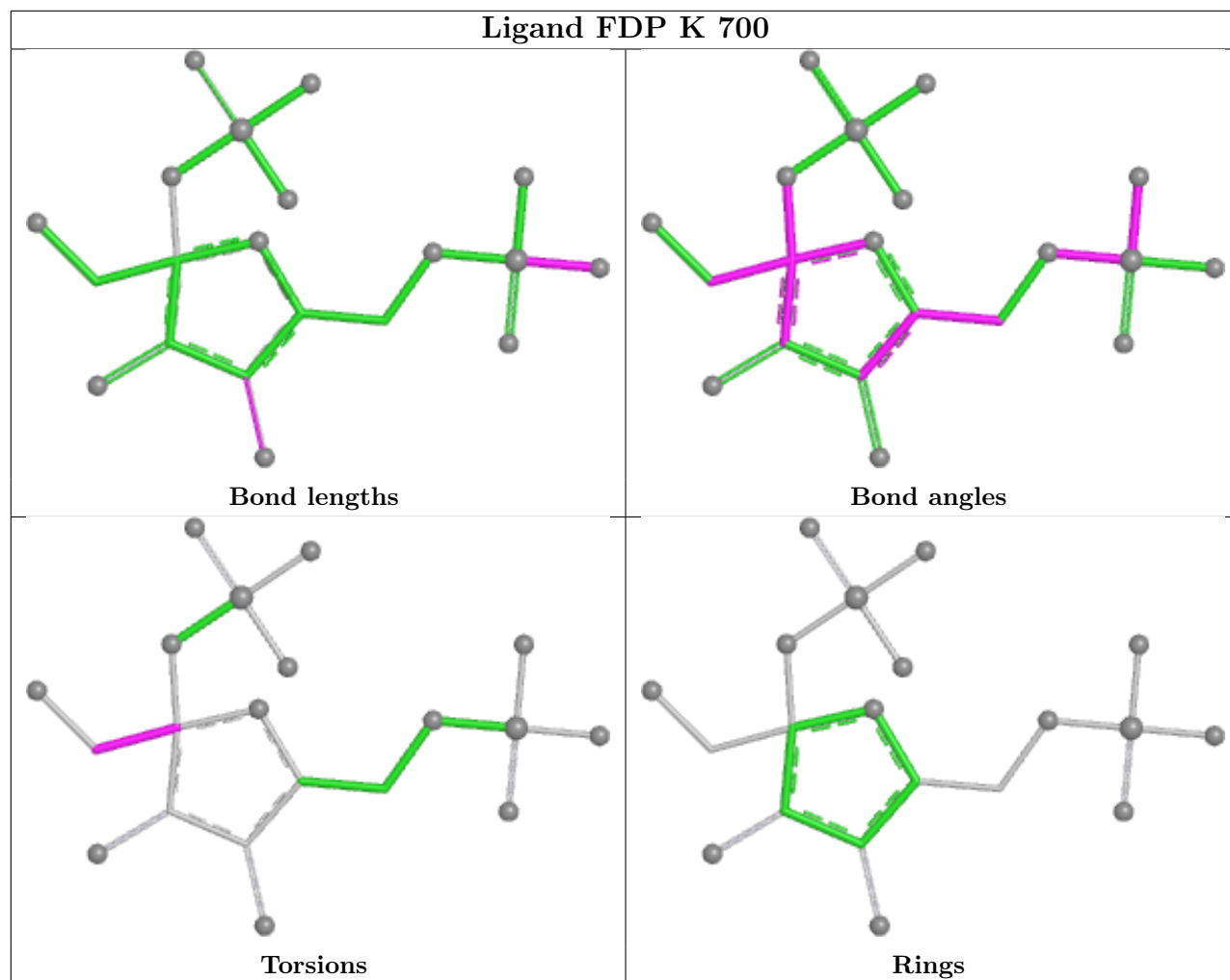
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



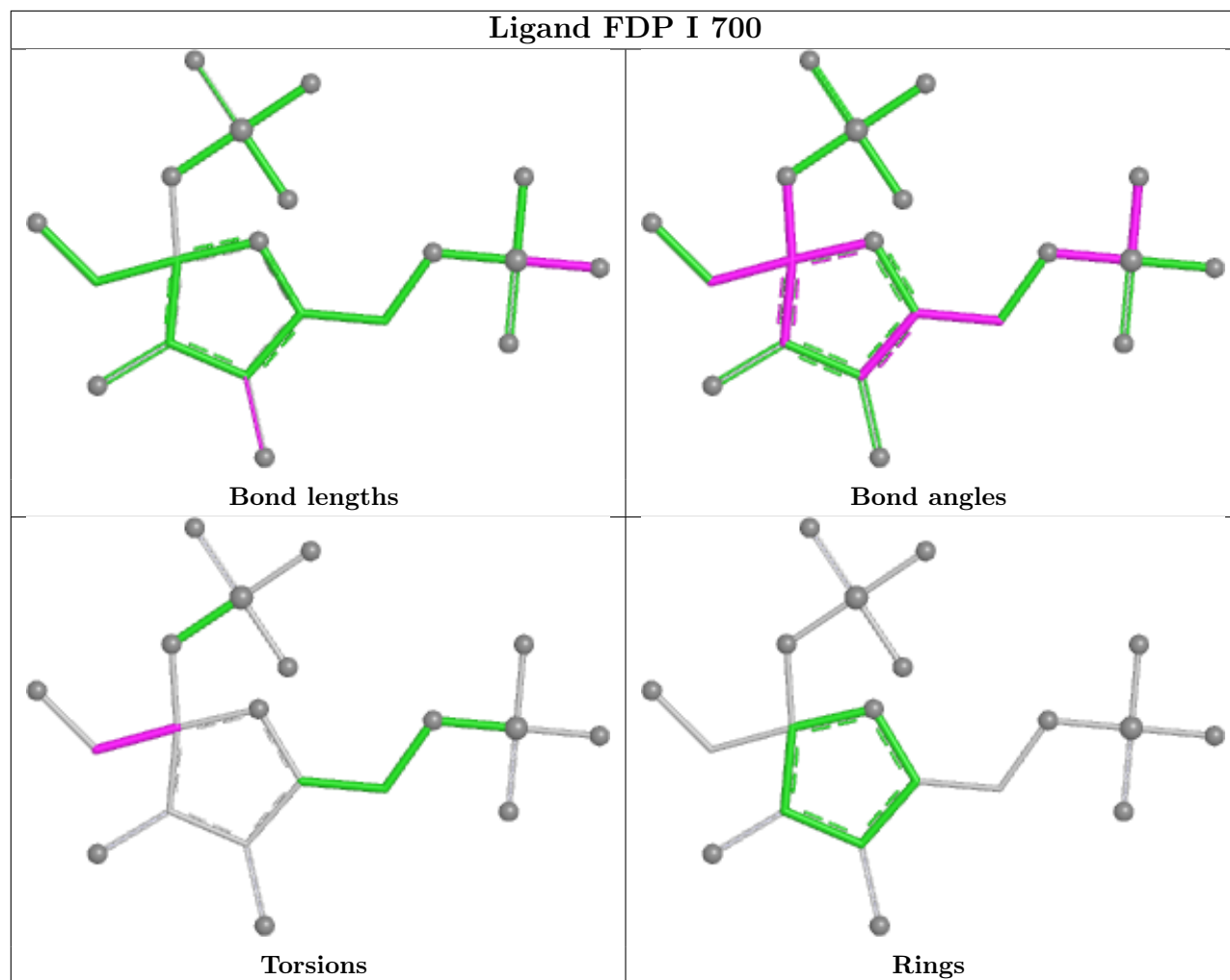


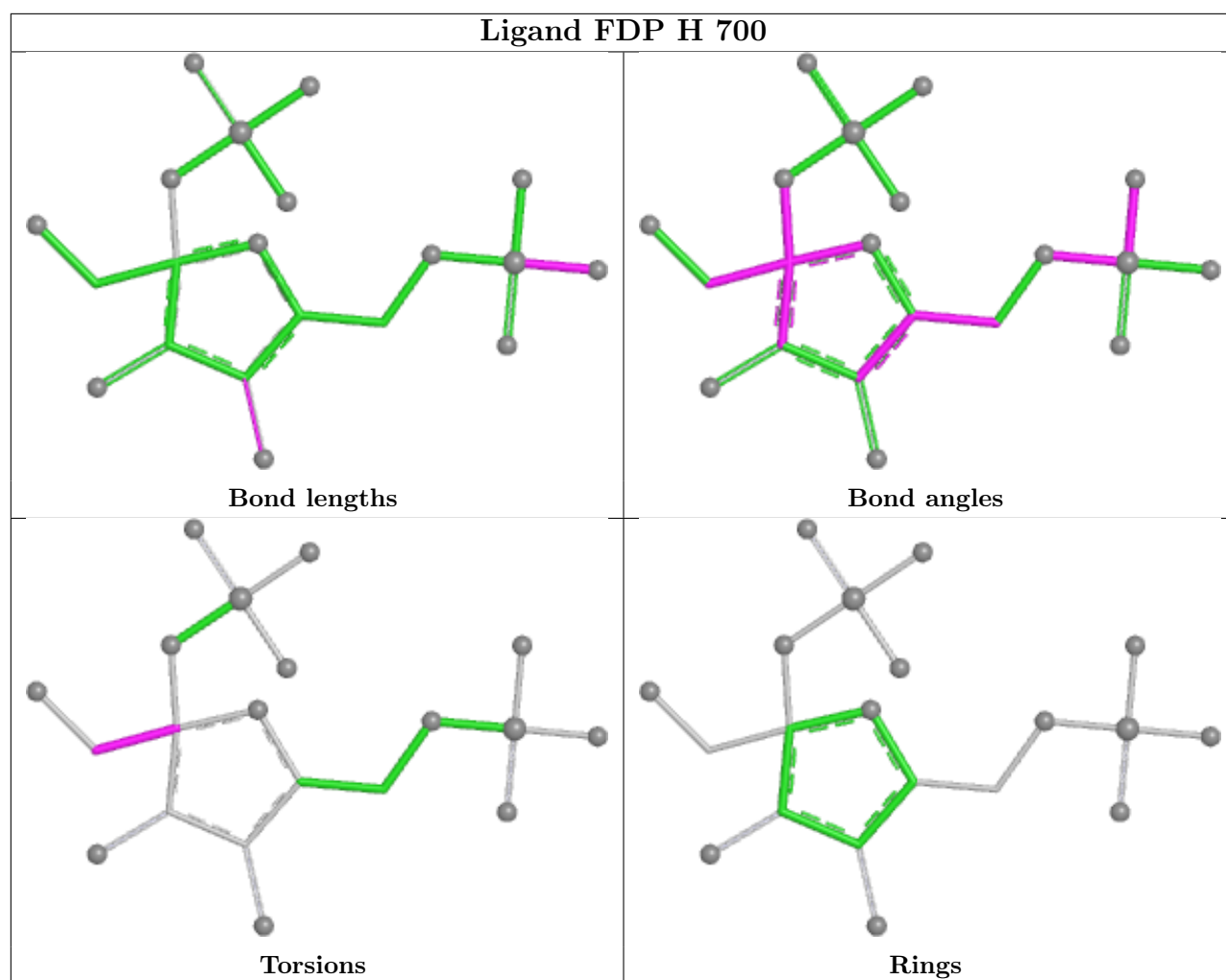


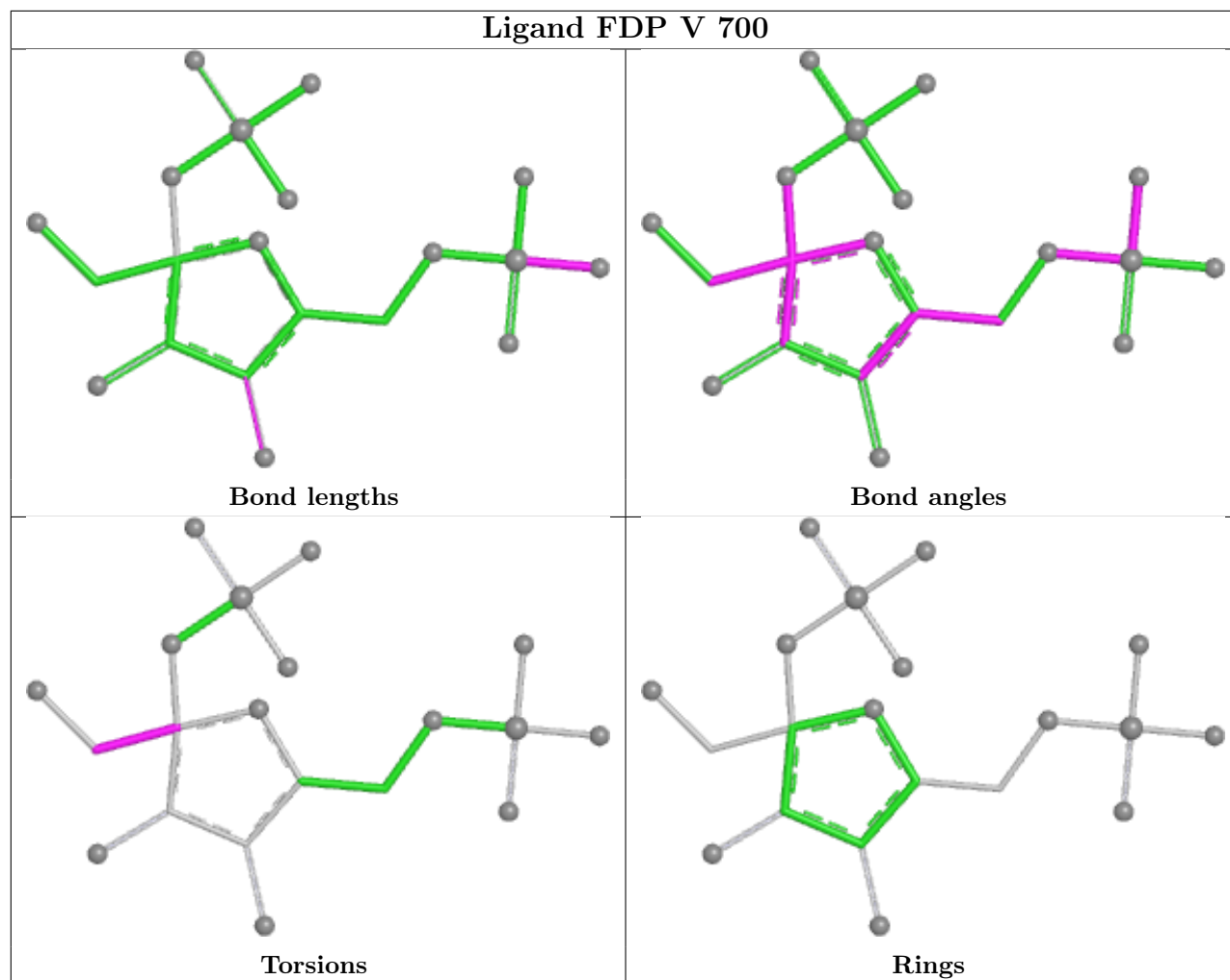


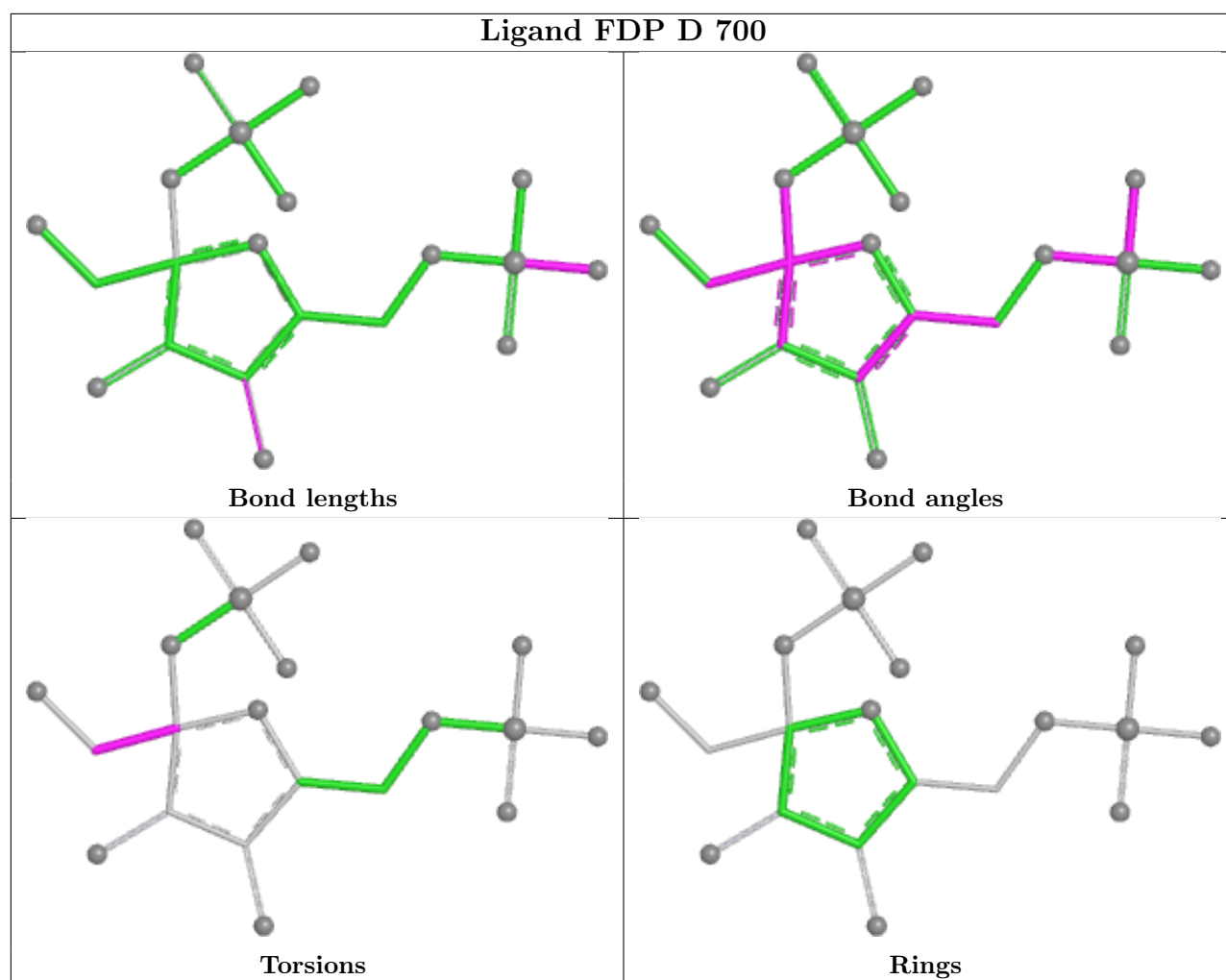


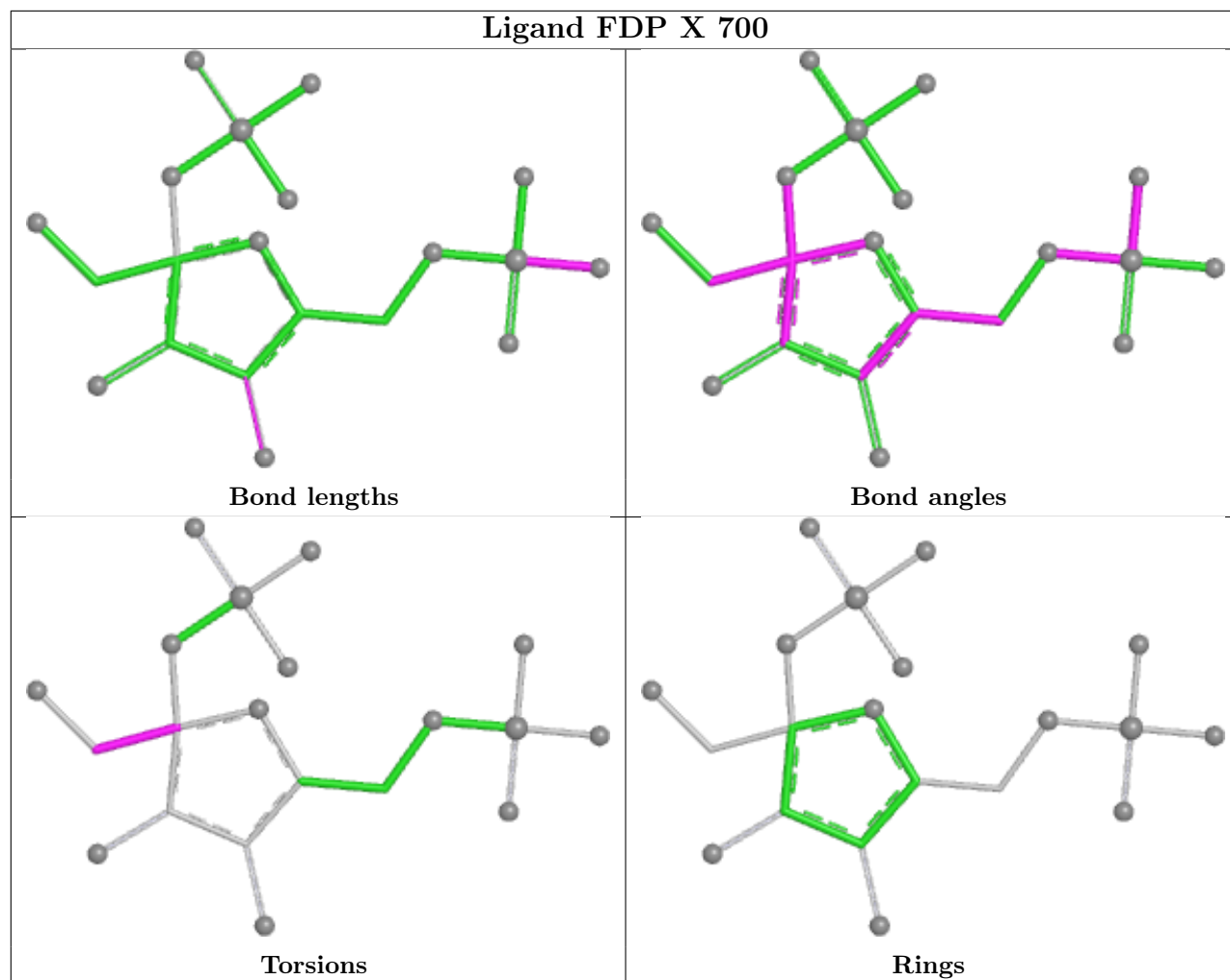
Ligand FDP I 700

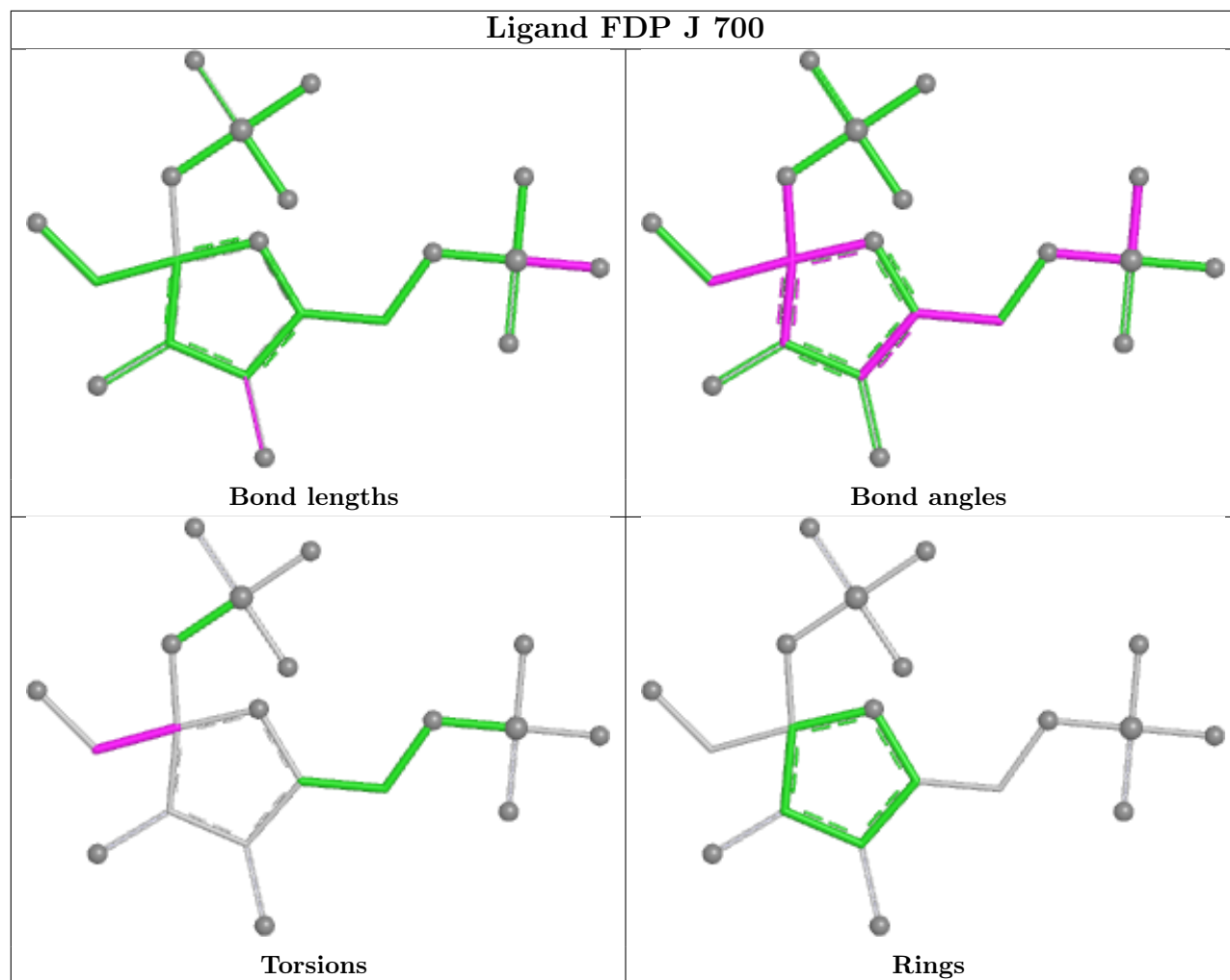




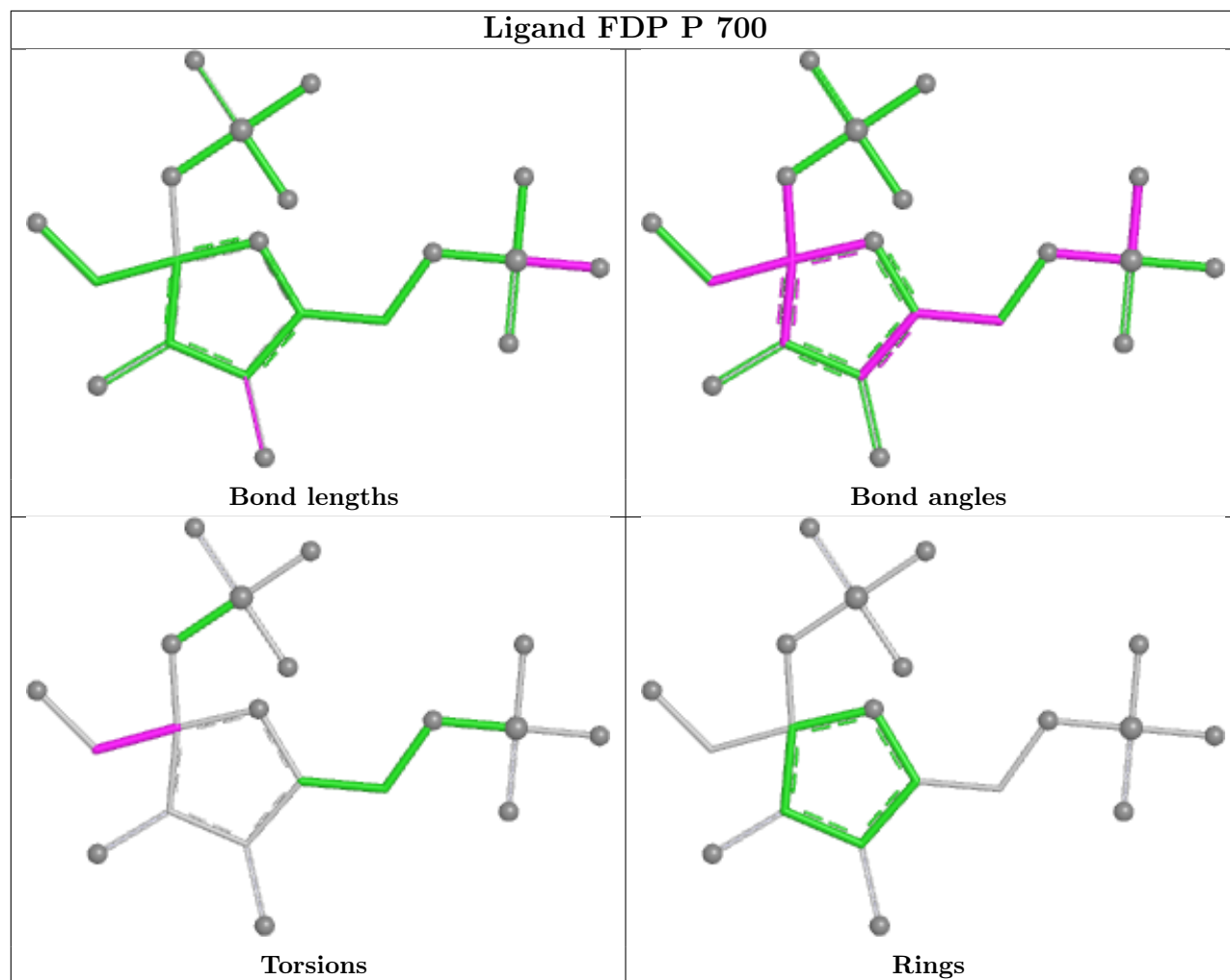


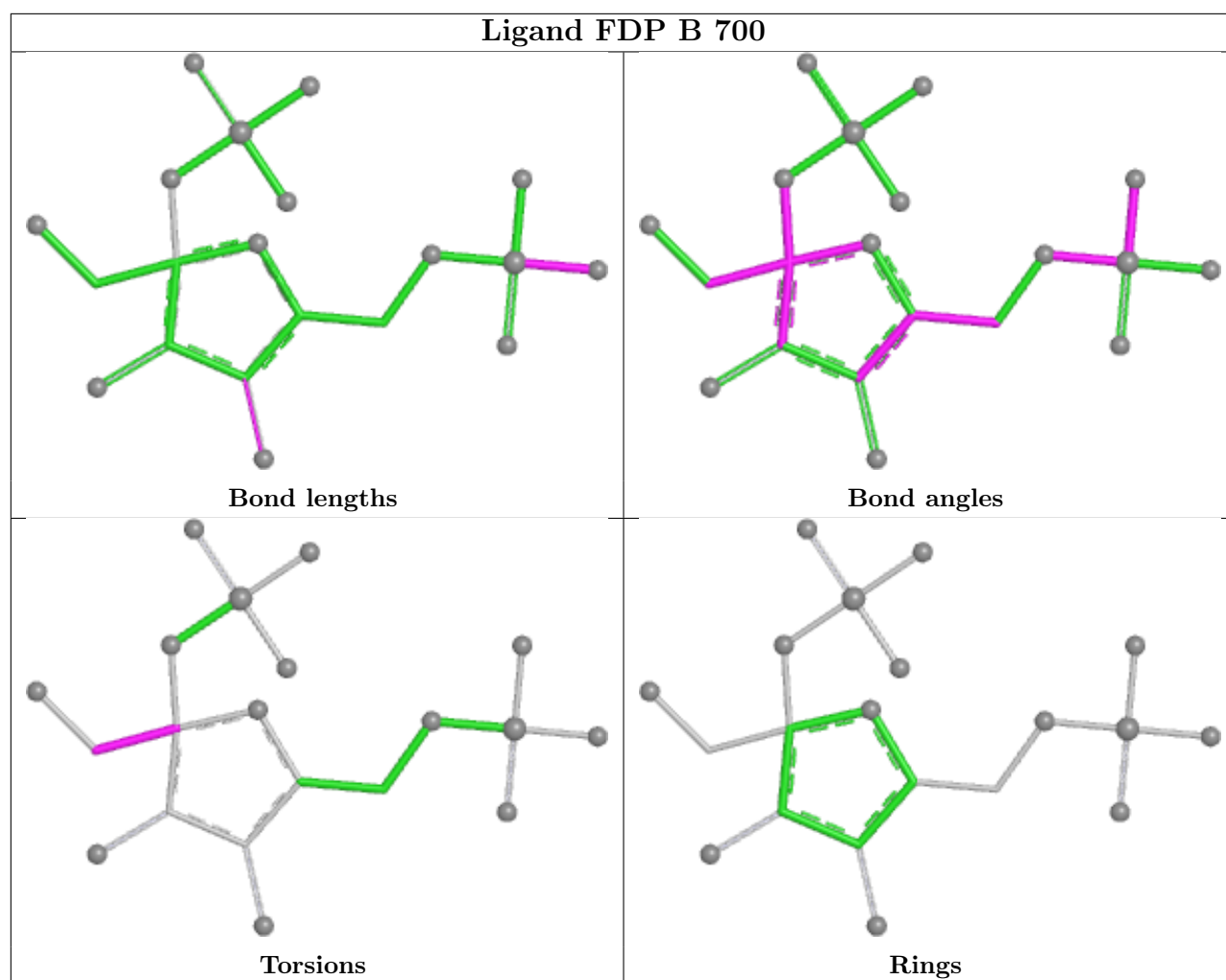




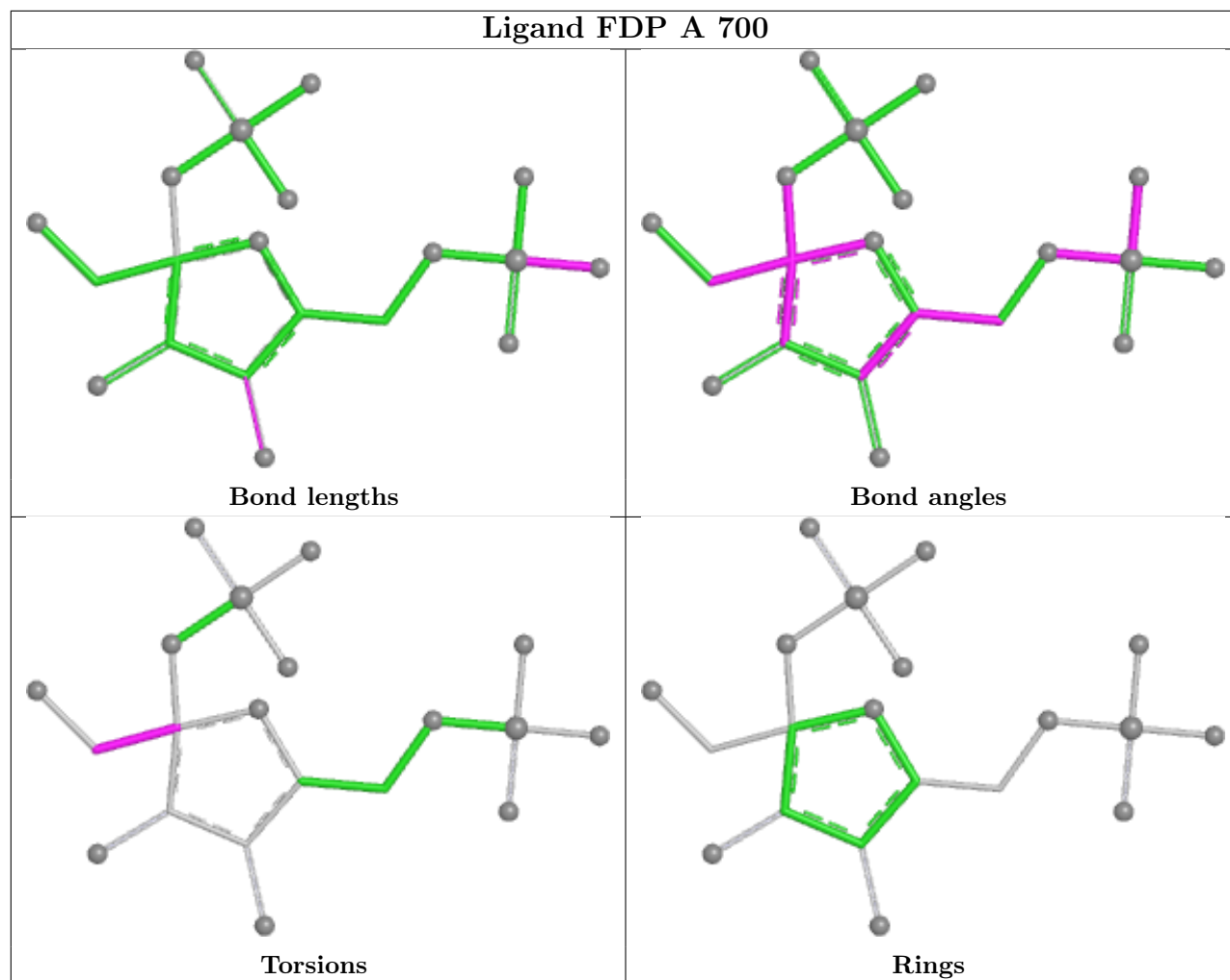


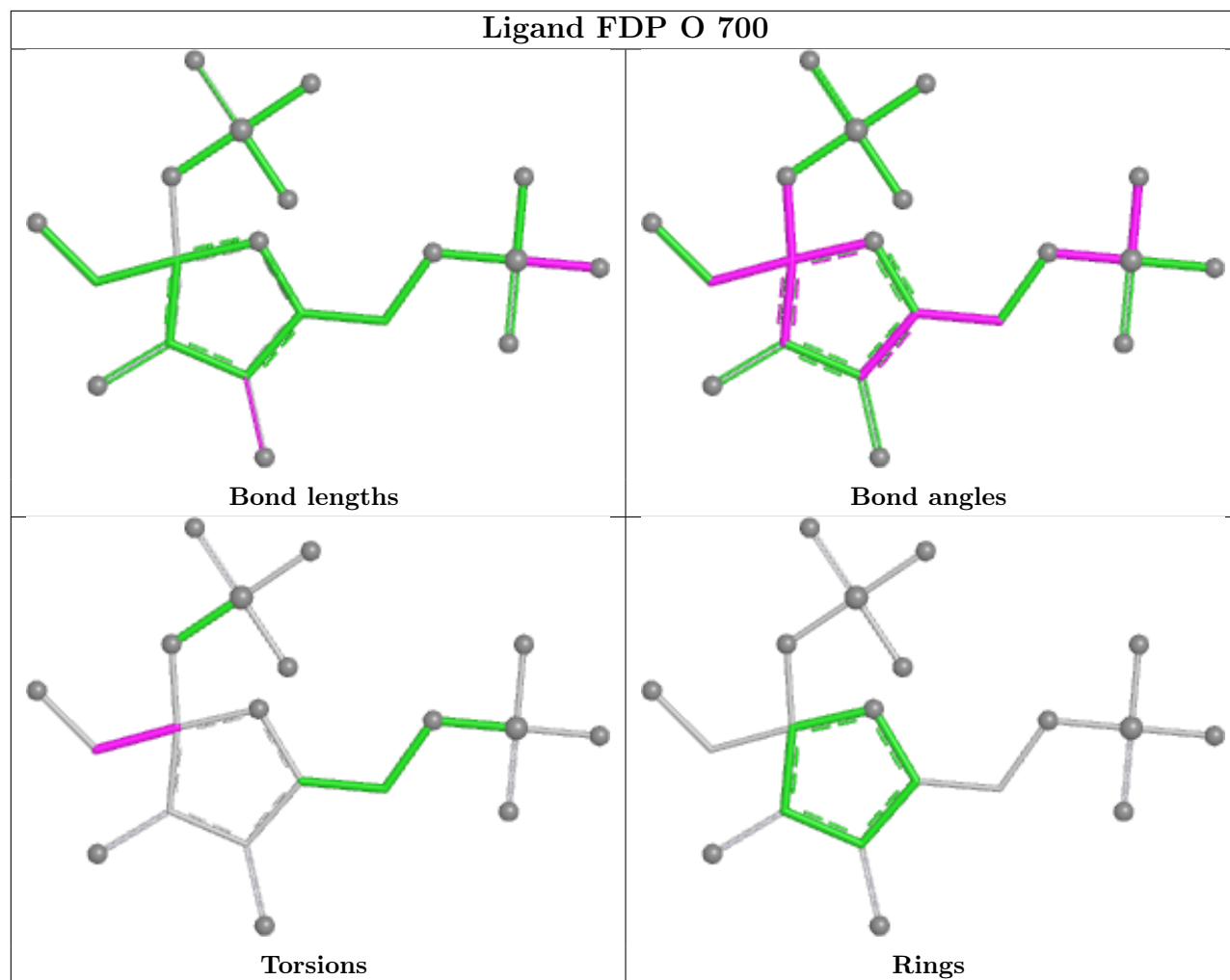
Ligand FDP P 700



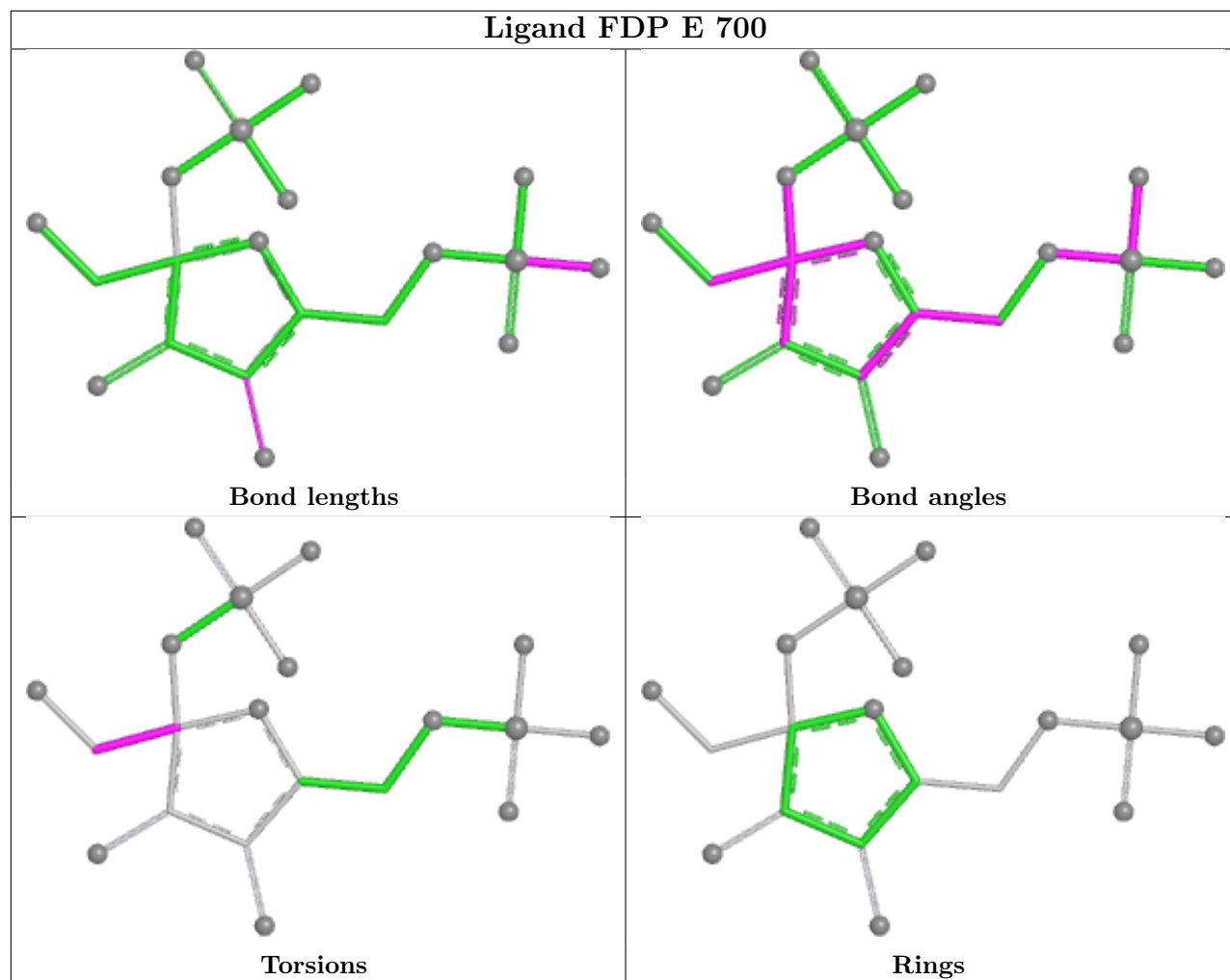


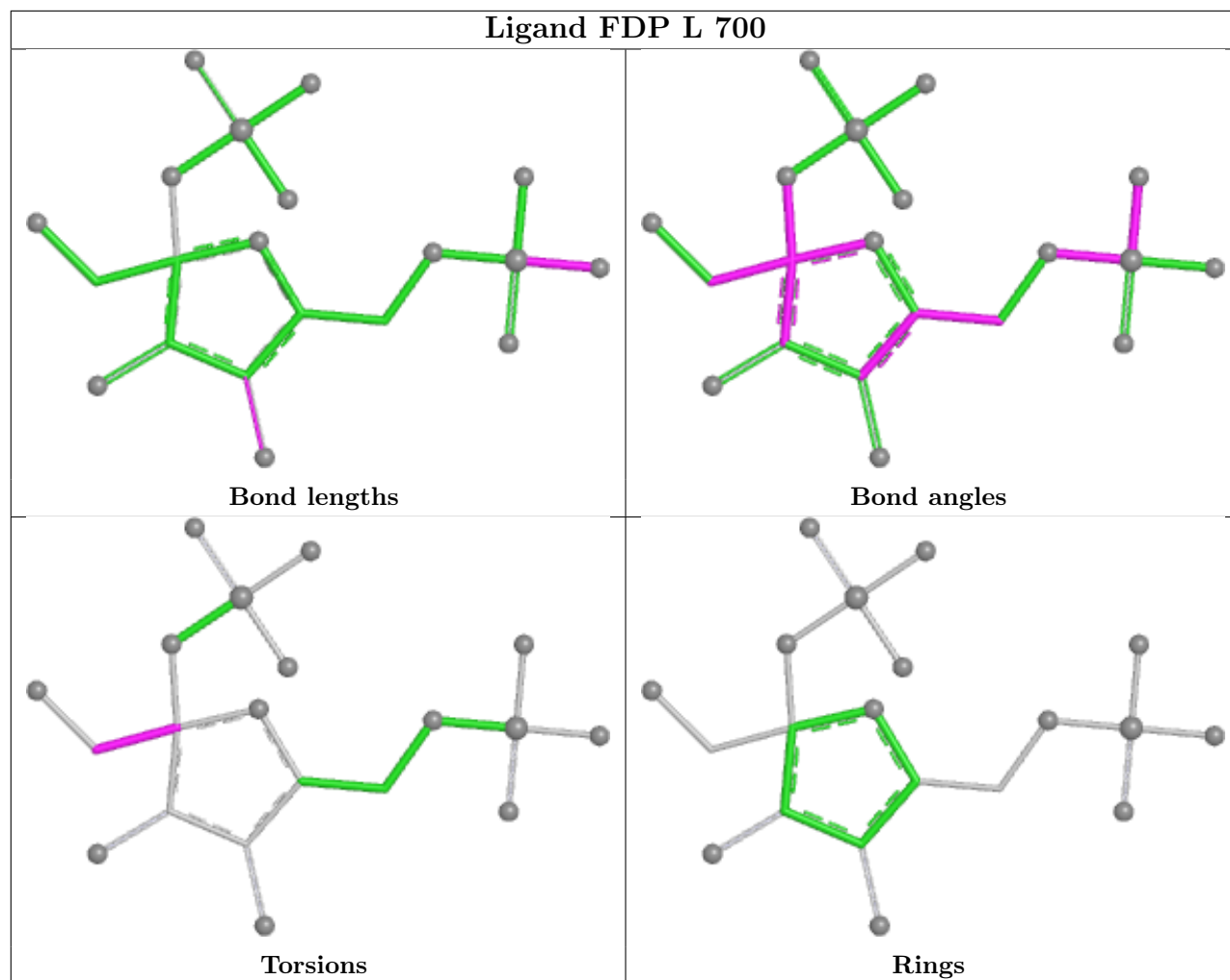
Ligand FDP A 700

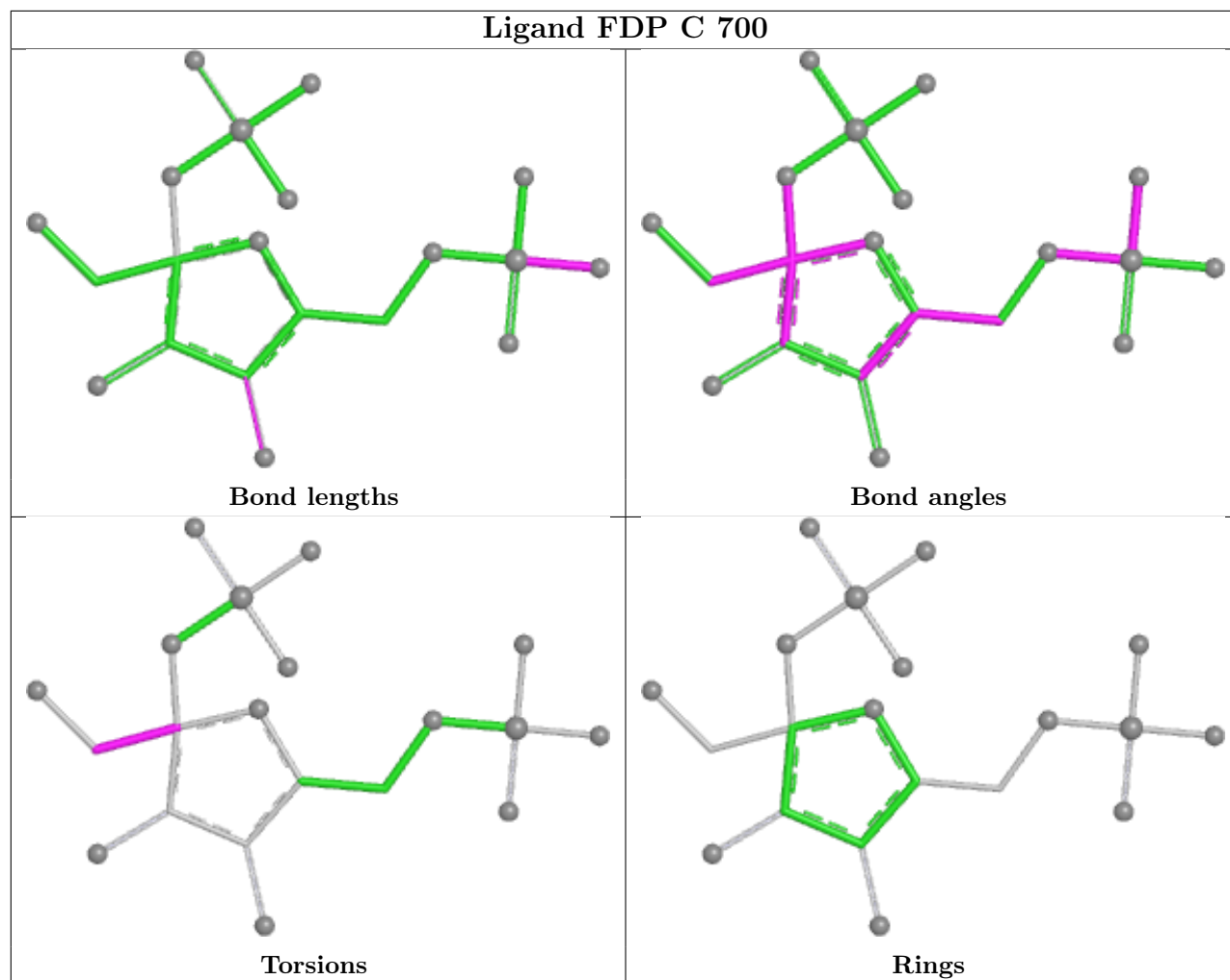


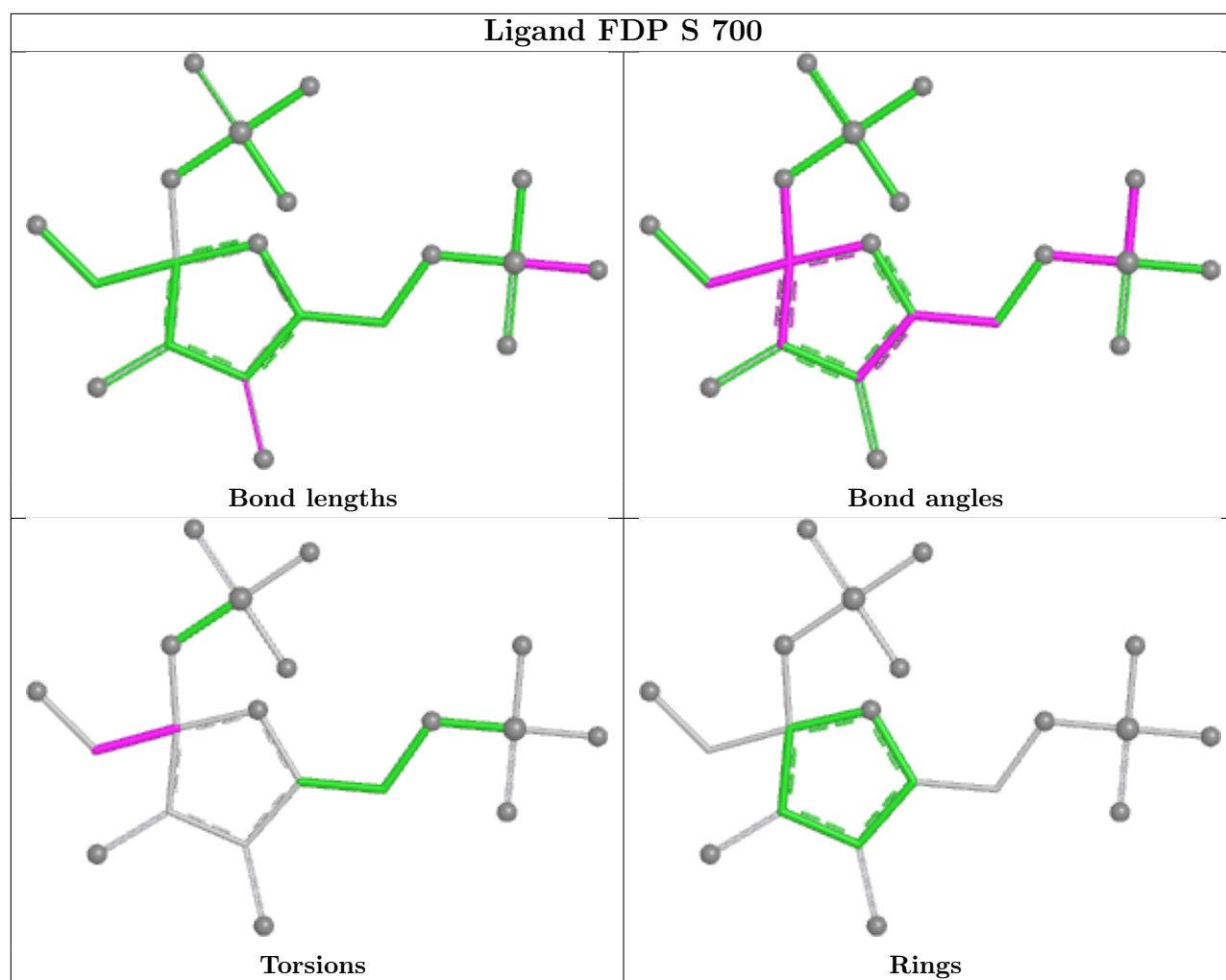


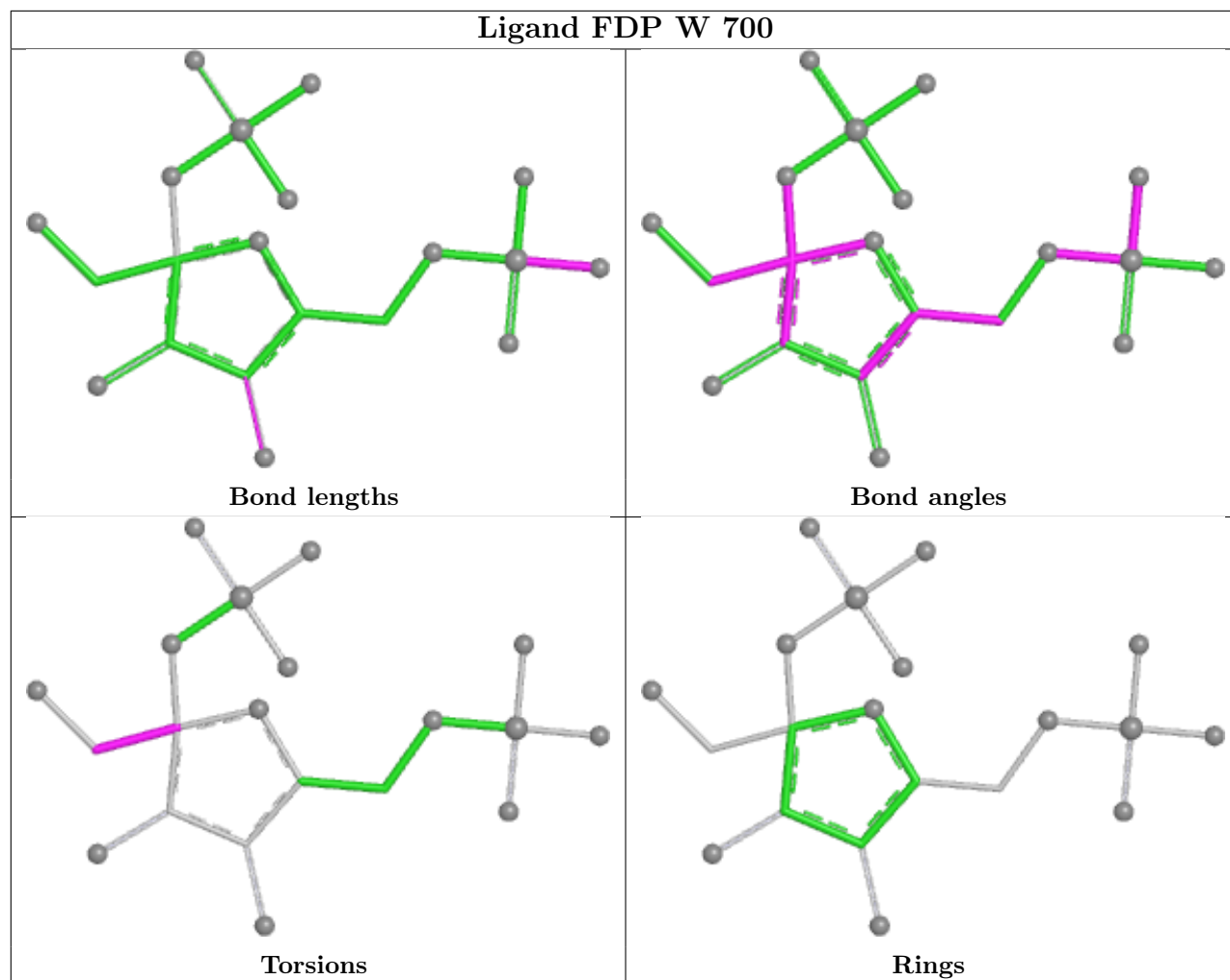
Ligand FDP E 700

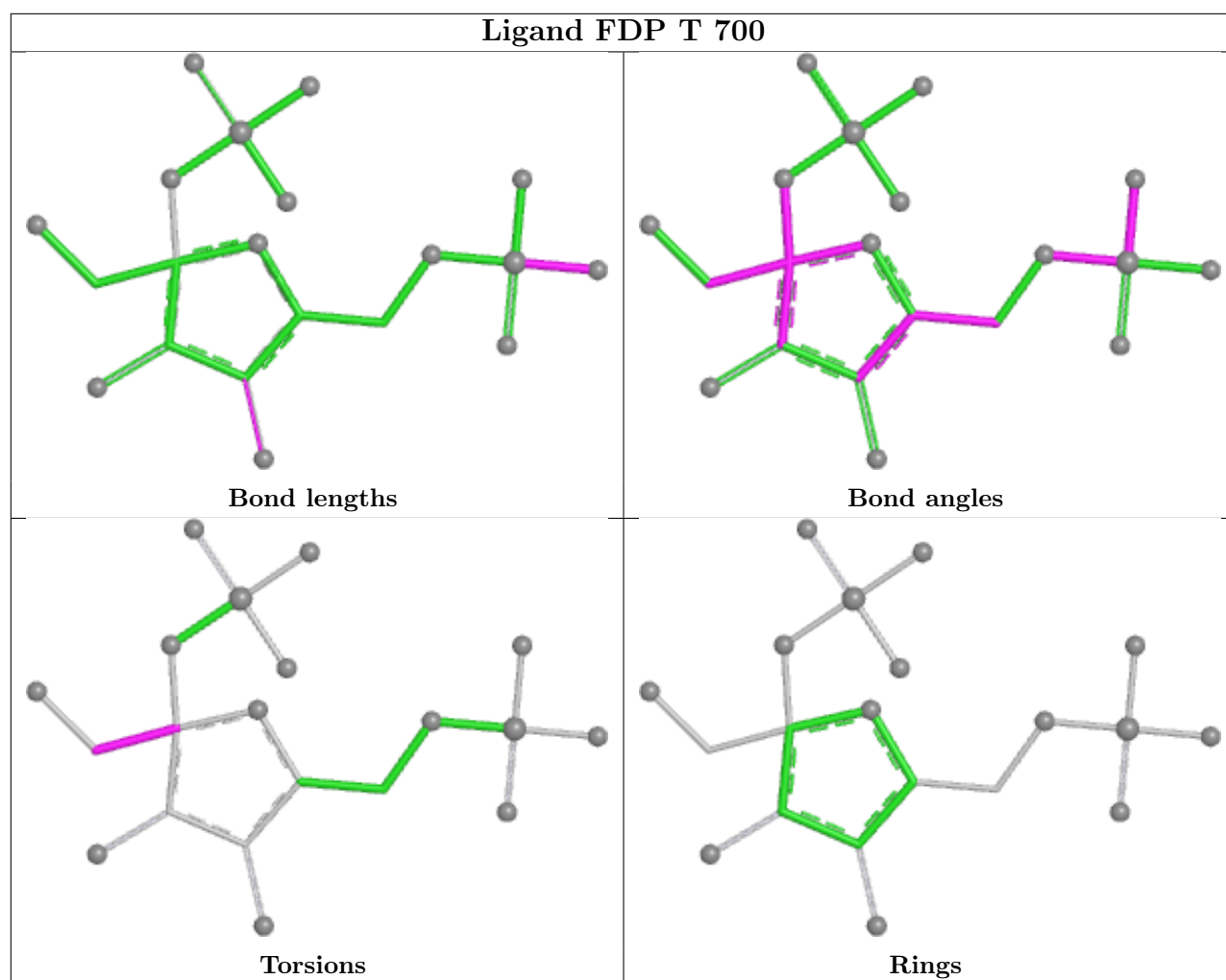


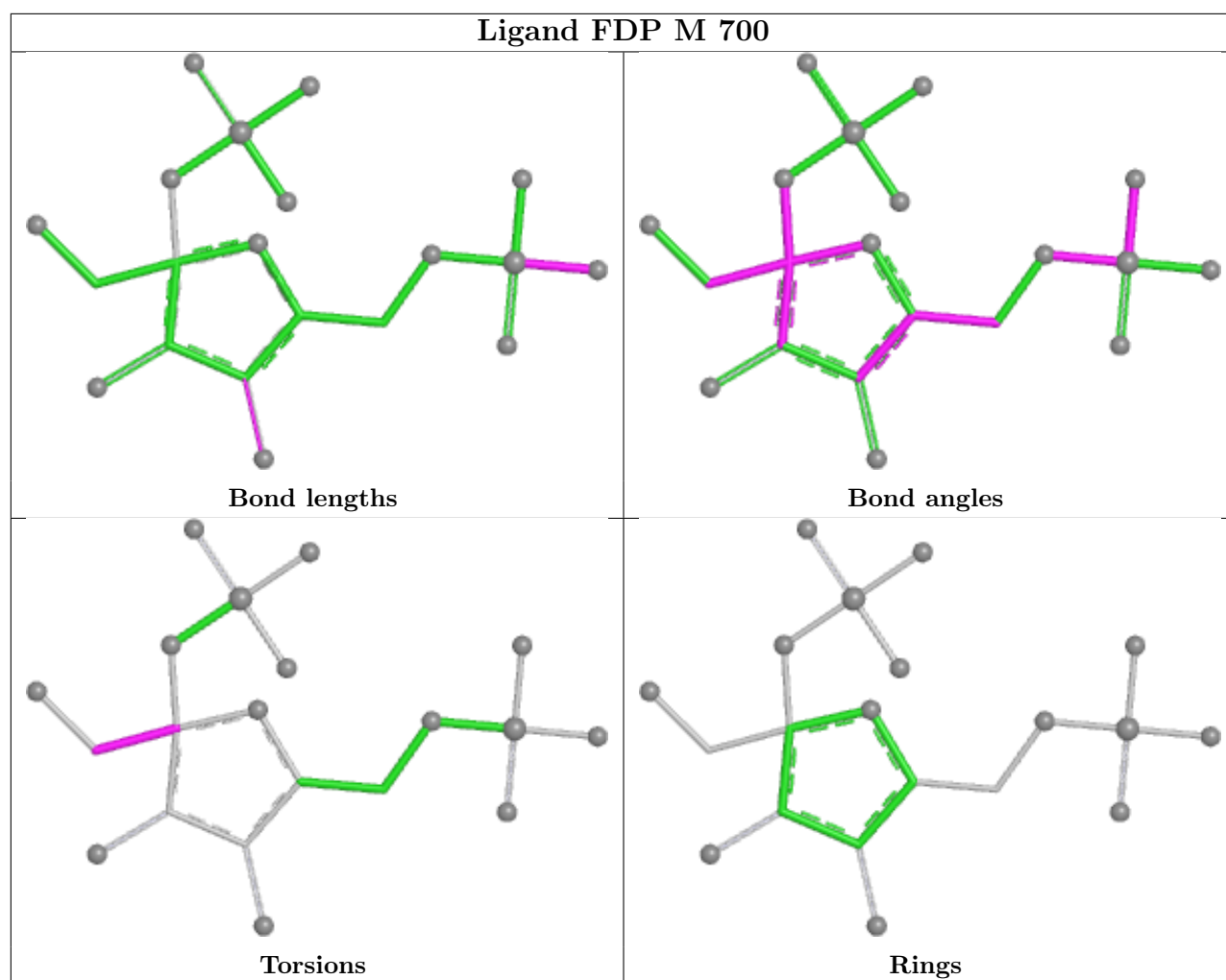




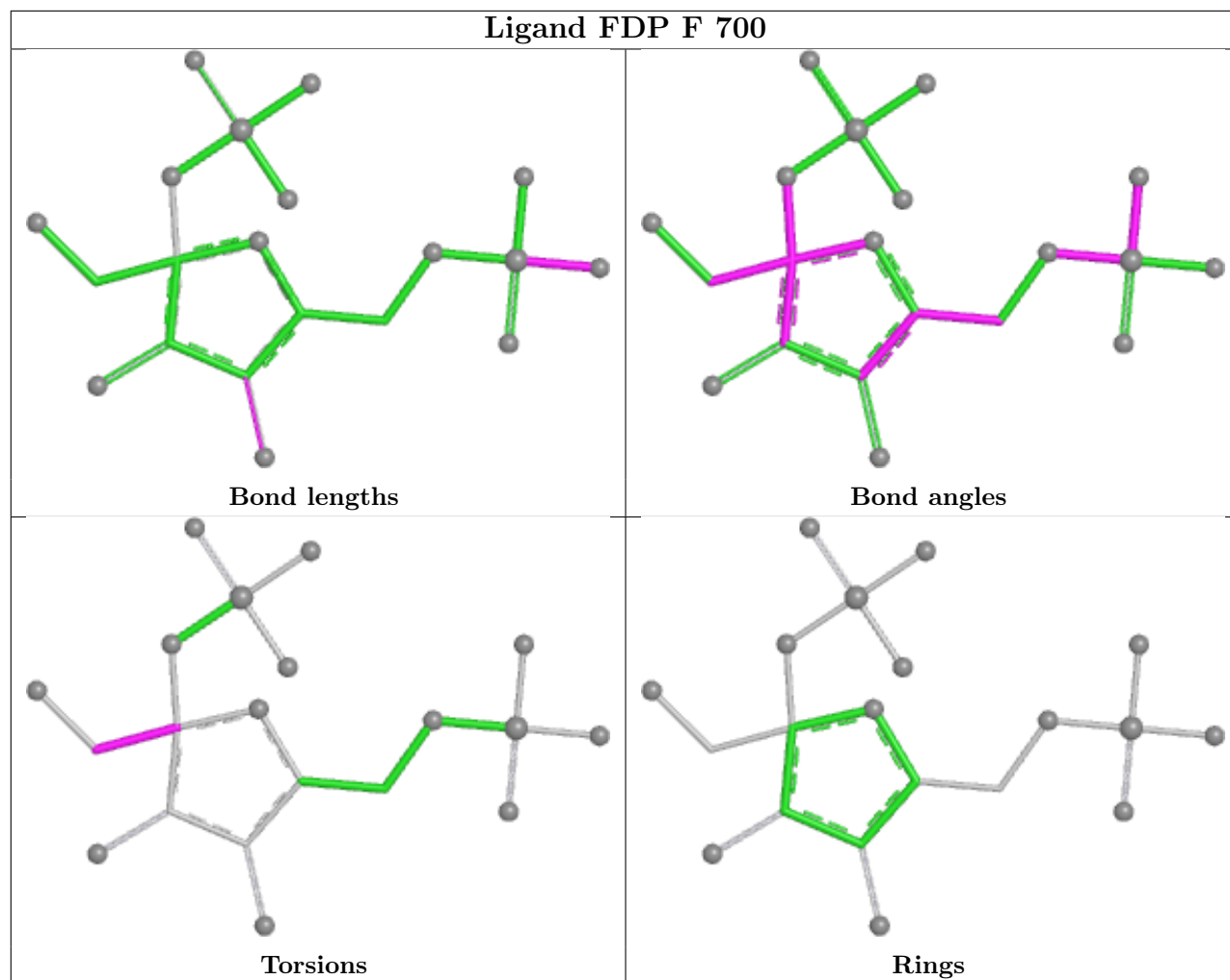


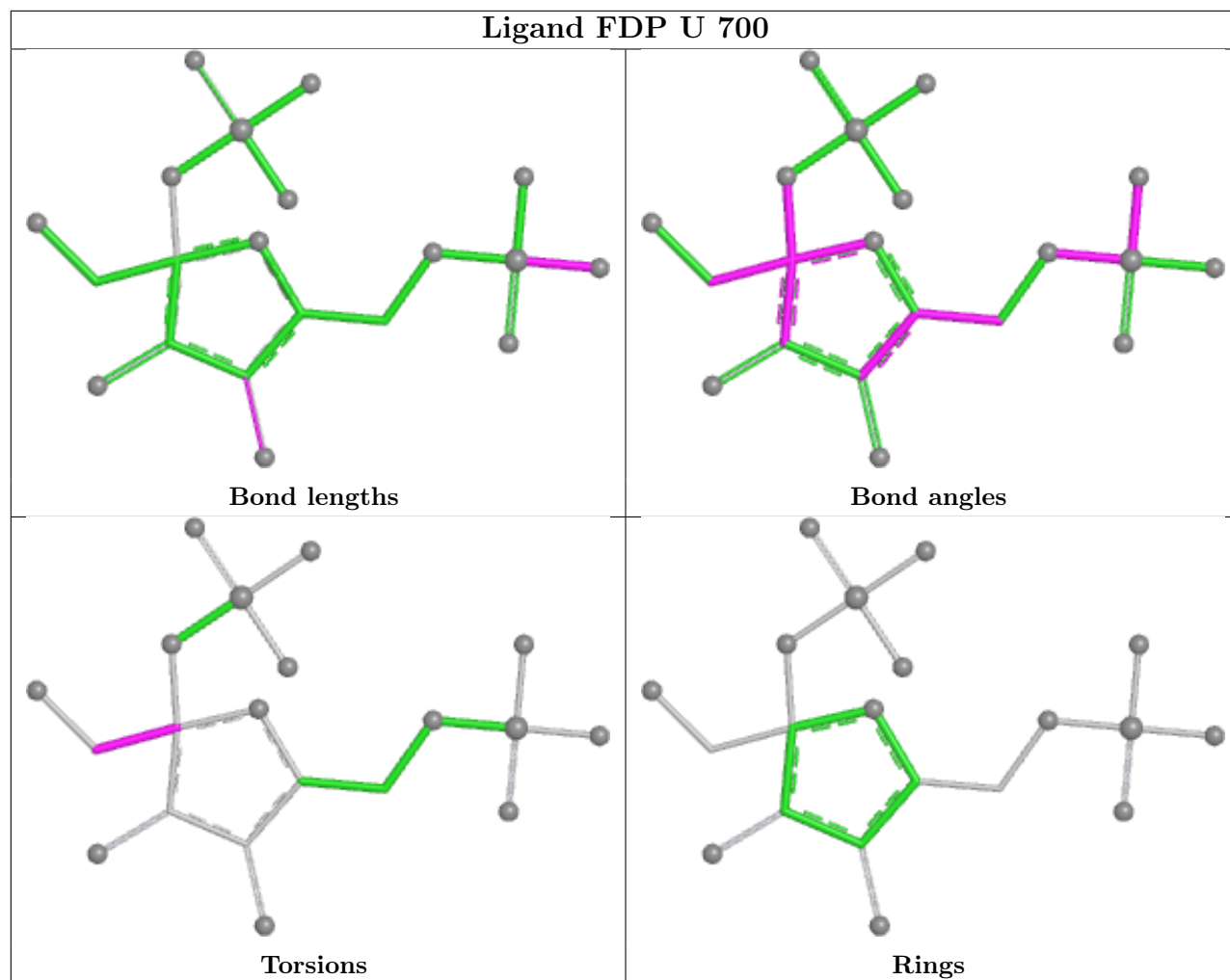






Ligand FDP F 700





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, 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	498/499 (99%)	-0.47	4 (0%) 82 69	13, 23, 36, 46	0
1	B	498/499 (99%)	-0.56	0 100 100	13, 23, 36, 46	0
1	C	498/499 (99%)	-0.63	1 (0%) 91 83	13, 23, 36, 46	0
1	D	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	E	498/499 (99%)	-0.63	0 100 100	13, 23, 36, 46	0
1	F	498/499 (99%)	-0.63	1 (0%) 91 83	13, 23, 36, 46	0
1	G	498/499 (99%)	-0.62	0 100 100	13, 23, 36, 46	0
1	H	498/499 (99%)	-0.65	0 100 100	13, 23, 36, 46	0
1	I	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	J	498/499 (99%)	-0.61	2 (0%) 88 77	13, 23, 36, 46	0
1	K	498/499 (99%)	-0.59	1 (0%) 91 83	13, 23, 36, 46	0
1	L	498/499 (99%)	-0.64	0 100 100	13, 23, 36, 46	0
1	M	498/499 (99%)	-0.63	0 100 100	13, 23, 36, 46	0
1	N	498/499 (99%)	-0.66	0 100 100	13, 23, 36, 46	0
1	O	498/499 (99%)	-0.53	0 100 100	13, 23, 36, 46	0
1	P	498/499 (99%)	-0.57	1 (0%) 91 83	13, 23, 36, 46	0
1	Q	498/499 (99%)	-0.63	0 100 100	13, 23, 36, 46	0
1	R	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	S	498/499 (99%)	-0.62	0 100 100	13, 23, 36, 46	0
1	T	498/499 (99%)	-0.57	0 100 100	13, 23, 36, 46	0
1	U	498/499 (99%)	-0.65	0 100 100	13, 23, 36, 46	0
1	V	498/499 (99%)	-0.60	0 100 100	13, 23, 36, 46	0
1	W	498/499 (99%)	-0.65	0 100 100	13, 23, 36, 46	0
1	X	498/499 (99%)	-0.61	1 (0%) 91 83	13, 23, 36, 46	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	11952/11976 (99%)	-0.61	11 (0%) 92 86	13, 23, 36, 46	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	4.4
1	J	107	CYS	3.6
1	C	158	GLU	2.9
1	P	104	GLY	2.9
1	A	302	MET	2.4

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FDP	I	700	20/20	0.97	0.07	25,32,34,35	0
2	FDP	K	700	20/20	0.97	0.09	25,32,34,35	0
2	FDP	B	700	20/20	0.98	0.07	25,32,34,35	0
2	FDP	G	700	20/20	0.98	0.08	25,32,34,35	0
2	FDP	M	700	20/20	0.98	0.06	25,32,34,35	0
2	FDP	N	700	20/20	0.98	0.06	25,32,34,35	0
2	FDP	X	700	20/20	0.98	0.07	25,32,34,35	0
2	FDP	H	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	C	700	20/20	0.99	0.07	25,32,34,35	0
2	FDP	J	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	D	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	L	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	E	700	20/20	0.99	0.07	25,32,34,35	0

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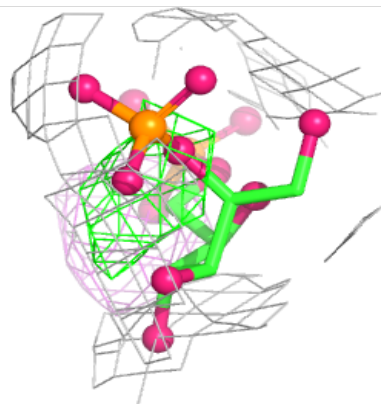
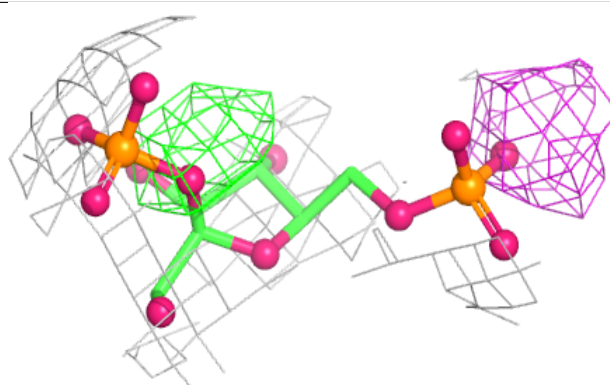
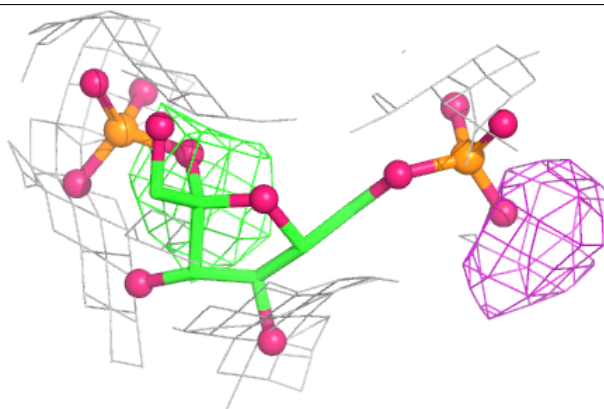
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FDP	F	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	O	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	P	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	Q	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	R	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	S	700	20/20	0.99	0.04	25,32,34,35	0
2	FDP	T	700	20/20	0.99	0.07	25,32,34,35	0
2	FDP	U	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	V	700	20/20	0.99	0.06	25,32,34,35	0
2	FDP	W	700	20/20	0.99	0.05	25,32,34,35	0
2	FDP	A	700	20/20	0.99	0.04	25,32,34,35	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.

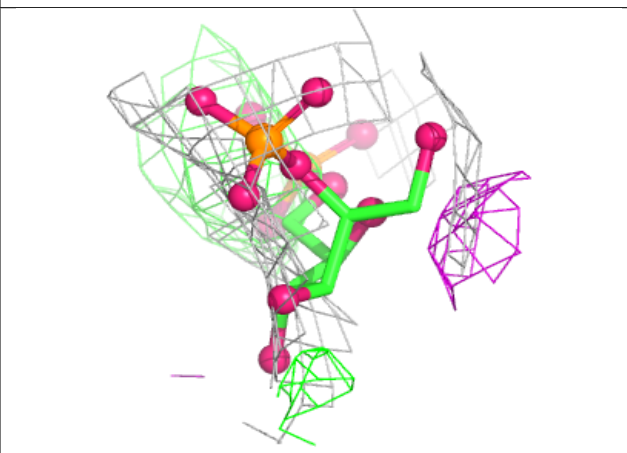
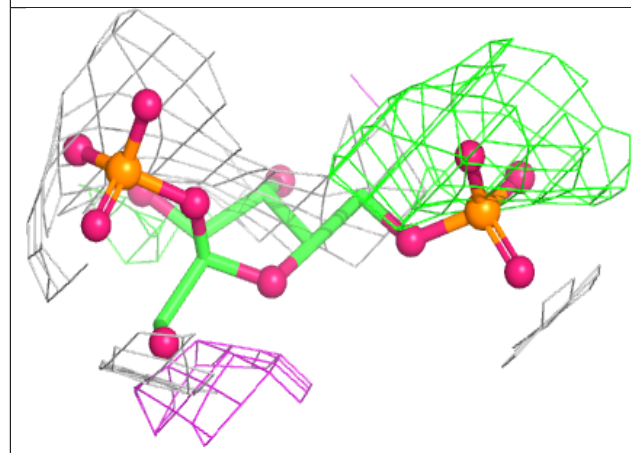
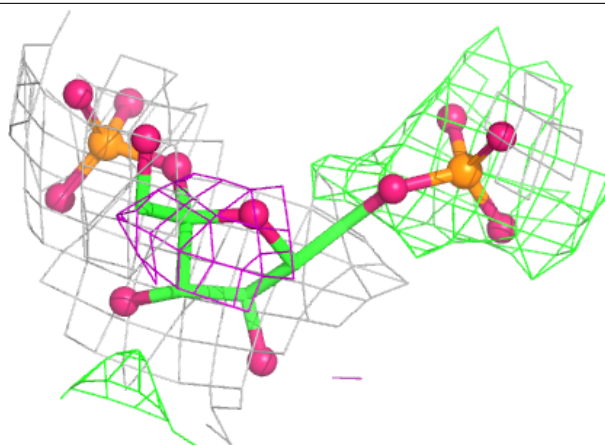
Electron density around FDP I 700:

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



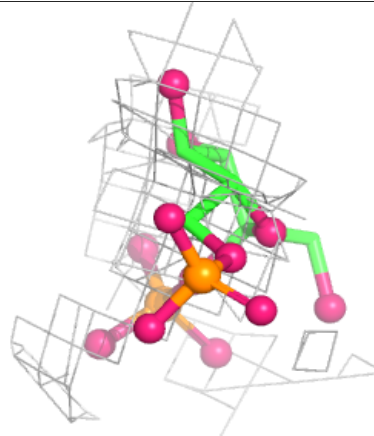
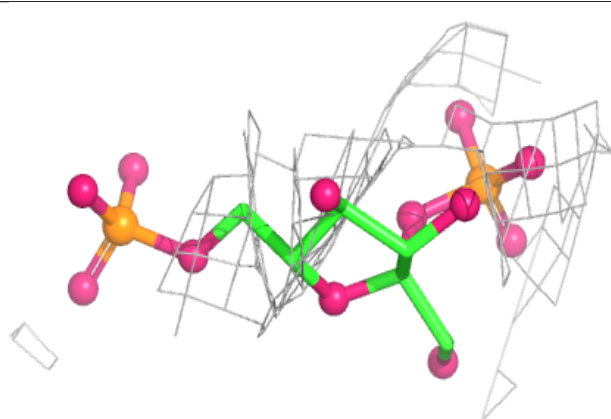
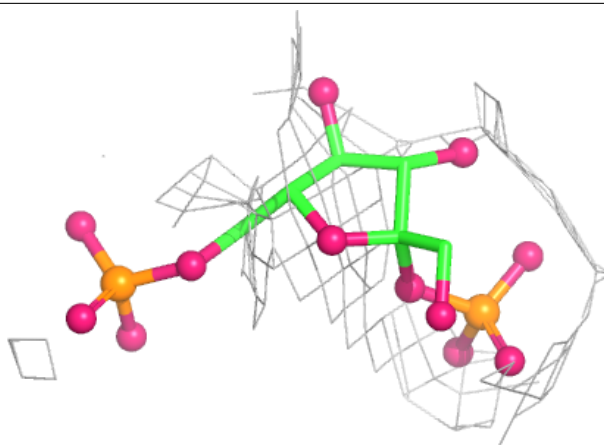
Electron density around FDP K 700:

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



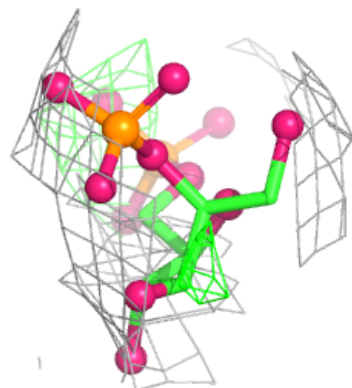
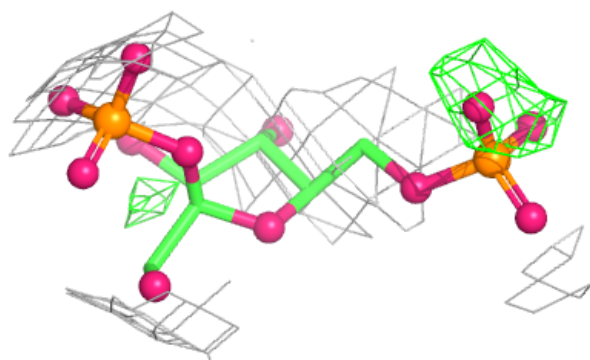
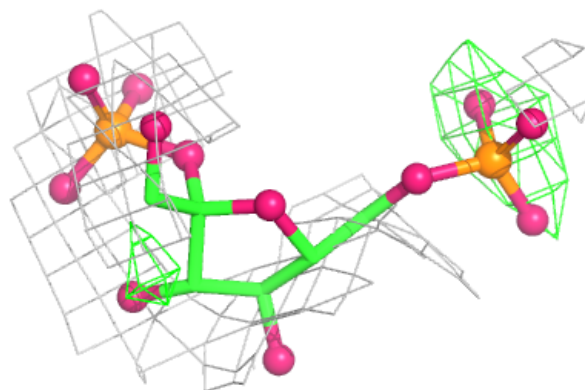
Electron density around FDP B 700:

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

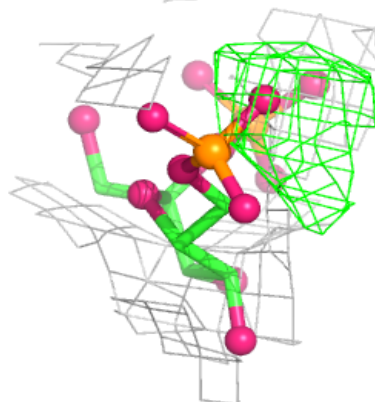
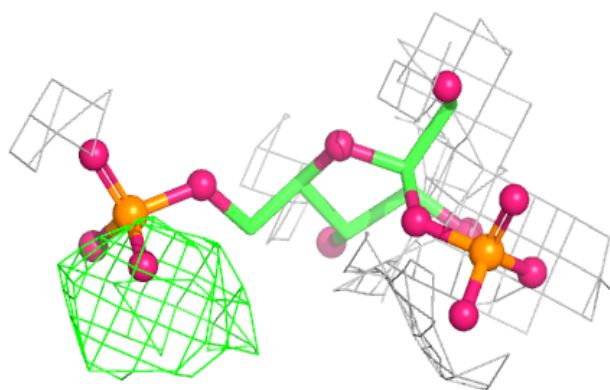
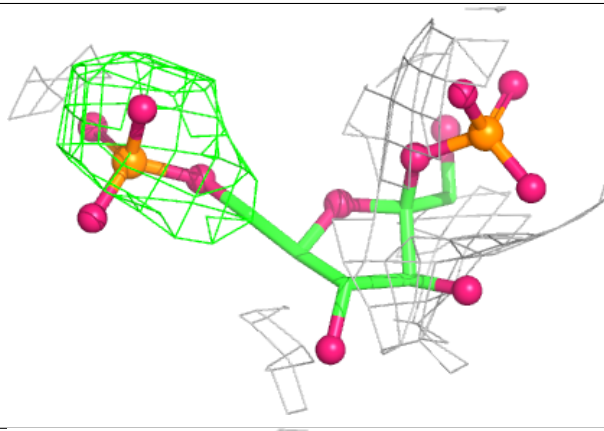


Electron density around FDP G 700:

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and green (positive)

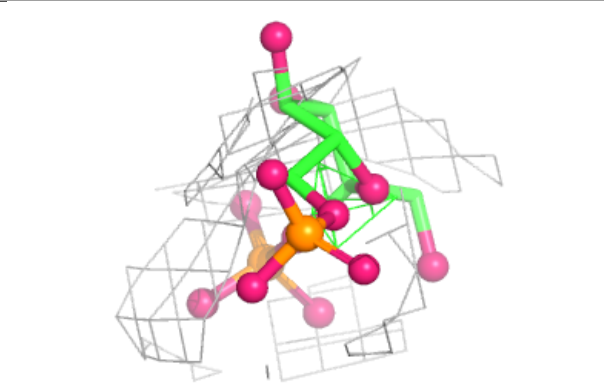
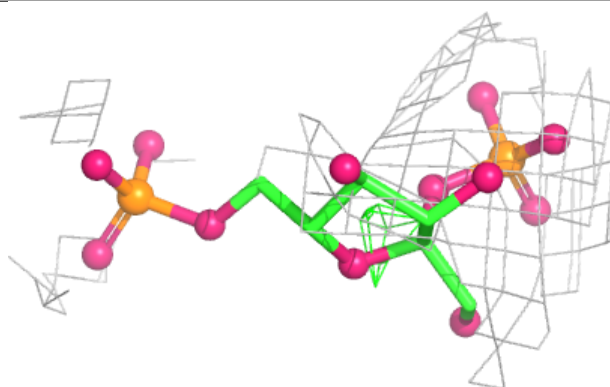
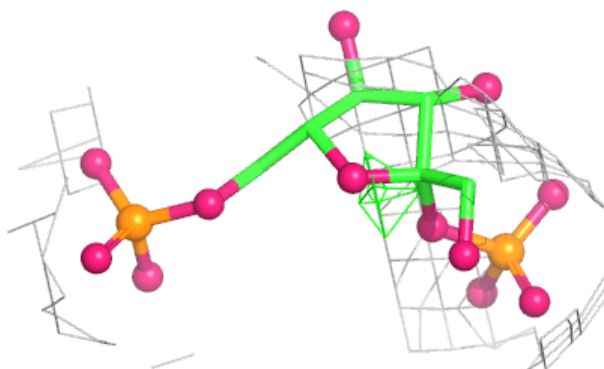
**Electron density around FDP M 700:**

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

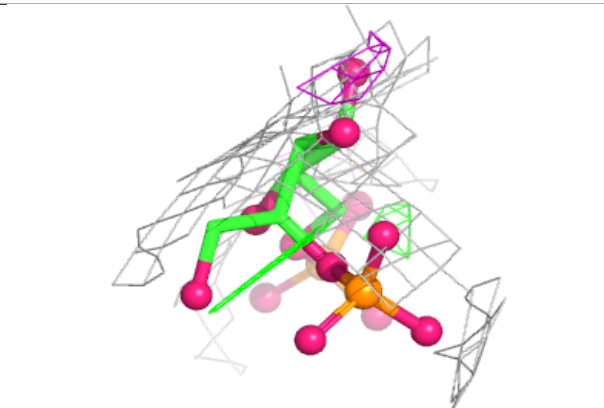
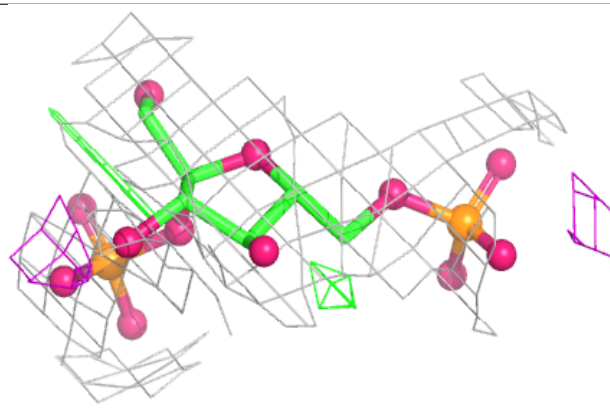
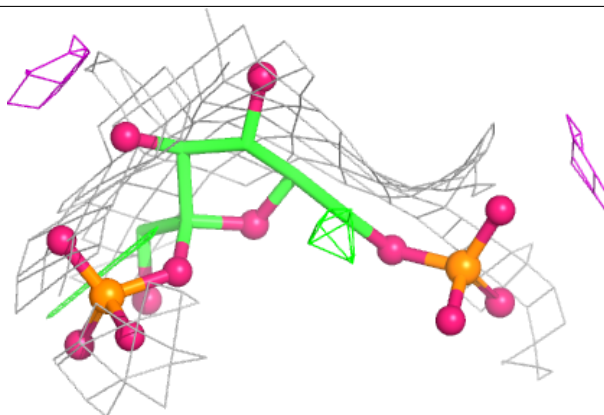


Electron density around FDP N 700:

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

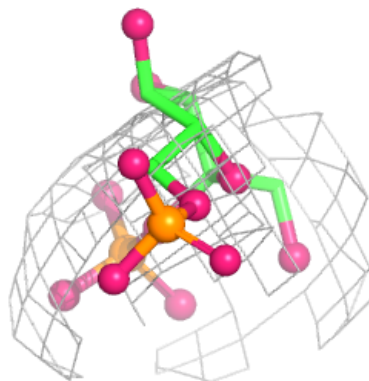
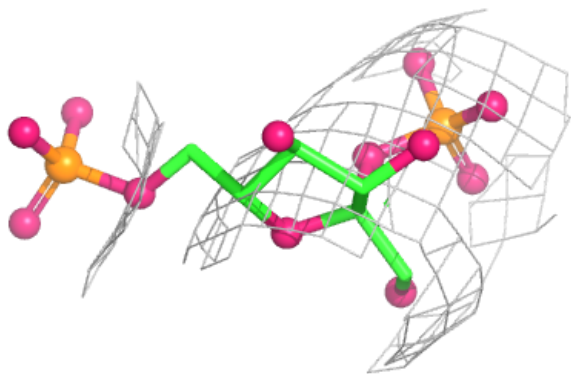
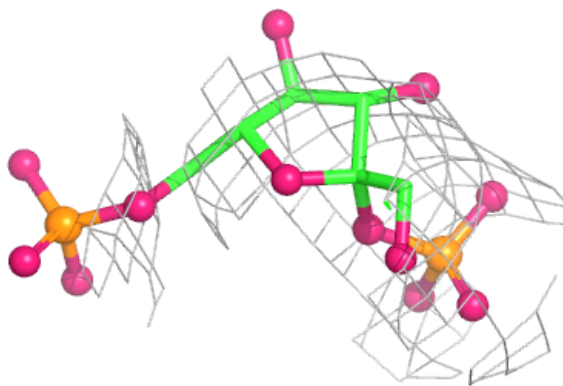
**Electron density around FDP X 700:**

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



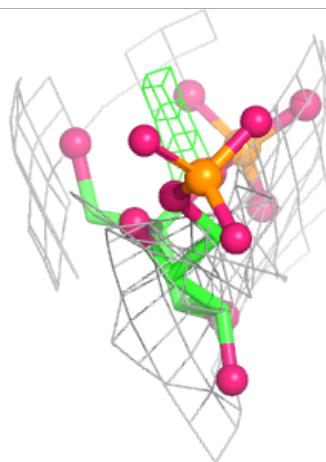
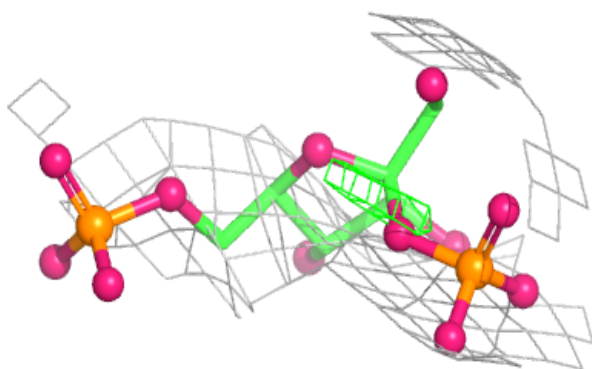
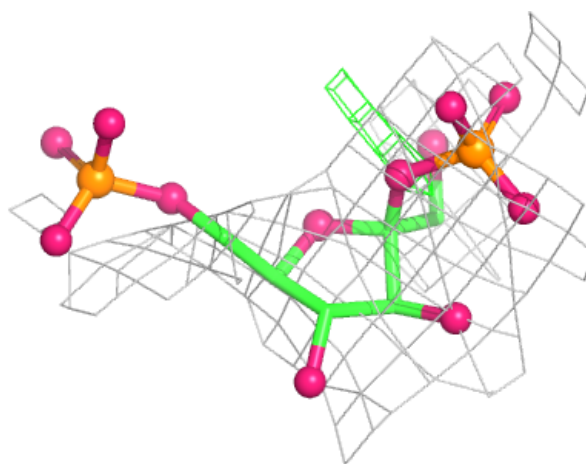
Electron density around FDP H 700:

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and green (positive)



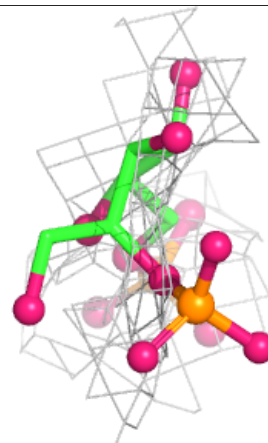
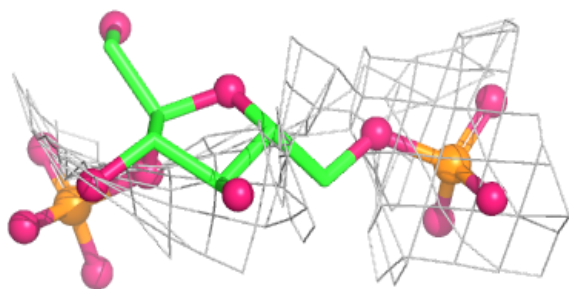
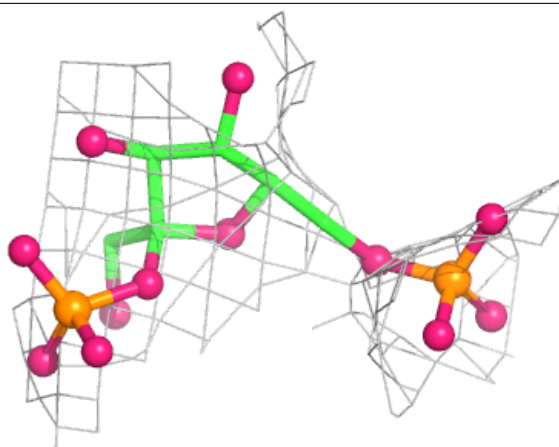
Electron density around FDP C 700:

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



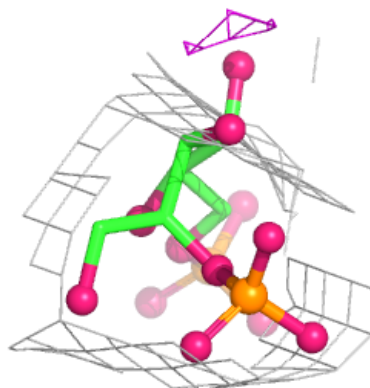
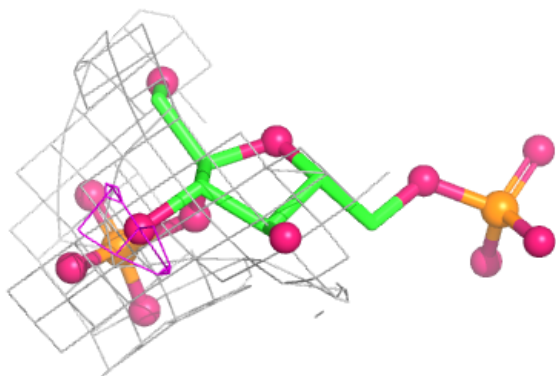
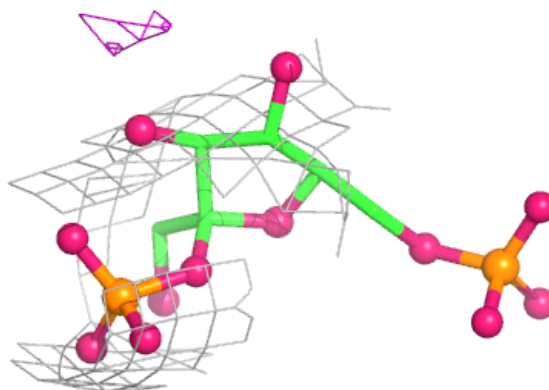
Electron density around FDP J 700:

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

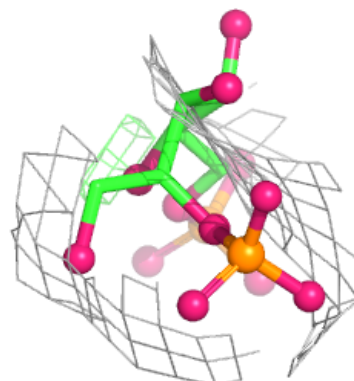
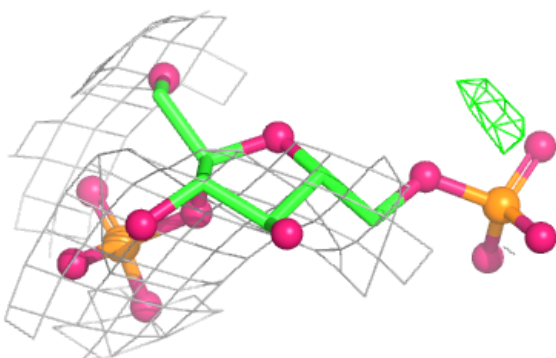
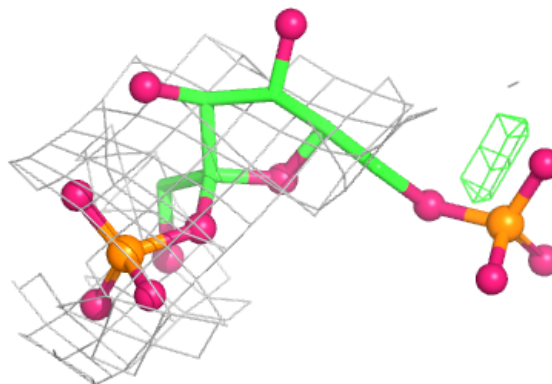


Electron density around FDP D 700:

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

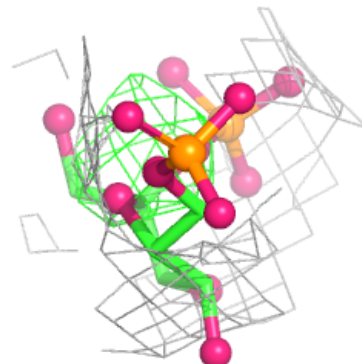
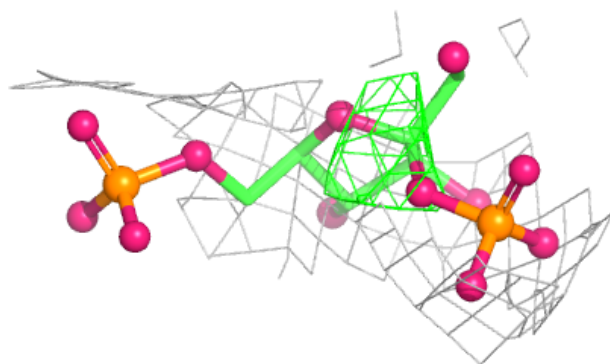
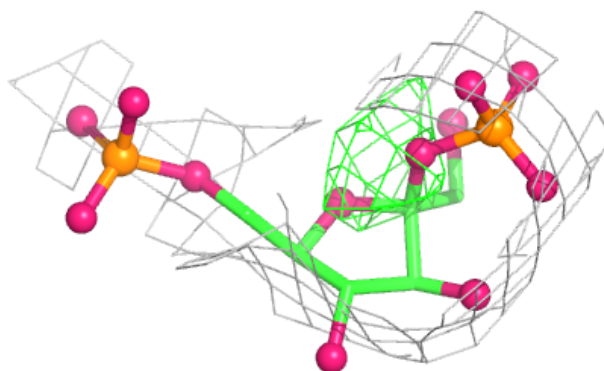
**Electron density around FDP L 700:**

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

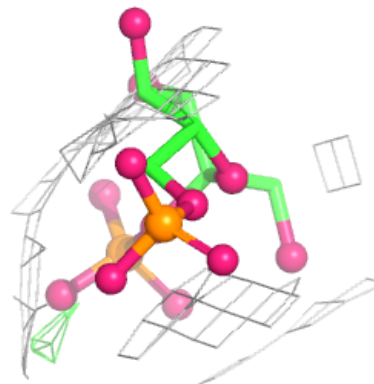
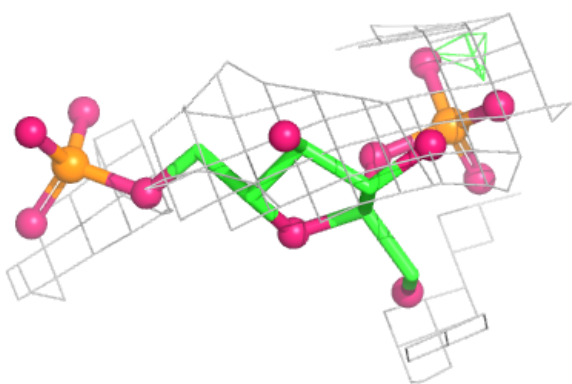
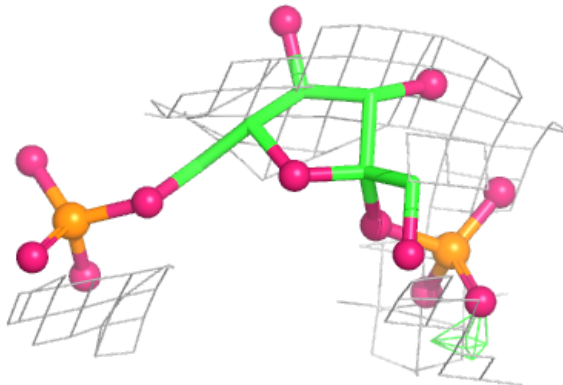


Electron density around FDP E 700:

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

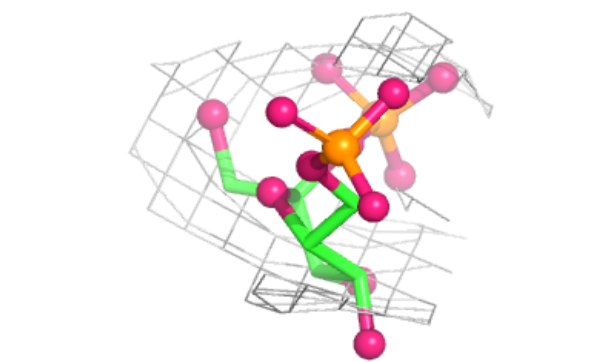
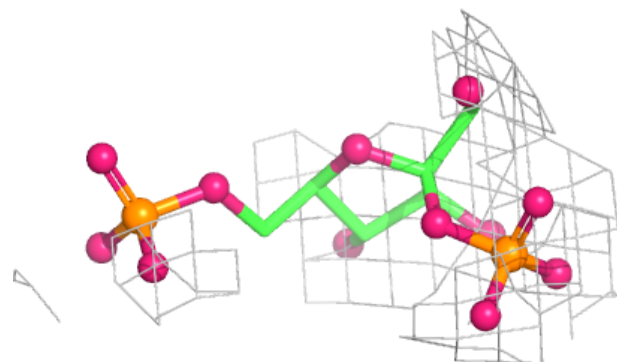
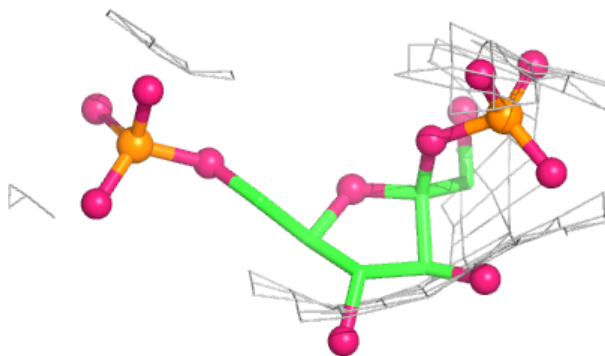
**Electron density around FDP F 700:**

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

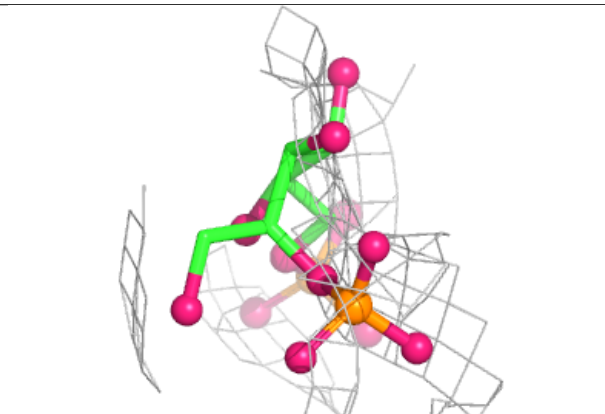
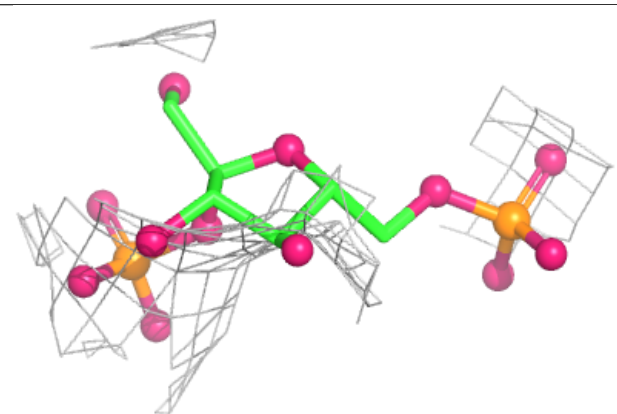
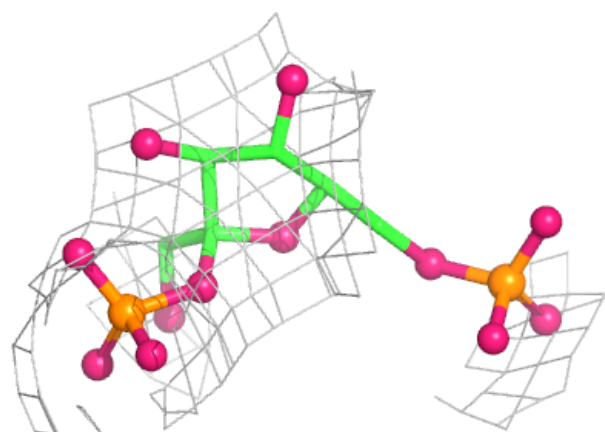


Electron density around FDP O 700:

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

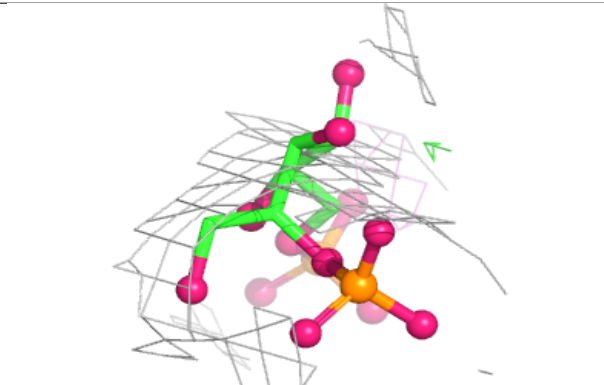
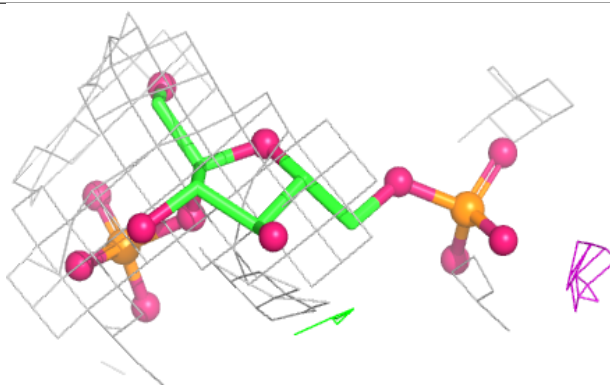
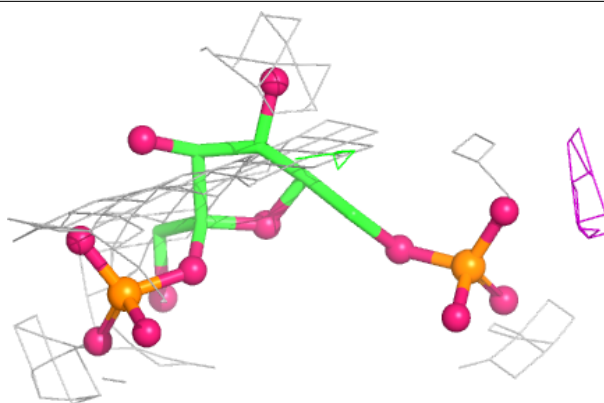
**Electron density around FDP P 700:**

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

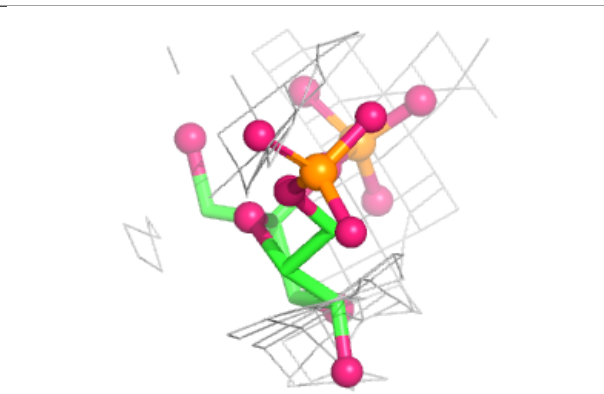
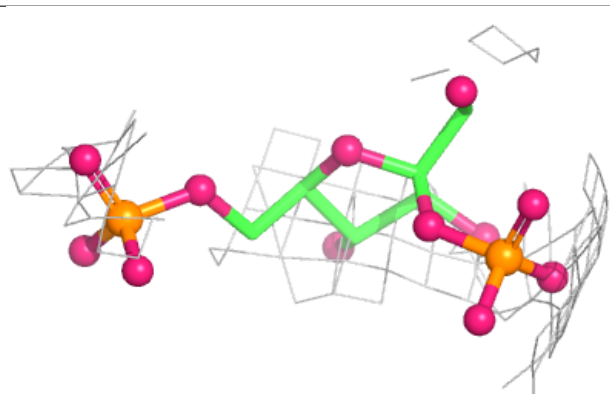
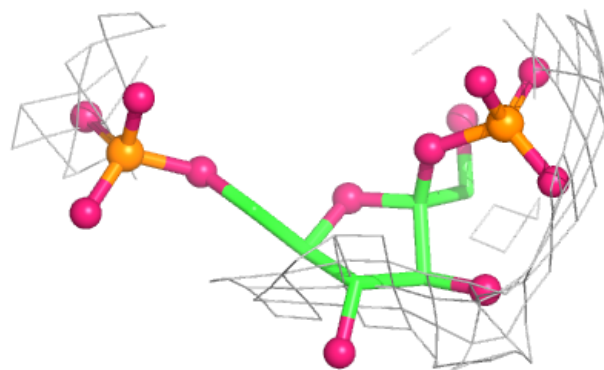


Electron density around FDP Q 700:

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

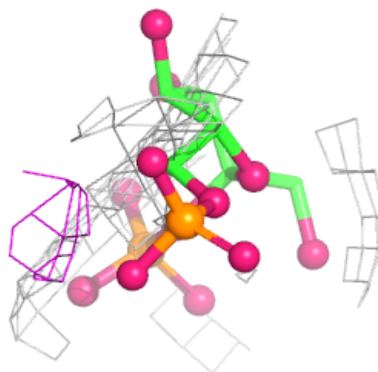
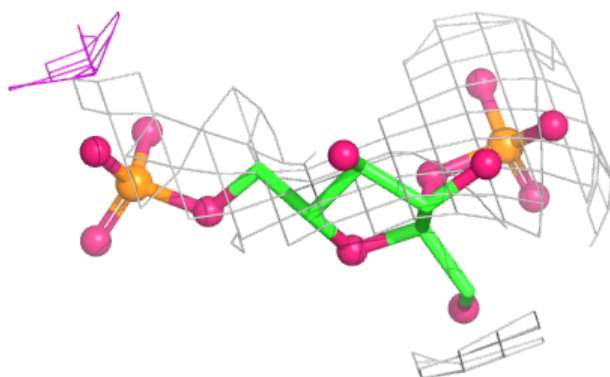
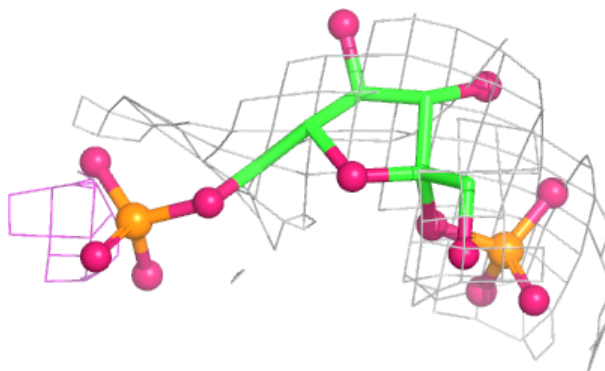
**Electron density around FDP R 700:**

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



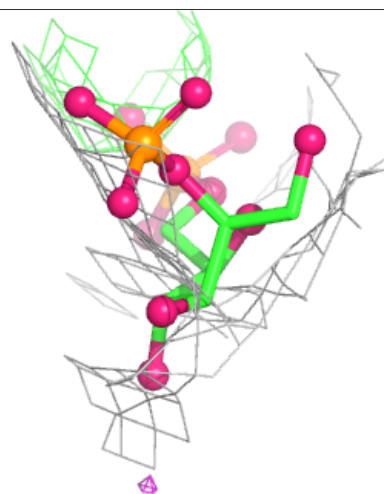
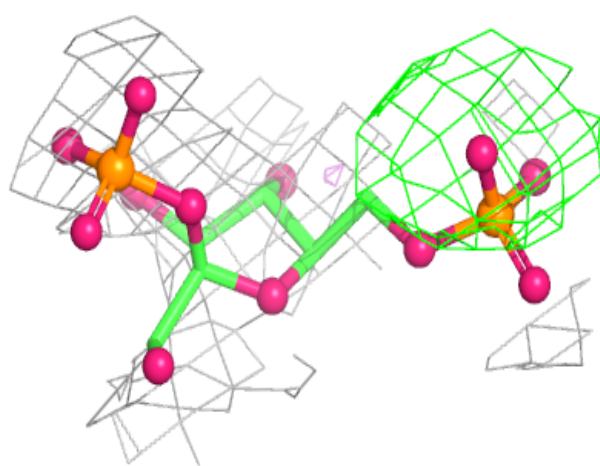
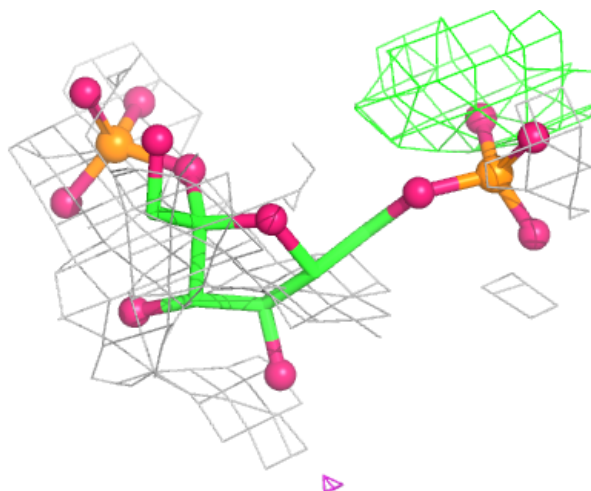
Electron density around FDP S 700:

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



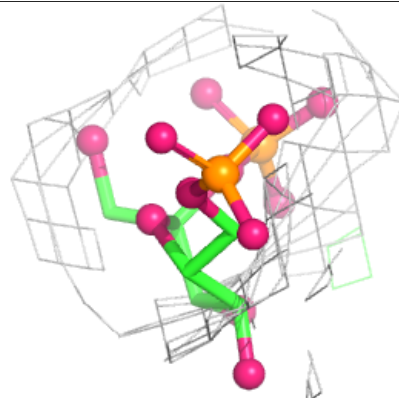
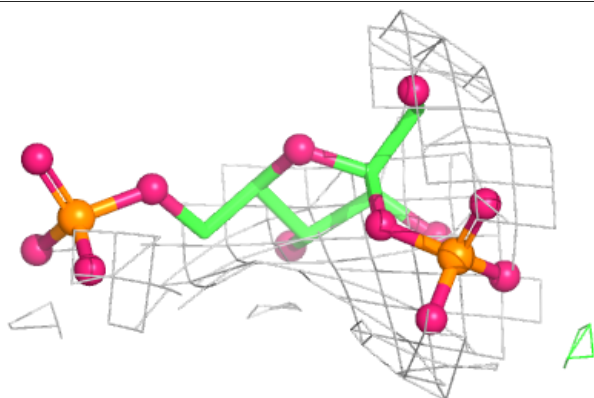
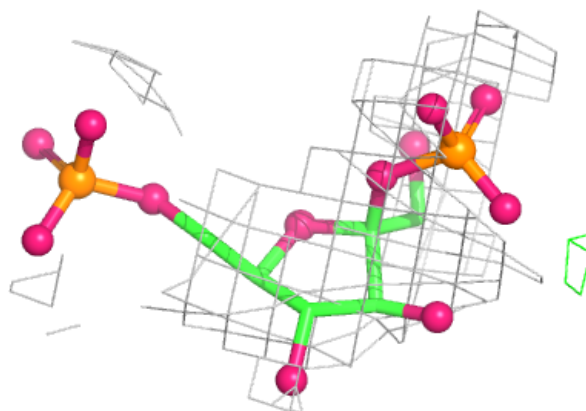
Electron density around FDP T 700:

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

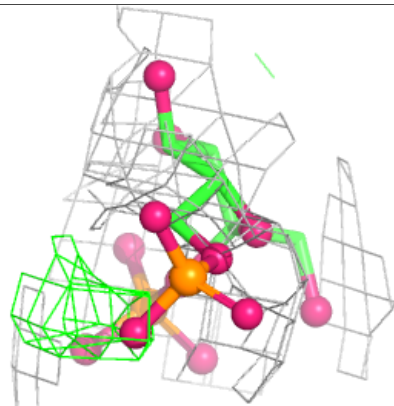
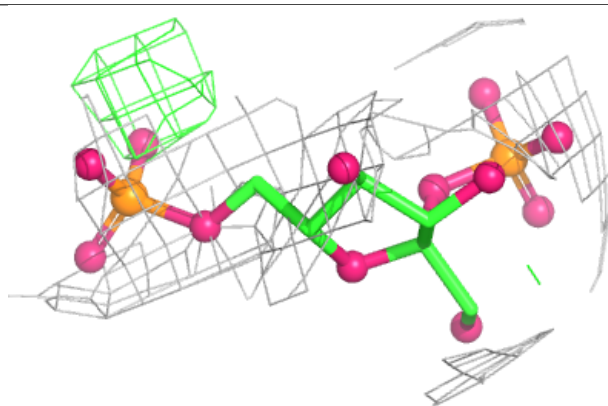
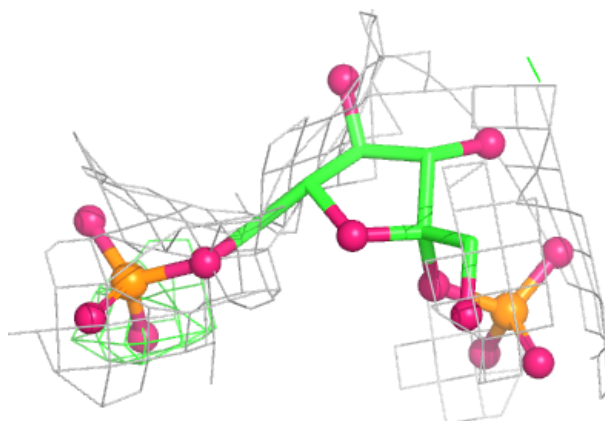


Electron density around FDP U 700:

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

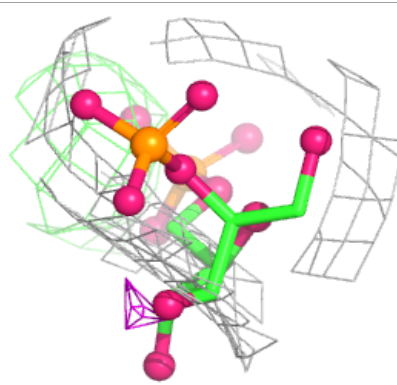
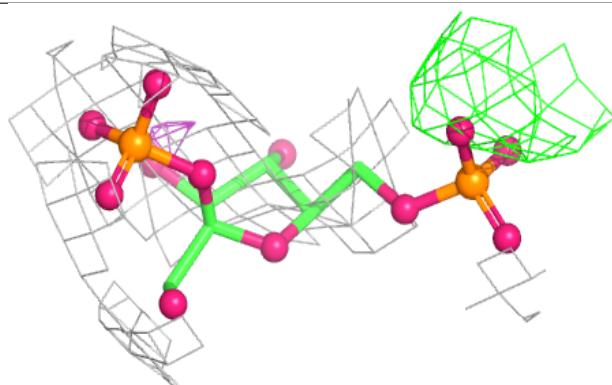
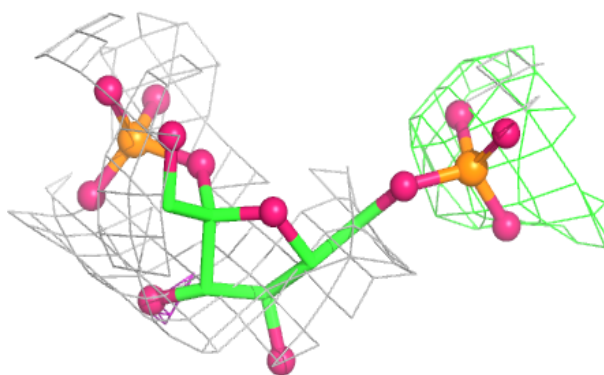
**Electron density around FDP V 700:**

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

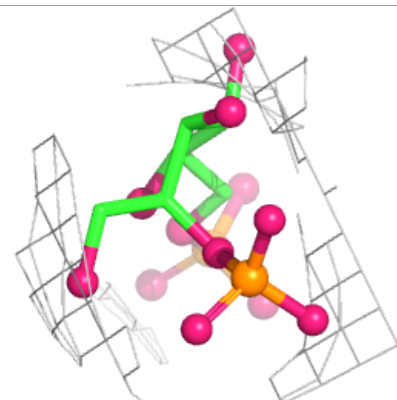
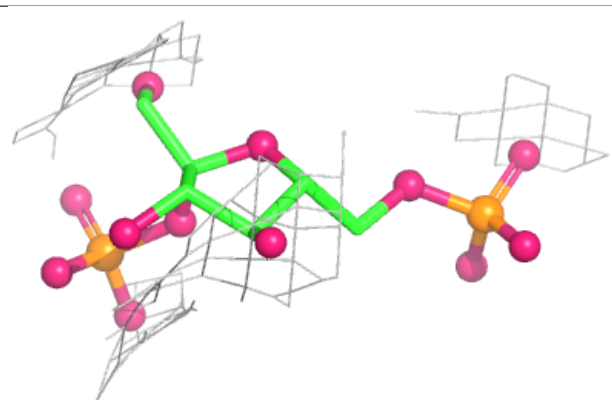
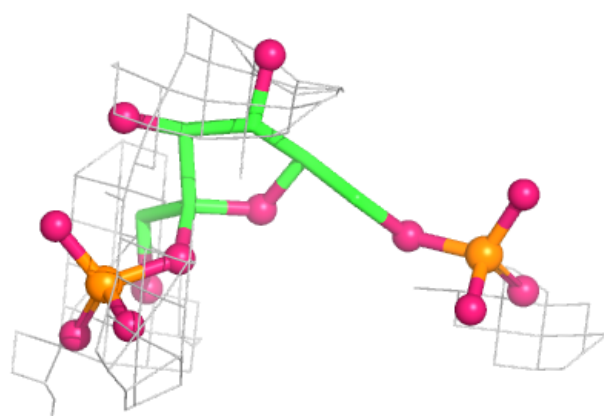


Electron density around FDP W 700:

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

**Electron density around FDP A 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.