



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:35 AM UTC

PDB ID : 3HQP / pdb_00003hqp
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

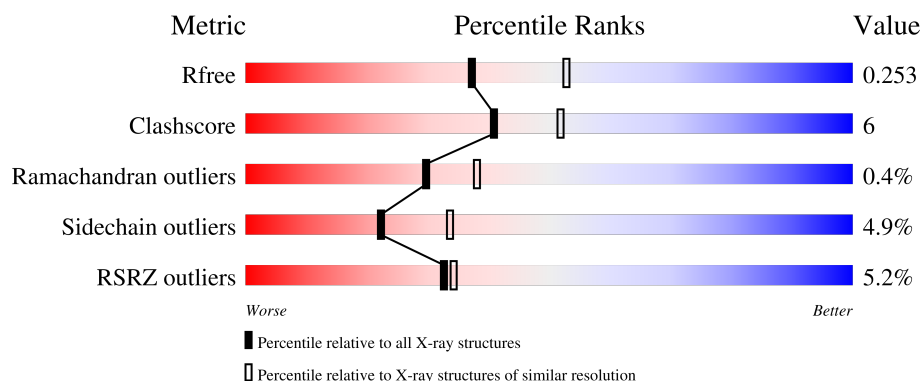
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	499	7% 86% 12% .
1	B	499	82% 16% .
1	C	499	% 85% 13% .
1	D	499	84% 14% .
1	E	499	5% 85% 13% .

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Mol	Chain	Length	Quality of chain
1	F	499	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OXL	B	510	-	X	-	-
4	OXL	E	510	-	X	-	-
4	OXL	G	510	-	X	-	-
4	OXL	I	510	-	X	-	-
4	OXL	J	510	-	X	-	-
4	OXL	N	510	-	X	-	-

2 Entry composition

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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	H	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	J	2	Total 2	Mg 2	0	0
2	K	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	M	2	Total 2	Mg 2	0	0
2	N	2	Total 2	Mg 2	0	0
2	P	2	Total 2	Mg 2	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

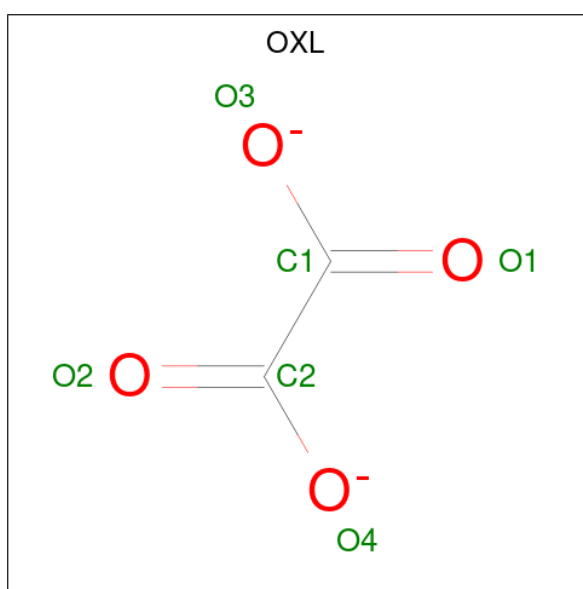
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	K 2	0	0
3	B	2	Total 2	K 2	0	0
3	C	2	Total 2	K 2	0	0
3	D	2	Total 2	K 2	0	0
3	E	2	Total 2	K 2	0	0
3	F	2	Total 2	K 2	0	0
3	G	2	Total 2	K 2	0	0
3	H	2	Total 2	K 2	0	0
3	I	2	Total 2	K 2	0	0
3	J	2	Total 2	K 2	0	0
3	K	2	Total 2	K 2	0	0
3	L	2	Total 2	K 2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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	2	Total	K	0	0
			2	2		
3	N	2	Total	K	0	0
			2	2		
3	O	2	Total	K	0	0
			2	2		
3	P	2	Total	K	0	0
			2	2		

- Molecule 4 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



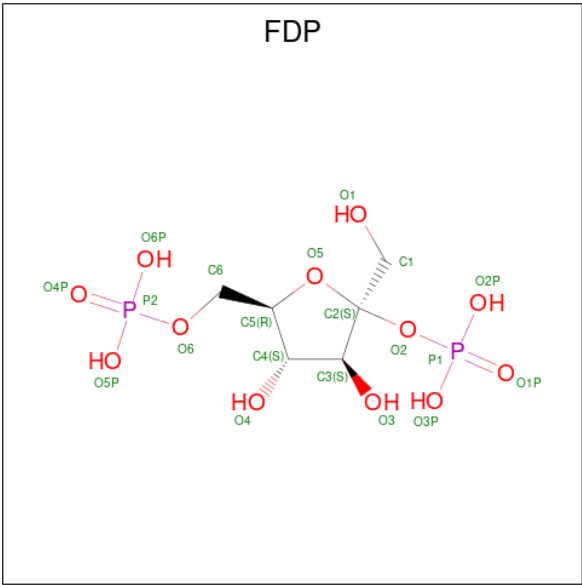
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	2	4		
4	B	1	Total	C	O	0	0
			6	2	4		
4	C	1	Total	C	O	0	0
			6	2	4		
4	D	1	Total	C	O	0	0
			6	2	4		
4	E	1	Total	C	O	0	0
			6	2	4		
4	F	1	Total	C	O	0	0
			6	2	4		
4	G	1	Total	C	O	0	0
			6	2	4		

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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 (CCD ID: FDP) (formula: C₆H₁₄O₁₂P₂).



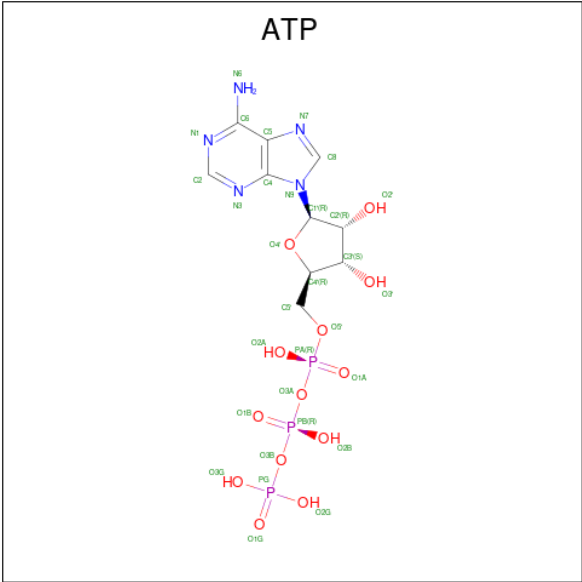
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			20	6	12	2		
5	B	1	Total	C	O	P	0	0
			20	6	12	2		
5	C	1	Total	C	O	P	0	0
			20	6	12	2		

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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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



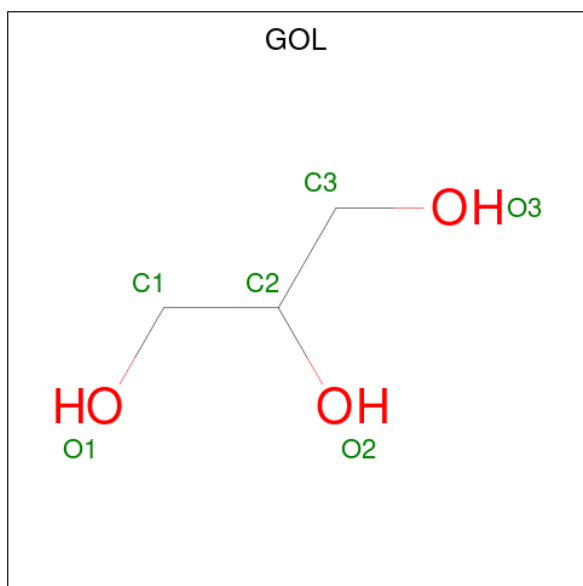
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	G	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 (CCD ID: 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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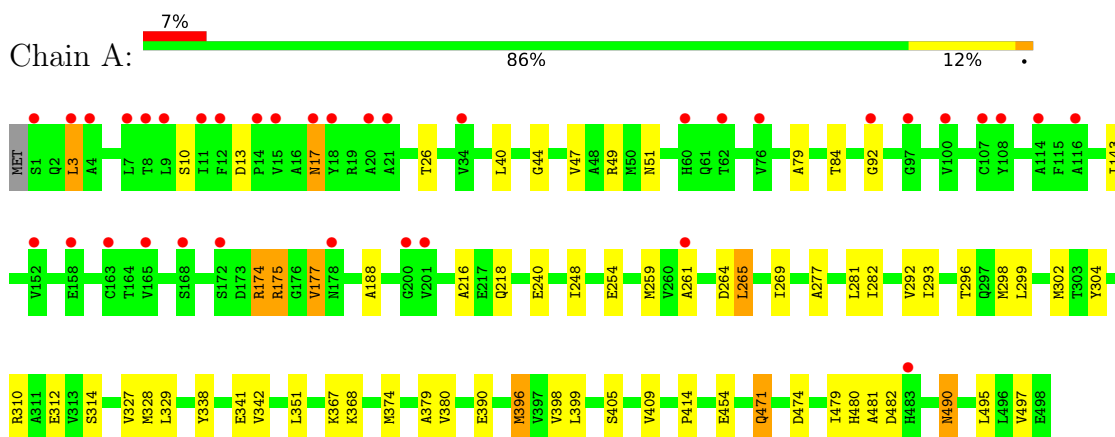
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	305	Total 305	O 305	0	0
8	D	400	Total 400	O 400	0	0
8	E	232	Total 232	O 232	0	0
8	F	187	Total 187	O 187	0	0
8	G	139	Total 139	O 139	0	0
8	H	215	Total 215	O 215	0	0
8	I	415	Total 415	O 415	0	0
8	J	499	Total 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

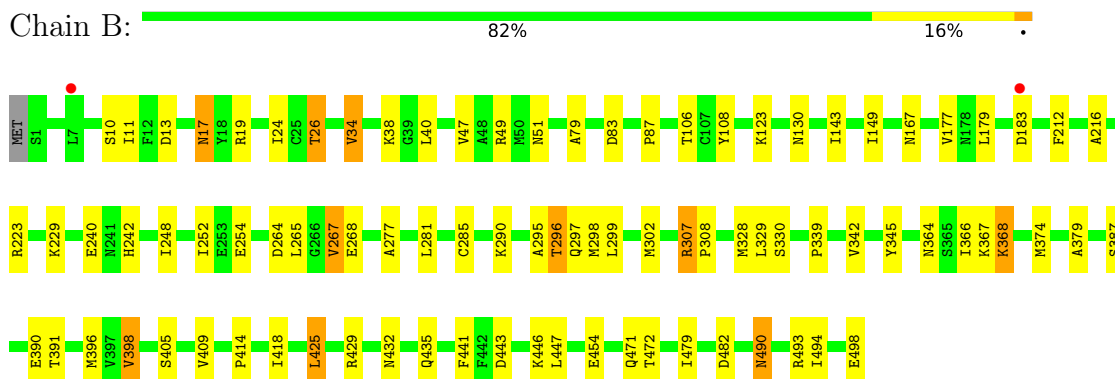
3 Residue-property plots

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.

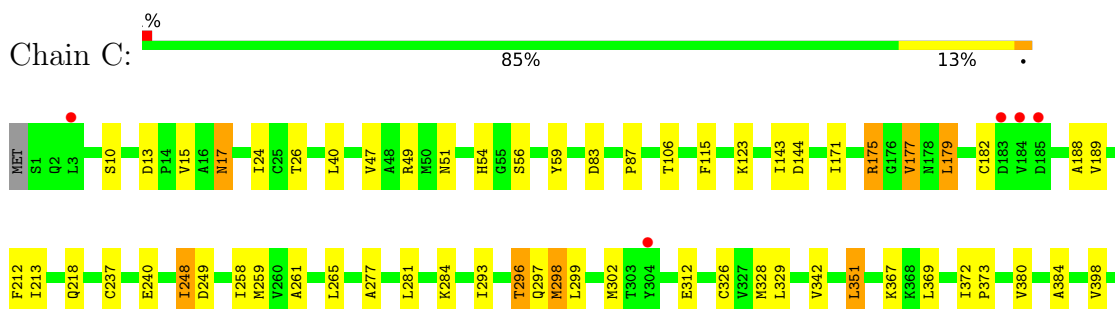
• Molecule 1: Pyruvate kinase

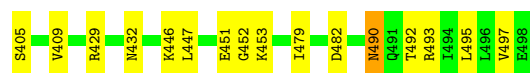


• Molecule 1: Pyruvate kinase



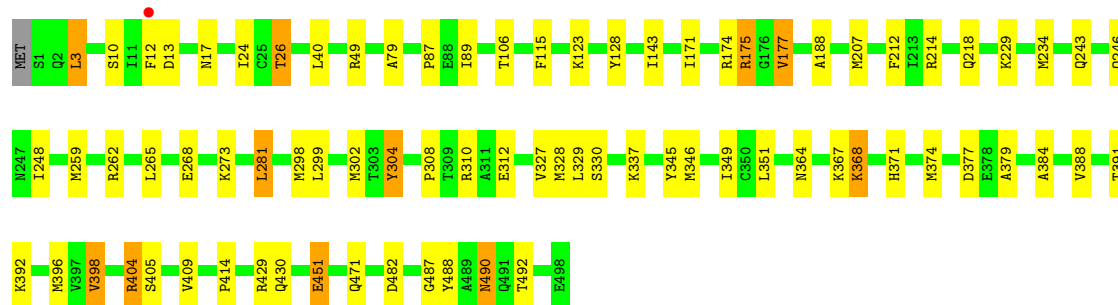
• Molecule 1: Pyruvate kinase





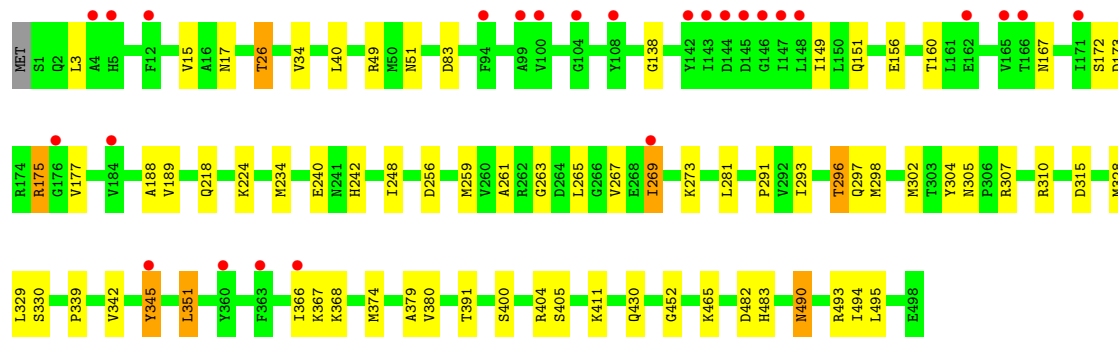
• Molecule 1: Pyruvate kinase

Chain D: 84% 14%



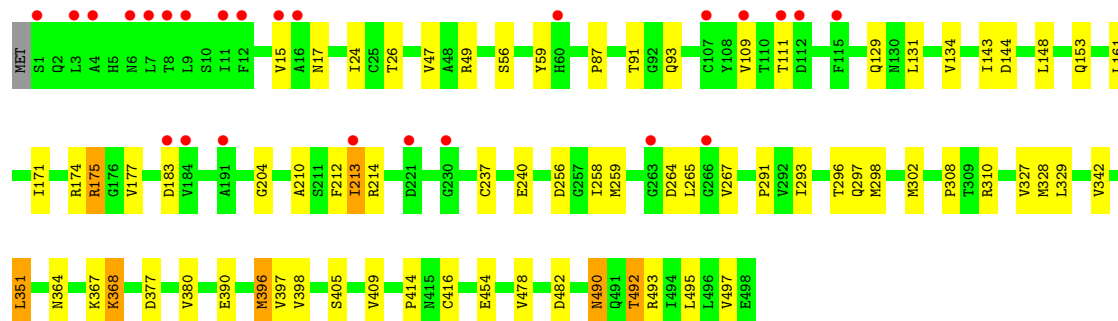
• Molecule 1: Pyruvate kinase

Chain E: 5% 85% 13%



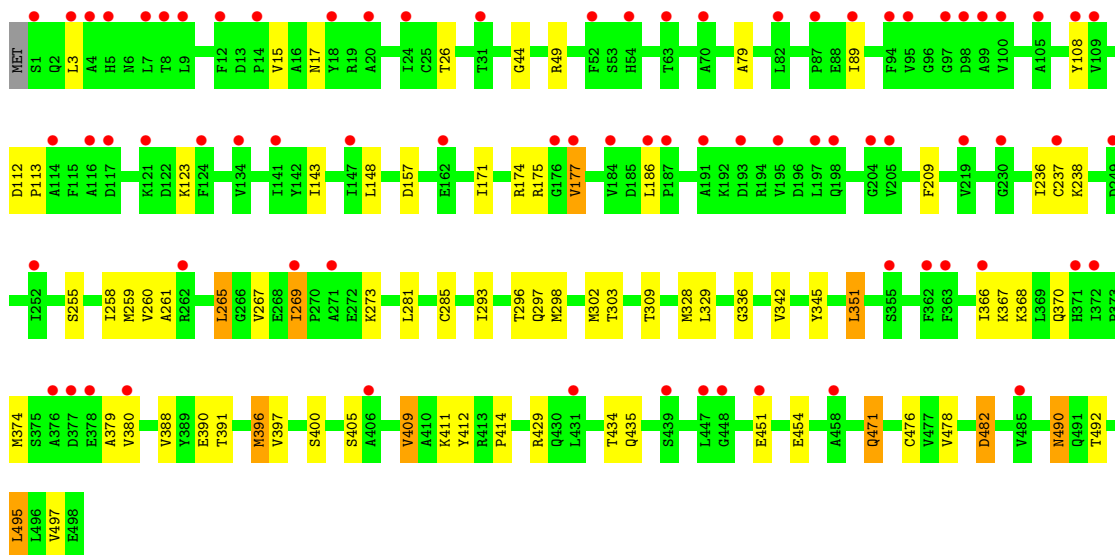
• Molecule 1: Pyruvate kinase

Chain F: 5% 85% 13%

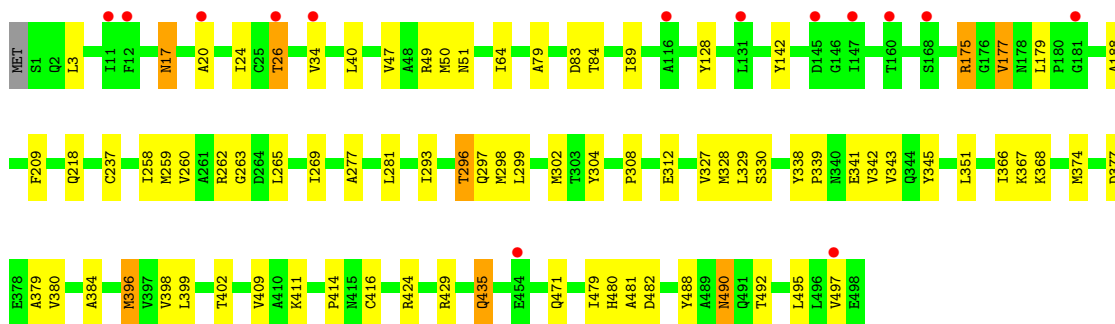
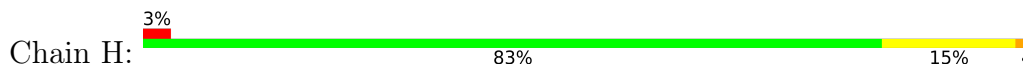


• Molecule 1: Pyruvate kinase

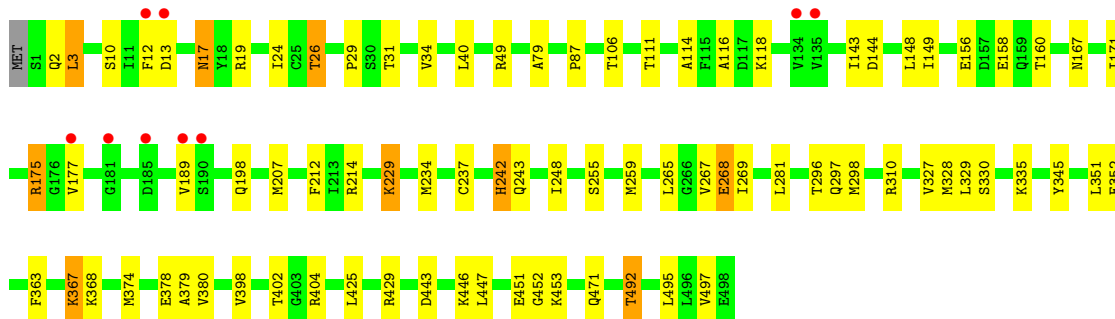
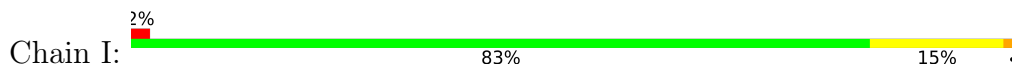
Chain G: 15% 84% 14%



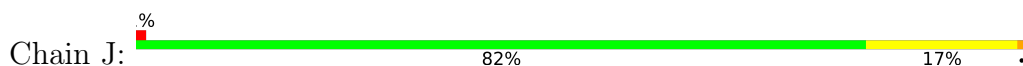
• Molecule 1: Pyruvate kinase

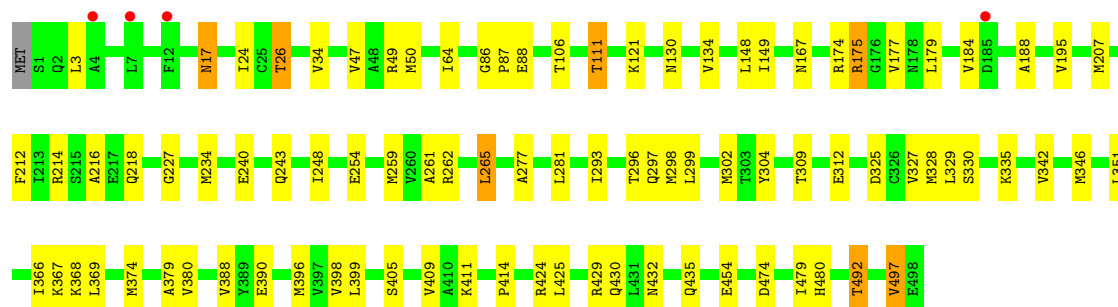


• Molecule 1: Pyruvate kinase

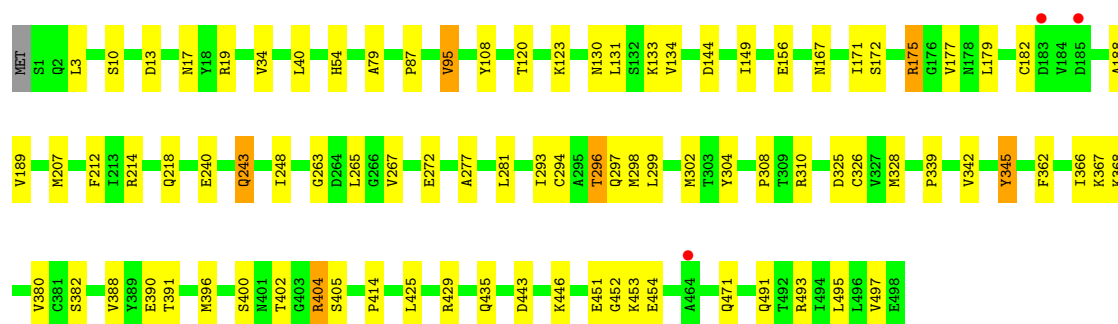
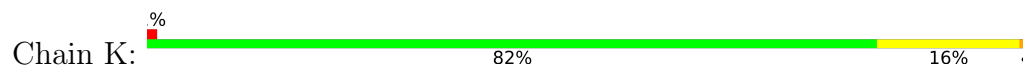


• Molecule 1: Pyruvate kinase

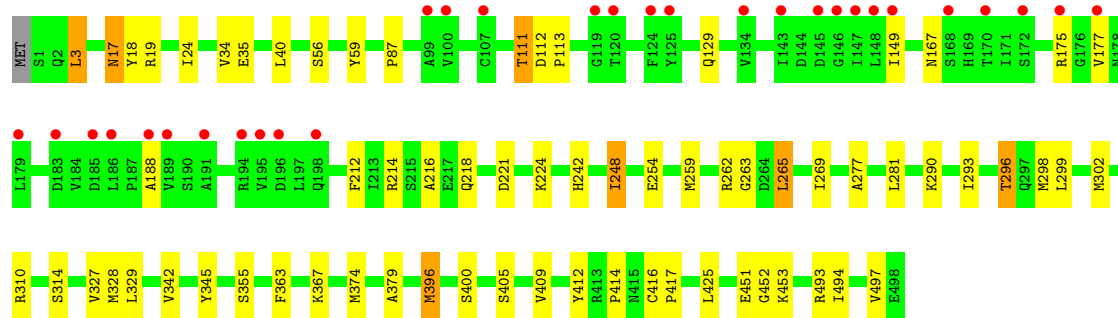
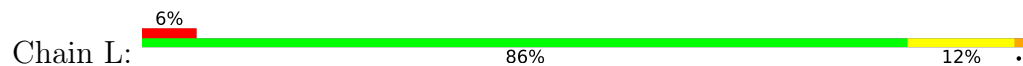




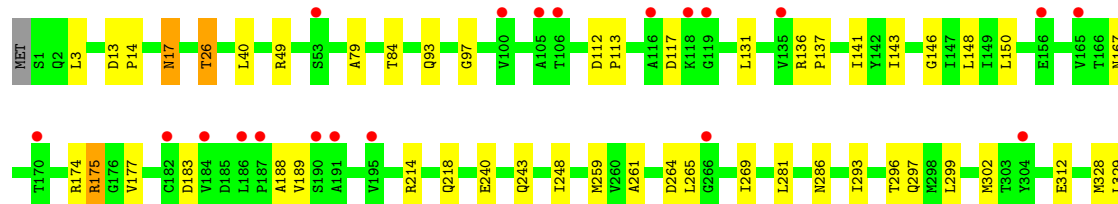
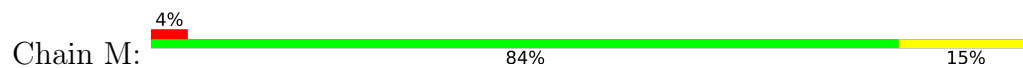
• Molecule 1: Pyruvate kinase

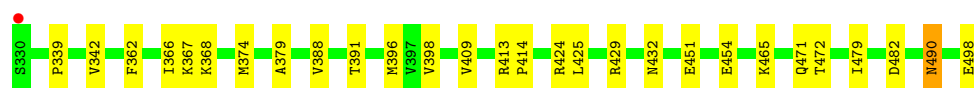


• Molecule 1: Pyruvate kinase

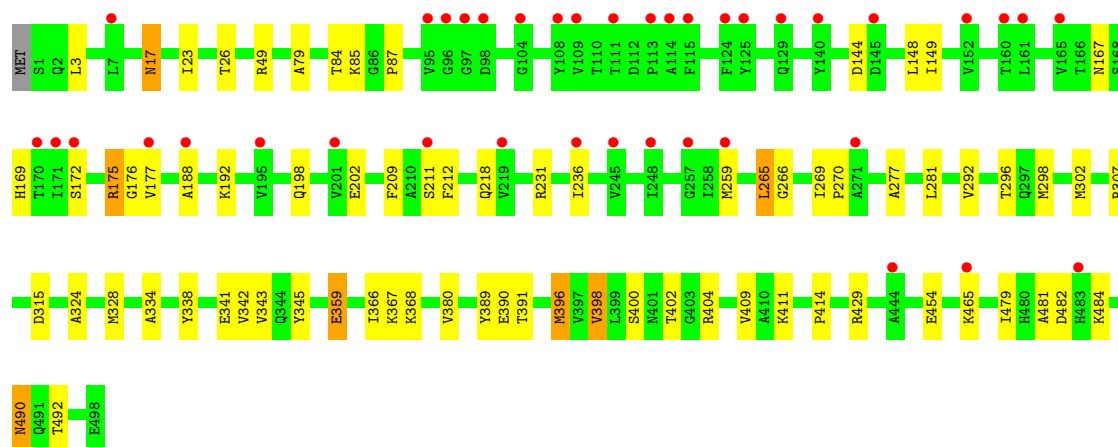
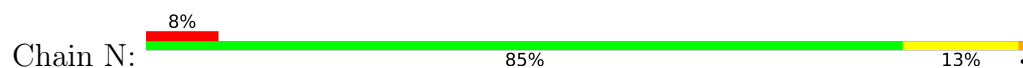


• Molecule 1: Pyruvate kinase

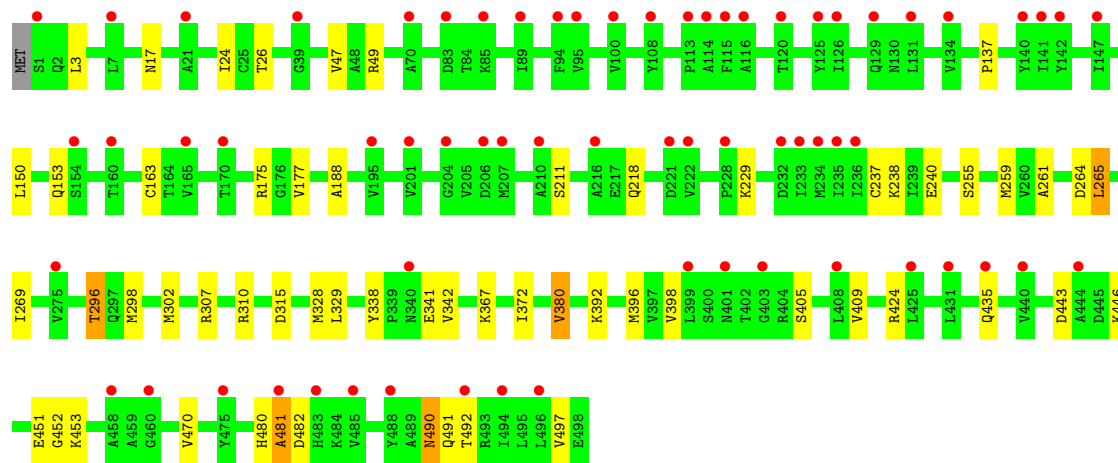
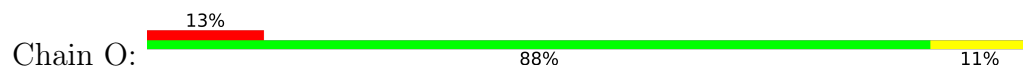




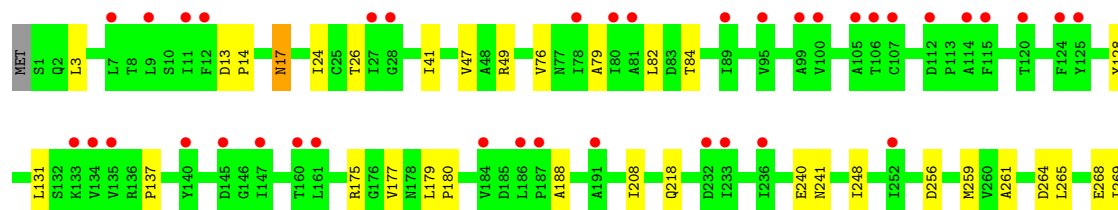
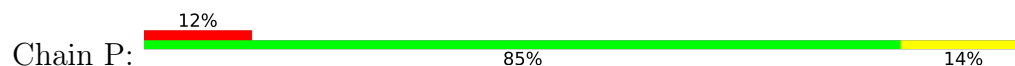
• Molecule 1: Pyruvate kinase

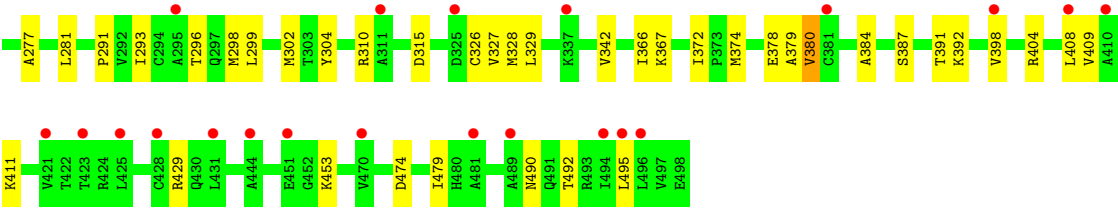


• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.49Å 151.14Å 160.32Å 89.73° 80.17° 71.64°	Depositor
Resolution (Å)	34.46 – 2.30 34.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (34.46-2.30) 94.6 (34.46-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	65997	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, GOL, K, OXL, 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	0.45	0/3876	0.81	0/5247
1	B	0.52	0/3856	0.84	1/5220 (0.0%)
1	C	0.48	0/3872	0.84	1/5242 (0.0%)
1	D	0.52	0/3867	0.83	1/5235 (0.0%)
1	E	0.48	0/3865	0.82	0/5232
1	F	0.49	0/3856	0.85	0/5220
1	G	0.45	0/3856	0.83	0/5220
1	H	0.50	0/3874	0.84	0/5244
1	I	0.59	0/3874	0.85	1/5245 (0.0%)
1	J	0.59	0/3882	0.87	3/5256 (0.1%)
1	K	0.59	0/3873	0.87	1/5243 (0.0%)
1	L	0.55	0/3856	0.88	3/5220 (0.1%)
1	M	0.49	0/3856	0.82	0/5220
1	N	0.48	0/3865	0.82	0/5232
1	O	0.48	0/3856	0.80	0/5220
1	P	0.48	0/3856	0.80	1/5220 (0.0%)
All	All	0.51	0/61840	0.84	12/83716 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	248	ILE	N-CA-C	7.00	117.75	110.62
1	P	404	ARG	N-CA-C	6.05	117.55	111.07
1	K	131	LEU	N-CA-C	5.68	118.20	111.33
1	B	267	VAL	CB-CA-C	-5.66	105.04	111.55
1	L	248	ILE	N-CA-C	5.59	116.33	110.62
1	C	248	ILE	N-CA-C	5.40	116.03	110.36
1	I	267	VAL	N-CA-C	-5.27	107.63	111.90
1	L	290	LYS	CA-C-N	5.17	125.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	290	LYS	C-N-CA	5.17	125.17	119.90
1	D	398	VAL	CB-CA-C	-5.14	103.00	110.81
1	J	227	GLY	CA-C-N	5.13	124.75	119.05
1	J	227	GLY	C-N-CA	5.13	124.75	119.05

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	54	0
1	B	3799	0	3801	70	0
1	C	3815	0	3814	52	0
1	D	3809	0	3807	65	0
1	E	3808	0	3808	44	0
1	F	3799	0	3801	55	0
1	G	3799	0	3801	47	0
1	H	3817	0	3821	55	0
1	I	3816	0	3815	56	0
1	J	3824	0	3820	68	0
1	K	3816	0	3811	55	0
1	L	3799	0	3802	44	0
1	M	3799	0	3802	46	0
1	N	3808	0	3807	41	0
1	O	3799	0	3802	40	0
1	P	3799	0	3802	41	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	20	0	10	0	0
5	G	20	0	10	1	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
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	4	0
8	K	462	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	798	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.

All (798) 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:HE2	1.18	1.15
1:J:298:MET:HE1	1:J:327:VAL:HB	1.36	1.07
1:C:26:THR:HG22	1:C:49:ARG:HD3	1.40	1.04
1:K:388:VAL:HG21	1:K:396:MET:CE	1.90	0.99
1:D:388:VAL:HG21	1:D:396:MET:HE2	1.50	0.93
1:A:396:MET:HE1	1:A:414:PRO:HG3	1.49	0.92
1:J:398[A]:VAL:HG11	1:J:409:VAL:HG21	1.50	0.92
1:H:26:THR:CG2	1:H:330:SER:HA	2.02	0.89
1:A:26:THR:HG22	1:A:49:ARG:HD3	1.55	0.89
1:N:396:MET:HE1	1:N:414:PRO:HG3	1.55	0.88
1:K:388:VAL:CG2	1:K:396:MET:HE2	2.03	0.88
3:I:504:K:K	8:I:678:HOH:O	1.86	0.87
1:F:26:THR:HG22	1:F:49:ARG:HD3	1.55	0.87
1:J:259:MET:HE2	1:J:328:MET:HE1	1.56	0.86
1:J:374:MET:CE	1:J:379:ALA:HA	2.05	0.86
1:B:396:MET:CE	1:B:414:PRO:HG3	2.06	0.85
1:C:398[A]:VAL:HG11	1:C:409:VAL:HG21	1.57	0.84
1:J:302:MET:HE3	1:J:342:VAL:HG23	1.57	0.84
5:N:700:FDP:H11	5:N:700:FDP:O3P	1.75	0.84
1:L:302:MET:HE3	1:L:342:VAL:HG23	1.59	0.84
1:I:26:THR:HG21	1:I:49:ARG:HH11	1.43	0.83
1:I:26:THR:HG23	1:I:329:LEU:O	1.78	0.83
1:D:298:MET:HE1	1:D:327:VAL:HB	1.61	0.83
1:J:111:THR:HG22	8:J:950:HOH:O	1.78	0.82
1:L:248:ILE:HG12	1:L:281:LEU:HD22	1.62	0.82
1:P:453:LYS:NZ	5:P:700:FDP:O1P	2.12	0.81
1:B:396:MET:HE3	1:B:418:ILE:HG12	1.62	0.81
1:J:380:VAL:HG13	1:J:492:THR:HG22	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:298:MET:HE1	1:J:327:VAL:CB	2.10	0.80
1:D:259:MET:HE2	1:D:328:MET:HE1	1.62	0.80
1:J:26:THR:HG23	1:J:329:LEU:O	1.80	0.80
1:A:17:ASN:H	1:A:17:ASN:HD22	1.28	0.80
1:D:26:THR:HG21	1:D:49:ARG:HH11	1.47	0.80
1:F:210:ALA:HB1	1:F:213:ILE:HD11	1.64	0.79
1:H:26:THR:HG23	1:H:330:SER:HA	1.61	0.79
1:G:26:THR:HG22	1:G:49:ARG:HD3	1.63	0.79
1:I:19:ARG:NH1	8:I:507:HOH:O	2.13	0.79
1:C:302:MET:HE3	1:C:342:VAL:HG23	1.63	0.78
1:B:297:GLN:HE21	1:D:310:ARG:H	1.31	0.78
1:L:374:MET:CE	1:L:379:ALA:HA	2.13	0.78
1:I:10:SER:HB3	1:I:13:ASP:OD1	1.82	0.78
1:B:396:MET:HE2	1:B:414:PRO:HG3	1.66	0.77
1:A:497:VAL:HB	8:A:748:HOH:O	1.84	0.76
1:A:482:ASP:H	1:A:490:ASN:HD21	1.34	0.76
1:F:210:ALA:CB	1:F:213:ILE:CD1	2.62	0.76
1:F:26:THR:HG21	1:F:49:ARG:HH11	1.49	0.76
1:M:26:THR:HG21	1:M:49:ARG:HH11	1.51	0.76
1:O:26:THR:HG21	1:O:49:ARG:HH11	1.48	0.76
1:A:175:ARG:HE	1:A:175:ARG:HA	1.49	0.75
1:F:210:ALA:CB	1:F:213:ILE:HD11	2.15	0.75
1:C:398[A]:VAL:HG12	1:C:479:ILE:HB	1.70	0.74
1:E:26:THR:HG22	1:E:49:ARG:HD3	1.67	0.74
1:L:259:MET:HE2	1:L:328:MET:HE1	1.70	0.73
1:B:298:MET:HE1	1:B:328:MET:H	1.52	0.73
1:E:374:MET:HE2	1:F:390:GLU:HB3	1.70	0.73
1:F:396:MET:HE1	1:F:414:PRO:CB	2.17	0.73
1:B:297:GLN:NE2	1:D:310:ARG:H	1.86	0.73
1:D:396:MET:HE1	1:D:414:PRO:CB	2.19	0.73
1:I:374:MET:CE	1:I:379:ALA:HA	2.18	0.73
1:D:364:ASN:O	1:D:368:LYS:HD3	1.89	0.72
1:D:451:GLU:CD	1:D:451:GLU:H	1.98	0.72
1:F:210:ALA:HB3	1:F:213:ILE:CD1	2.19	0.72
1:G:171:ILE:HB	1:G:175:ARG:HG3	1.72	0.72
1:I:24:ILE:HG21	1:I:328:MET:HE2	1.72	0.72
1:M:398:VAL:HG11	1:M:409:VAL:HG21	1.72	0.72
1:A:396:MET:HE1	1:A:414:PRO:CG	2.19	0.72
1:K:298:MET:CE	1:K:328:MET:H	2.03	0.71
1:A:374:MET:HE3	1:A:379:ALA:HA	1.72	0.71
1:F:396:MET:HE1	1:F:414:PRO:CG	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:MET:HE1	1:G:414:PRO:CB	2.21	0.71
1:M:259:MET:HE2	1:M:328:MET:HE1	1.73	0.71
1:D:214:ARG:HB2	1:D:243:GLN:HG3	1.73	0.70
1:H:398[A]:VAL:HG11	1:H:409:VAL:HG21	1.72	0.70
1:M:396:MET:HE1	1:M:414:PRO:HG3	1.72	0.70
1:D:248:ILE:HG12	1:D:281:LEU:HD22	1.71	0.70
1:D:87:PRO:HD2	1:D:212:PHE:HB2	1.73	0.70
1:F:396:MET:HE1	1:F:414:PRO:HG3	1.73	0.70
1:N:269:ILE:HG13	1:N:270:PRO:HD2	1.74	0.70
1:C:384:ALA:HB2	1:C:492:THR:HG21	1.74	0.69
1:I:297:GLN:HE21	1:K:310:ARG:H	1.41	0.69
1:E:259:MET:HE2	1:E:328:MET:HE1	1.73	0.69
1:J:396:MET:HE1	1:J:414:PRO:CB	2.23	0.69
1:B:398:VAL:HG11	1:B:409:VAL:HG21	1.75	0.69
1:C:175:ARG:HH22	6:C:1001:ATP:HO3'	1.38	0.69
1:M:214:ARG:HB2	1:M:243:GLN:HG3	1.74	0.69
1:O:480:HIS:CB	1:O:481:ALA:HB3	2.23	0.69
1:J:297:GLN:HE21	1:L:310:ARG:H	1.39	0.68
1:C:405:SER:O	1:C:409:VAL:HG23	1.93	0.68
1:J:277:ALA:O	1:J:281:LEU:HG	1.93	0.68
1:I:26:THR:HG21	1:I:49:ARG:NH1	2.07	0.68
1:B:298:MET:CE	1:B:328:MET:H	2.05	0.68
1:D:374:MET:CE	1:D:379:ALA:HA	2.24	0.68
1:G:26:THR:HG21	1:G:49:ARG:HH11	1.59	0.68
1:A:259:MET:HE2	1:A:328:MET:HE1	1.76	0.68
1:A:398:VAL:HG11	1:A:409:VAL:HG21	1.74	0.68
1:D:487:GLY:HA2	1:I:229:LYS:HG3	1.74	0.68
1:K:188:ALA:HB1	1:K:218:GLN:HG3	1.77	0.67
1:F:259:MET:HE2	1:F:328:MET:HE1	1.77	0.67
1:I:87:PRO:HD2	1:I:212:PHE:HB2	1.76	0.67
1:J:26:THR:CG2	1:J:330:SER:HA	2.24	0.67
1:C:26:THR:CG2	1:C:49:ARG:HD3	2.22	0.67
6:D:1001:ATP:H8	6:D:1001:ATP:H5'1	1.59	0.67
1:B:26:THR:HG21	1:B:49:ARG:HH11	1.60	0.66
1:A:17:ASN:HD22	1:A:17:ASN:N	1.93	0.66
1:D:26:THR:HG23	1:D:330:SER:HA	1.77	0.66
1:E:298:MET:HE1	1:E:328:MET:H	1.60	0.66
1:M:26:THR:HG23	1:M:329:LEU:O	1.96	0.66
1:F:310:ARG:H	1:H:297:GLN:HE21	1.45	0.65
1:J:398[A]:VAL:HG12	1:J:479:ILE:HB	1.76	0.65
1:N:398:VAL:HG11	1:N:409:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:THR:HG23	1:E:329:LEU:O	1.97	0.65
1:I:374:MET:HE2	1:I:379:ALA:HA	1.79	0.65
1:I:380:VAL:HG13	1:I:492:THR:HG22	1.78	0.65
1:J:297:GLN:NE2	1:L:310:ARG:H	1.94	0.65
1:P:398:VAL:HG11	1:P:409:VAL:HG21	1.77	0.65
1:F:210:ALA:HB1	1:F:213:ILE:CD1	2.25	0.65
1:I:26:THR:CG2	1:I:49:ARG:HH11	2.08	0.65
1:D:298:MET:HE1	1:D:327:VAL:CB	2.26	0.65
1:B:396:MET:HE1	1:B:414:PRO:HG3	1.78	0.65
1:J:298:MET:HE3	1:J:346:MET:HE1	1.78	0.64
1:O:480:HIS:CA	1:O:481:ALA:HB3	2.26	0.64
1:F:298:MET:HE1	1:F:327:VAL:HB	1.78	0.64
1:M:175:ARG:HE	1:M:175:ARG:HA	1.62	0.64
1:O:398:VAL:HG11	1:O:409:VAL:HG21	1.78	0.64
1:E:482:ASP:H	1:E:490:ASN:HD21	1.43	0.64
1:J:26:THR:HG23	1:J:330:SER:HA	1.77	0.64
1:L:19:ARG:NH1	8:L:527:HOH:O	2.30	0.64
1:N:396:MET:HE1	1:N:414:PRO:CG	2.26	0.64
1:A:482:ASP:H	1:A:490:ASN:ND2	1.95	0.64
1:I:297:GLN:NE2	1:K:310:ARG:H	1.95	0.64
1:D:482:ASP:H	1:D:490:ASN:HD21	1.45	0.64
1:H:396:MET:HE1	1:H:414:PRO:CB	2.27	0.64
1:O:480:HIS:HB3	1:O:482:ASP:H	1.63	0.64
1:B:87:PRO:HD2	1:B:212:PHE:HB2	1.79	0.63
1:B:26:THR:HG23	1:B:329:LEU:O	1.98	0.63
1:O:480:HIS:HA	1:O:481:ALA:HB3	1.79	0.63
1:A:398:VAL:HG12	1:A:479:ILE:HB	1.81	0.63
1:I:352:GLU:HG2	1:K:272:GLU:O	1.98	0.63
1:I:446:LYS:HG3	1:I:447:LEU:HG	1.81	0.63
1:J:240:GLU:HB3	1:J:261:ALA:HB3	1.79	0.63
1:M:374:MET:HE3	1:M:379:ALA:HA	1.81	0.63
1:B:49:ARG:NH2	1:B:83:ASP:OD2	2.32	0.62
1:D:26:THR:HG23	1:D:329:LEU:O	2.00	0.62
1:E:26:THR:HG21	1:E:49:ARG:HH11	1.64	0.62
1:J:396:MET:HE1	1:J:414:PRO:HG3	1.80	0.62
1:K:396:MET:HE1	1:K:414:PRO:CB	2.29	0.62
1:O:480:HIS:HA	1:O:481:ALA:CB	2.30	0.62
1:K:19:ARG:NH1	8:K:519:HOH:O	2.33	0.62
1:O:259:MET:HE2	1:O:328:MET:HE1	1.80	0.62
1:B:277:ALA:O	1:B:281:LEU:HG	1.99	0.62
1:C:26:THR:HG21	1:C:49:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:VAL:HG13	1:H:492:THR:HG23	1.82	0.61
1:H:262:ARG:NH2	1:H:298:MET:HG2	2.14	0.61
1:D:388:VAL:HG21	1:D:396:MET:CE	2.27	0.61
1:J:207:MET:HE2	1:J:234:MET:CE	2.30	0.61
1:M:143:ILE:HB	1:M:148:LEU:HB3	1.81	0.61
1:J:396:MET:HE1	1:J:414:PRO:CG	2.31	0.61
1:K:298:MET:HE1	1:K:328:MET:H	1.64	0.61
1:O:480:HIS:HB3	1:O:481:ALA:HB3	1.82	0.61
1:E:242:HIS:HA	1:E:269:ILE:HD11	1.81	0.61
1:A:277:ALA:O	1:A:281:LEU:HG	2.00	0.61
1:H:482:ASP:H	1:H:490:ASN:HD21	1.46	0.61
1:E:298:MET:CE	1:E:328:MET:H	2.14	0.61
1:F:26:THR:CG2	1:F:49:ARG:HH11	2.12	0.61
1:B:248:ILE:HG12	1:B:281:LEU:HD22	1.81	0.60
1:J:298:MET:HE2	1:J:328:MET:H	1.65	0.60
1:A:17:ASN:H	1:A:17:ASN:ND2	1.99	0.60
1:B:26:THR:HG23	1:B:330:SER:HA	1.83	0.60
1:L:396:MET:HE1	1:L:414:PRO:CB	2.31	0.60
1:E:293:ILE:HG21	1:E:328:MET:HE3	1.84	0.60
1:G:366:ILE:HD13	1:G:411:LYS:O	2.01	0.60
1:J:298:MET:CE	1:J:327:VAL:HB	2.23	0.60
1:B:26:THR:HG22	1:B:49:ARG:HE	1.66	0.60
1:H:398[A]:VAL:HG12	1:H:479:ILE:HB	1.84	0.60
1:O:26:THR:HG22	1:O:49:ARG:HD3	1.84	0.59
1:K:396:MET:HE1	1:K:414:PRO:HB3	1.85	0.59
1:B:17:ASN:HD22	1:B:17:ASN:H	1.50	0.59
1:J:174:ARG:HD2	7:J:499:GOL:H11	1.85	0.59
1:F:240:GLU:HB2	1:F:264:ASP:HB2	1.84	0.59
1:H:479:ILE:HG12	1:H:492:THR:HG22	1.84	0.59
1:B:374:MET:HE3	1:B:379:ALA:HA	1.83	0.59
1:D:345:TYR:O	1:D:349:ILE:HG13	2.02	0.59
1:B:482:ASP:H	1:B:490:ASN:HD21	1.51	0.59
1:F:144:ASP:HB2	1:F:175:ARG:HG3	1.85	0.59
1:J:374:MET:HE2	1:J:379:ALA:HA	1.84	0.59
1:A:3:LEU:HD13	1:C:369:LEU:HD12	1.85	0.58
1:A:474:ASP:O	1:A:497:VAL:HG22	2.03	0.58
1:M:26:THR:HG21	1:M:49:ARG:NH1	2.18	0.58
1:A:405:SER:O	1:A:409:VAL:HG23	2.04	0.58
1:G:259:MET:HE2	1:G:328:MET:HE1	1.85	0.58
1:H:396:MET:HE2	1:H:416:CYS:SG	2.44	0.58
1:K:325:ASP:HA	1:K:435:GLN:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:175:ARG:NE	1:N:175:ARG:HA	2.18	0.58
1:B:398:VAL:HG12	1:B:479:ILE:HB	1.85	0.58
1:H:277:ALA:O	1:H:281:LEU:HG	2.04	0.58
1:A:26:THR:HG21	1:A:49:ARG:HH11	1.68	0.58
1:C:259:MET:HE2	1:C:328:MET:HE1	1.84	0.58
1:E:188:ALA:HB1	1:E:218:GLN:HG3	1.86	0.58
1:K:175:ARG:NH2	6:K:1001:ATP:O3'	2.36	0.58
1:D:371:HIS:ND1	8:D:706:HOH:O	2.33	0.57
1:E:175:ARG:NH2	6:E:1001:ATP:O3'	2.35	0.57
1:F:482:ASP:H	1:F:490:ASN:HD21	1.51	0.57
1:K:108:TYR:CE1	1:K:156:GLU:HG3	2.38	0.57
1:J:216:ALA:HB1	1:J:254:GLU:HG3	1.84	0.57
1:D:487:GLY:CA	1:I:229:LYS:HG3	2.35	0.57
1:N:259:MET:HE2	1:N:328:MET:HE1	1.86	0.57
1:J:259:MET:CE	1:J:328:MET:HE1	2.31	0.57
1:J:398[A]:VAL:CG1	1:J:409:VAL:HG21	2.31	0.57
1:L:298:MET:HE1	1:L:327:VAL:HB	1.87	0.57
1:N:188:ALA:HB1	1:N:218:GLN:HG3	1.87	0.57
1:J:26:THR:HG21	1:J:49:ARG:HH11	1.69	0.56
1:F:87:PRO:HD2	1:F:212:PHE:HB2	1.87	0.56
1:K:248:ILE:HG12	1:K:281:LEU:HD22	1.87	0.56
1:K:380:VAL:HG23	1:L:494:ILE:HD12	1.86	0.56
1:A:310:ARG:H	1:C:297:GLN:HE21	1.54	0.56
1:D:396:MET:HE1	1:D:414:PRO:HB3	1.86	0.56
1:J:299:LEU:HD22	1:J:302:MET:HE2	1.86	0.56
1:L:405:SER:O	1:L:409:VAL:HG23	2.06	0.56
1:M:293:ILE:HG21	1:M:328:MET:HE3	1.87	0.56
1:O:480:HIS:CA	1:O:481:ALA:CB	2.84	0.56
1:H:384:ALA:CB	1:H:479:ILE:HD11	2.35	0.56
1:M:482:ASP:H	1:M:490:ASN:HD21	1.53	0.56
1:D:490:ASN:HD22	1:D:490:ASN:H	1.53	0.56
1:F:93:GLN:HE21	1:F:174:ARG:HH21	1.54	0.56
1:M:398:VAL:HG12	1:M:479:ILE:HB	1.88	0.56
1:O:26:THR:CG2	1:O:49:ARG:HH11	2.17	0.56
1:B:19:ARG:NH1	8:B:513:HOH:O	2.39	0.55
1:B:26:THR:CG2	1:B:49:ARG:HE	2.18	0.55
1:I:3:LEU:HD11	1:K:366:ILE:HG13	1.87	0.55
1:I:10:SER:OG	1:I:12:PHE:HD2	1.89	0.55
1:J:374:MET:HE1	1:J:379:ALA:HA	1.87	0.55
1:N:400:SER:OG	1:N:402:THR:O	2.19	0.55
1:J:335:LYS:HE2	8:J:634:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:ILE:HD13	1:E:411:LYS:O	2.05	0.55
1:I:79:ALA:HB2	1:I:429:ARG:O	2.07	0.55
1:I:363:PHE:CZ	1:I:367:LYS:HE3	2.42	0.55
1:J:369:LEU:HD12	1:L:3:LEU:HD13	1.89	0.55
1:P:24:ILE:HG12	1:P:47:VAL:HB	1.89	0.55
1:D:298:MET:CE	1:D:327:VAL:HB	2.35	0.55
1:F:364:ASN:O	1:F:368:LYS:HD3	2.07	0.55
1:O:302:MET:HE3	1:O:342:VAL:HG23	1.87	0.55
1:P:26:THR:HG21	1:P:49:ARG:HH11	1.70	0.55
1:B:364:ASN:O	1:B:368:LYS:HD3	2.06	0.55
1:F:210:ALA:HB3	1:F:213:ILE:HD13	1.88	0.55
1:N:84:THR:HB	1:N:211:SER:H	1.72	0.55
1:A:374:MET:HE2	1:B:390:GLU:HB3	1.88	0.55
1:G:396:MET:HE1	1:G:414:PRO:HB3	1.89	0.55
1:H:259:MET:HE2	1:H:328:MET:HE1	1.87	0.55
1:H:293:ILE:HG21	1:H:328:MET:HE3	1.88	0.55
1:I:298:MET:CE	1:I:328:MET:H	2.19	0.55
1:N:148:LEU:HD13	1:N:169:HIS:HB3	1.89	0.55
1:A:26:THR:CG2	1:A:49:ARG:HH11	2.20	0.54
1:B:374:MET:CE	1:B:379:ALA:HA	2.36	0.54
1:O:26:THR:HG21	1:O:49:ARG:NH1	2.20	0.54
1:M:490:ASN:HD22	1:M:490:ASN:H	1.56	0.54
1:F:175:ARG:NH2	6:F:1001:ATP:O3'	2.41	0.54
1:P:248:ILE:HG12	1:P:281:LEU:HD22	1.89	0.54
1:C:87:PRO:HD2	1:C:212:PHE:HB2	1.87	0.54
1:C:188:ALA:HB1	1:C:218:GLN:HG3	1.89	0.54
1:C:277:ALA:O	1:C:281:LEU:HG	2.07	0.54
1:F:302:MET:HE2	1:F:308:PRO:HB3	1.90	0.54
1:H:374:MET:CE	1:H:379:ALA:HA	2.37	0.54
1:M:374:MET:HE2	1:N:390:GLU:HB3	1.88	0.54
1:N:149:ILE:H	1:N:167:ASN:HD21	1.55	0.54
1:K:214:ARG:HB2	1:K:243:GLN:HG3	1.89	0.54
1:A:390:GLU:HB3	1:B:374:MET:HE2	1.89	0.54
1:J:405:SER:O	1:J:409:VAL:HG23	2.08	0.54
1:D:79:ALA:HB2	1:D:429:ARG:O	2.08	0.54
1:G:26:THR:CG2	1:G:49:ARG:HH11	2.21	0.54
1:H:51:ASN:HA	1:H:83:ASP:HB3	1.87	0.54
1:B:295:ALA:HB1	1:B:328:MET:HE2	1.89	0.54
1:M:374:MET:CE	1:M:379:ALA:HA	2.38	0.54
1:C:10:SER:HB3	1:C:13:ASP:OD2	2.08	0.54
1:C:240:GLU:HB3	1:C:261:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:443:ASP:HB3	1:I:446:LYS:HG2	1.90	0.54
1:M:79:ALA:HB2	1:M:429:ARG:O	2.07	0.54
1:F:143:ILE:HB	1:F:148:LEU:HB3	1.88	0.54
1:I:116:ALA:HB3	7:I:499:GOL:H11	1.89	0.54
1:A:259:MET:CE	1:A:328:MET:HE1	2.37	0.53
1:N:380:VAL:HG13	1:N:492:THR:HG23	1.90	0.53
1:H:302:MET:HE3	1:H:342:VAL:HG23	1.90	0.53
1:H:396:MET:HE1	1:H:414:PRO:CG	2.38	0.53
1:L:293:ILE:HG21	1:L:328:MET:HE3	1.90	0.53
1:P:259:MET:HE2	1:P:328:MET:HE1	1.90	0.53
1:M:188:ALA:HB1	1:M:218:GLN:HG3	1.90	0.53
1:C:179:LEU:HB3	1:C:182:CYS:HB2	1.91	0.53
1:D:188:ALA:HB1	1:D:218:GLN:HG3	1.89	0.53
1:D:246:GLN:HG3	8:D:1886:HOH:O	2.07	0.53
1:L:262:ARG:NH2	1:L:298:MET:HG2	2.24	0.53
1:O:380:VAL:HG13	1:O:492:THR:HG23	1.89	0.53
1:I:207:MET:HE2	1:I:234:MET:HE3	1.91	0.53
1:N:482:ASP:H	1:N:490:ASN:HD21	1.56	0.53
1:A:302:MET:HE3	1:A:342:VAL:HG23	1.91	0.53
1:K:302:MET:HE3	1:K:342:VAL:HG23	1.91	0.53
1:C:299:LEU:HD22	1:C:302:MET:HE2	1.90	0.53
1:D:234:MET:HE2	1:D:430:GLN:HG2	1.90	0.53
1:I:248:ILE:HG12	1:I:281:LEU:HD22	1.90	0.52
1:P:240:GLU:HB3	1:P:261:ALA:HB3	1.92	0.52
1:A:47:VAL:HG22	1:A:79:ALA:HB3	1.92	0.52
1:A:374:MET:CE	1:A:379:ALA:HA	2.39	0.52
1:D:298:MET:CE	1:D:328:MET:H	2.21	0.52
1:C:298:MET:CE	1:C:328:MET:H	2.23	0.52
1:C:175:ARG:NH2	6:C:1001:ATP:O3'	2.32	0.52
1:E:374:MET:CE	1:E:379:ALA:HA	2.39	0.52
1:L:87:PRO:HD2	1:L:212:PHE:HB2	1.91	0.52
1:D:268:GLU:HG3	8:D:610:HOH:O	2.09	0.52
1:G:303:THR:HG23	1:G:336:GLY:HA2	1.91	0.52
1:A:310:ARG:H	1:C:297:GLN:NE2	2.07	0.52
1:G:482:ASP:H	1:G:490:ASN:HD21	1.58	0.52
1:M:17:ASN:H	1:M:17:ASN:HD22	1.57	0.52
1:M:297:GLN:HE21	1:O:310:ARG:H	1.58	0.52
1:P:17:ASN:H	1:P:17:ASN:HD22	1.57	0.52
1:B:299:LEU:HD13	1:B:302:MET:HE3	1.91	0.52
1:H:188:ALA:HB1	1:H:218:GLN:HG3	1.91	0.52
1:A:175:ARG:NH2	6:A:1001:ATP:O3'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:THR:HG23	1:B:498:GLU:HA	1.92	0.52
1:C:296:THR:HG22	1:C:297:GLN:HG3	1.91	0.52
1:A:248:ILE:HG12	1:A:281:LEU:HD22	1.91	0.52
1:B:149:ILE:H	1:B:167:ASN:HD21	1.57	0.52
1:B:366:ILE:HG13	1:D:3:LEU:HD11	1.92	0.52
1:H:298:MET:CE	1:H:328:MET:H	2.22	0.52
1:J:17:ASN:C	1:J:17:ASN:HD22	2.18	0.52
1:J:298:MET:CE	1:J:328:MET:H	2.22	0.52
1:K:10:SER:HB3	1:K:13:ASP:OD1	2.10	0.52
1:B:17:ASN:HD22	1:B:17:ASN:N	2.08	0.51
1:C:17:ASN:N	1:C:17:ASN:HD22	2.07	0.51
1:N:26:THR:HG23	1:N:334:ALA:HB2	1.92	0.51
1:P:128:TYR:HB3	1:P:131:LEU:HD22	1.92	0.51
1:P:366:ILE:HD13	1:P:411:LYS:O	2.10	0.51
1:L:149:ILE:H	1:L:167:ASN:HD21	1.59	0.51
1:J:184:VAL:HG23	1:J:184:VAL:O	2.11	0.51
1:M:136:ARG:HB3	1:M:137:PRO:HD2	1.91	0.51
1:E:298:MET:HG2	1:E:315:ASP:OD2	2.11	0.51
1:G:108:TYR:HB2	1:G:123:LYS:HG3	1.92	0.51
1:O:443:ASP:HB3	1:O:446:LYS:HG2	1.93	0.51
1:C:429:ARG:O	1:C:432:ASN:HB2	2.11	0.51
1:J:234:MET:HE2	1:J:430:GLN:HG2	1.93	0.51
1:K:299:LEU:HD13	1:K:302:MET:CE	2.41	0.51
1:A:293:ILE:HG21	1:A:328:MET:HE3	1.92	0.51
1:B:387:SER:O	1:B:391:THR:HG22	2.11	0.51
1:O:24:ILE:HG12	1:O:47:VAL:HB	1.92	0.51
1:P:298:MET:HG2	1:P:315:ASP:OD2	2.10	0.51
1:B:297:GLN:NE2	1:D:310:ARG:HG2	2.25	0.51
1:I:298:MET:HE1	1:I:328:MET:H	1.76	0.51
1:L:263:GLY:CA	1:L:296:THR:HG21	2.41	0.51
1:C:380:VAL:HG13	1:C:492:THR:HG23	1.92	0.51
1:E:302:MET:HE3	1:E:342:VAL:HG23	1.93	0.51
1:L:298:MET:CE	1:L:328:MET:H	2.24	0.51
5:N:700:FDP:O3P	5:N:700:FDP:C1	2.55	0.51
1:O:188:ALA:HB1	1:O:218:GLN:HG3	1.92	0.51
1:B:446:LYS:HG3	1:B:447:LEU:HG	1.92	0.50
1:N:17:ASN:H	1:N:17:ASN:ND2	2.09	0.50
1:F:26:THR:HG23	1:F:329:LEU:O	2.11	0.50
1:G:237:CYS:SG	1:G:255:SER:HB3	2.50	0.50
1:J:374:MET:CE	1:J:379:ALA:CA	2.84	0.50
1:C:144:ASP:HB2	1:C:175:ARG:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:277:ALA:O	1:P:281:LEU:HG	2.10	0.50
1:D:374:MET:HE3	1:D:379:ALA:HA	1.90	0.50
1:K:452:GLY:C	1:K:453:LYS:HG2	2.37	0.50
1:B:268:GLU:HG3	8:B:615:HOH:O	2.10	0.50
1:C:26:THR:HG21	1:C:49:ARG:NH1	2.27	0.50
1:J:297:GLN:NE2	1:L:310:ARG:HG2	2.26	0.50
1:A:338:TYR:HB3	1:A:341:GLU:HB2	1.92	0.50
1:I:3:LEU:CD1	1:K:366:ILE:HG13	2.41	0.50
1:I:268:GLU:HG3	8:I:568:HOH:O	2.12	0.50
1:K:277:ALA:O	1:K:281:LEU:HG	2.12	0.50
1:N:266:GLY:HA3	1:P:310:ARG:HE	1.76	0.50
1:O:405:SER:HB2	5:O:700:FDP:O4P	2.12	0.50
1:C:26:THR:HG23	1:C:329:LEU:O	2.11	0.50
1:H:481:ALA:HA	1:H:490:ASN:HD22	1.76	0.50
1:O:380:VAL:HG21	1:O:490:ASN:HA	1.94	0.50
1:D:207:MET:HE2	1:D:234:MET:CE	2.42	0.50
1:E:452:GLY:HA2	1:E:483:HIS:CE1	2.47	0.50
1:F:405:SER:O	1:F:409:VAL:HG23	2.11	0.50
1:O:480:HIS:HB3	1:O:482:ASP:N	2.25	0.50
1:P:380:VAL:HG21	1:P:490:ASN:HA	1.94	0.50
1:M:93:GLN:HB2	1:M:117:ASP:HA	1.94	0.49
1:M:131:LEU:H	1:M:131:LEU:HD23	1.76	0.49
1:O:372:ILE:HG22	1:P:392:LYS:HE2	1.94	0.49
1:C:17:ASN:ND2	1:C:17:ASN:H	2.10	0.49
1:C:372:ILE:HG22	1:D:392:LYS:HE2	1.94	0.49
1:P:240:GLU:HB2	1:P:264:ASP:HB2	1.94	0.49
1:E:15:VAL:HB	1:E:351:LEU:HD22	1.94	0.49
1:A:471:GLN:O	1:A:497:VAL:HG23	2.13	0.49
1:B:26:THR:CG2	1:B:330:SER:HA	2.43	0.49
1:M:26:THR:HG22	1:M:49:ARG:HD3	1.94	0.49
1:N:302:MET:HE3	1:N:342:VAL:HG23	1.94	0.49
1:D:26:THR:HG21	1:D:49:ARG:NH1	2.21	0.49
1:E:156:GLU:HB2	1:E:160:THR:HB	1.94	0.49
1:A:380:VAL:HG23	1:B:494:ILE:HD12	1.94	0.49
1:H:83:ASP:HA	1:H:209:PHE:HB2	1.94	0.49
1:N:277:ALA:O	1:N:281:LEU:HG	2.13	0.49
1:H:298:MET:HE2	1:H:328:MET:H	1.78	0.49
1:J:87:PRO:HD2	1:J:212:PHE:HB2	1.95	0.49
1:K:299:LEU:HD13	1:K:302:MET:HE3	1.93	0.49
1:F:129:GLN:CD	1:F:129:GLN:H	2.20	0.49
1:J:262:ARG:NH2	1:J:298:MET:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:366:ILE:HD13	1:J:411:LYS:O	2.12	0.49
1:A:240:GLU:HB3	1:A:261:ALA:HB3	1.94	0.48
1:F:240:GLU:HA	1:F:265:LEU:HB2	1.93	0.48
1:I:24:ILE:CG2	1:I:328:MET:HE2	2.40	0.48
1:N:17:ASN:H	1:N:17:ASN:HD22	1.61	0.48
1:F:26:THR:HG21	1:F:49:ARG:NH1	2.24	0.48
1:F:298:MET:HE1	1:F:327:VAL:CB	2.43	0.48
1:J:388:VAL:HG21	1:J:396:MET:HE2	1.94	0.48
1:J:429:ARG:O	1:J:432:ASN:HB2	2.13	0.48
1:K:130:ASN:HD21	1:K:133:LYS:HD3	1.77	0.48
1:O:26:THR:HG23	1:O:329:LEU:O	2.12	0.48
1:O:338:TYR:HB3	1:O:341:GLU:HB2	1.94	0.48
1:A:175:ARG:HA	1:A:175:ARG:NE	2.23	0.48
1:B:396:MET:CE	1:B:418:ILE:HG12	2.38	0.48
1:I:26:THR:CG2	1:I:330:SER:HA	2.44	0.48
1:K:149:ILE:H	1:K:167:ASN:HD21	1.61	0.48
1:N:298:MET:HG2	1:N:315:ASP:OD2	2.14	0.48
1:B:490:ASN:HD22	1:B:490:ASN:H	1.62	0.48
1:M:396:MET:HE1	1:M:414:PRO:CG	2.43	0.48
1:M:26:THR:CG2	1:M:49:ARG:HH11	2.21	0.48
1:P:378:GLU:HG3	1:P:408:LEU:HD11	1.95	0.48
1:K:491:GLN:OE1	1:K:493:ARG:HD2	2.13	0.48
1:O:453:LYS:HG3	1:O:480:HIS:HD2	1.78	0.48
1:P:387:SER:O	1:P:391:THR:HG22	2.14	0.48
1:C:54:HIS:HE1	6:C:1001:ATP:O2B	1.97	0.48
1:D:298:MET:HE2	1:D:328:MET:H	1.79	0.48
1:I:149:ILE:H	1:I:167:ASN:HD21	1.60	0.48
1:P:302:MET:HE3	1:P:342:VAL:HG23	1.96	0.48
1:P:398:VAL:HG12	1:P:479:ILE:HB	1.96	0.48
1:D:26:THR:CG2	1:D:49:ARG:HH11	2.23	0.48
1:J:298:MET:HE3	1:J:346:MET:CE	2.42	0.48
1:N:366:ILE:HD13	1:N:411:LYS:O	2.13	0.48
1:B:396:MET:HE2	1:B:414:PRO:CG	2.39	0.48
1:J:26:THR:CG2	1:J:329:LEU:O	2.58	0.48
1:D:259:MET:CE	1:D:328:MET:HE1	2.37	0.48
1:G:400:SER:OG	5:G:700:FDP:O4P	2.28	0.48
1:B:302:MET:HE1	1:B:345:TYR:CB	2.43	0.47
1:H:396:MET:HE1	1:H:414:PRO:HG3	1.96	0.47
1:L:24:ILE:HG21	1:L:328:MET:HE2	1.96	0.47
1:C:171:ILE:HB	1:C:175:ARG:HG2	1.95	0.47
1:E:26:THR:HG21	1:E:49:ARG:NH1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:SER:O	1:K:175:ARG:CD	2.62	0.47
1:G:388:VAL:HG21	1:G:396:MET:HE2	1.95	0.47
1:H:34:VAL:HG12	8:H:829:HOH:O	2.15	0.47
1:J:26:THR:HG21	1:J:330:SER:HA	1.95	0.47
1:O:150:LEU:HB3	1:O:163:CYS:HB3	1.96	0.47
1:O:240:GLU:HB3	1:O:261:ALA:HB3	1.96	0.47
1:G:476:CYS:HB3	1:G:495:LEU:HD12	1.96	0.47
1:I:310:ARG:HG2	1:K:297:GLN:OE1	2.14	0.47
1:P:384:ALA:HB2	1:P:492:THR:HG21	1.95	0.47
1:D:26:THR:CG2	1:D:330:SER:HA	2.42	0.47
1:G:79:ALA:HB2	1:G:429:ARG:O	2.13	0.47
1:I:156:GLU:HB2	1:I:160:THR:HB	1.96	0.47
1:G:405:SER:O	1:G:409:VAL:HG23	2.15	0.47
1:J:130[B]:ASN:ND2	8:J:694:HOH:O	2.47	0.47
1:K:95:VAL:HG13	1:K:120:THR:HG22	1.97	0.47
1:K:263:GLY:CA	1:K:296:THR:HG21	2.44	0.47
1:A:240:GLU:HB2	1:A:264:ASP:HB2	1.95	0.47
1:E:269:ILE:HG23	1:E:273:LYS:HB2	1.97	0.47
1:E:490:ASN:H	1:E:490:ASN:HD22	1.62	0.47
1:H:24:ILE:HB	1:H:328:MET:HG3	1.95	0.47
1:I:207:MET:HE2	1:I:234:MET:CE	2.44	0.47
1:N:338:TYR:HB3	1:N:341:GLU:HB2	1.97	0.47
1:P:26:THR:CG2	1:P:49:ARG:HH11	2.28	0.47
1:F:396:MET:HE2	1:F:416:CYS:SG	2.55	0.47
1:H:299:LEU:HD23	1:H:312:GLU:HB3	1.96	0.47
1:O:453:LYS:HE3	1:O:481:ALA:HB1	1.96	0.47
1:P:299:LEU:HD12	1:P:329:LEU:HD21	1.97	0.47
1:D:451:GLU:CD	1:D:451:GLU:N	2.71	0.47
1:E:263:GLY:CA	1:E:296:THR:HG21	2.45	0.47
1:N:198:GLN:HE21	1:N:202:GLU:HG3	1.80	0.47
1:A:26:THR:HG23	1:A:329:LEU:O	2.14	0.47
1:C:17:ASN:HD22	1:C:17:ASN:H	1.63	0.47
1:G:186:LEU:HB3	8:G:611:HOH:O	2.15	0.47
1:G:302:MET:HE3	1:G:342:VAL:HG23	1.97	0.47
1:H:79:ALA:HB2	1:H:429:ARG:O	2.15	0.47
1:F:397:VAL:HB	1:F:478:VAL:HG22	1.97	0.46
1:I:402:THR:OG1	1:I:404:ARG:HB2	2.14	0.46
1:B:10:SER:HB3	1:B:13:ASP:CG	2.41	0.46
1:H:26:THR:HG21	1:H:49:ARG:HH11	1.79	0.46
1:N:79:ALA:HB2	1:N:429:ARG:O	2.16	0.46
1:P:256:ASP:O	1:P:291:PRO:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ALA:HB1	1:A:254:GLU:HG3	1.97	0.46
1:C:248:ILE:HG12	1:C:281:LEU:HD22	1.98	0.46
1:D:89:ILE:HG22	1:D:177:VAL:HG13	1.97	0.46
1:D:404:ARG:HD3	8:D:628:HOH:O	2.14	0.46
1:G:143:ILE:HB	1:G:148:LEU:HB3	1.97	0.46
1:G:261:ALA:O	1:G:265:LEU:HB2	2.16	0.46
1:H:142:TYR:O	1:H:177:VAL:HA	2.15	0.46
1:F:56:SER:H	1:F:59:TYR:HB3	1.81	0.46
1:G:374:MET:CE	1:G:379:ALA:HA	2.45	0.46
1:I:144:ASP:HB2	1:I:175:ARG:HG3	1.98	0.46
1:D:10:SER:HB3	1:D:13:ASP:OD1	2.15	0.46
1:E:310:ARG:H	1:G:297:GLN:NE2	2.12	0.46
1:K:172:SER:O	1:K:175:ARG:HD3	2.16	0.46
1:E:297:GLN:HE21	1:G:309:THR:HB	1.81	0.46
1:G:260:VAL:HG22	1:G:281:LEU:HD12	1.96	0.46
1:M:388:VAL:HG21	1:M:396:MET:HE2	1.97	0.46
1:C:51:ASN:HA	1:C:83:ASP:HB3	1.97	0.46
1:E:494:ILE:HD12	1:F:380:VAL:HG23	1.98	0.46
1:L:298:MET:HE1	1:L:327:VAL:CB	2.45	0.46
1:A:188:ALA:HB1	1:A:218:GLN:HG3	1.98	0.46
1:D:384:ALA:HB2	1:D:492:THR:HG21	1.98	0.46
1:F:131:LEU:HA	1:F:134:VAL:HB	1.98	0.46
1:B:405:SER:O	1:B:409:VAL:HG23	2.16	0.46
1:D:24:ILE:HG21	1:D:328:MET:HE2	1.97	0.46
1:E:172:SER:O	1:E:175:ARG:HD3	2.16	0.46
1:F:302:MET:HE3	1:F:342:VAL:HG23	1.98	0.46
1:O:392:LYS:HE2	1:P:372:ILE:HG22	1.98	0.46
1:H:47:VAL:HG22	1:H:79:ALA:HB3	1.98	0.46
1:K:443:ASP:OD2	1:K:446:LYS:HE2	2.16	0.46
1:B:374:MET:HE3	1:B:379:ALA:CA	2.46	0.45
1:C:249:ASP:OD1	1:C:284:LYS:NZ	2.45	0.45
1:E:138:GLY:HA2	1:E:151:GLN:HE21	1.81	0.45
1:K:294:CYS:O	1:K:298:MET:HE2	2.16	0.45
1:L:242:HIS:HD2	8:L:662:HOH:O	1.99	0.45
1:M:17:ASN:HD22	1:M:17:ASN:N	2.13	0.45
1:H:298:MET:HE1	1:H:327:VAL:CB	2.47	0.45
1:I:26:THR:HG23	1:I:330:SER:HA	1.98	0.45
1:M:141:ILE:HB	1:M:150:LEU:HB2	1.97	0.45
1:N:292:VAL:HG13	1:N:324:ALA:HA	1.98	0.45
1:P:79:ALA:HB2	1:P:429:ARG:O	2.17	0.45
1:P:293:ILE:HG12	1:P:326:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:GLY:C	1:C:453:LYS:HG2	2.41	0.45
1:G:26:THR:HG23	1:G:329:LEU:O	2.16	0.45
1:A:396:MET:HE1	1:A:414:PRO:CB	2.45	0.45
1:A:396:MET:CE	1:A:414:PRO:HG3	2.34	0.45
1:D:304:TYR:HA	1:D:337:LYS:HD3	1.97	0.45
1:H:17:ASN:N	1:H:17:ASN:HD22	2.12	0.45
1:I:143:ILE:HB	1:I:148:LEU:HB3	1.98	0.45
1:K:339:PRO:O	1:K:342:VAL:HG12	2.15	0.45
1:M:299:LEU:HD23	1:M:312:GLU:HB3	1.98	0.45
1:G:209:PHE:HB3	1:G:238:LYS:HD2	1.98	0.45
1:A:299:LEU:HD23	1:A:312:GLU:HB3	1.97	0.45
1:H:175:ARG:NH2	6:H:1001:ATP:O3'	2.48	0.45
1:H:338:TYR:HB3	1:H:341:GLU:HB2	1.97	0.45
1:I:171:ILE:HB	1:I:175:ARG:HG2	1.98	0.45
1:P:82:LEU:HB3	1:P:208:ILE:HD13	1.99	0.45
1:B:443:ASP:HB3	1:B:446:LYS:HG2	1.99	0.45
1:N:398:VAL:HG12	1:N:479:ILE:HB	1.99	0.45
1:P:188:ALA:HB1	1:P:218:GLN:HG3	1.98	0.45
1:P:374:MET:HE3	1:P:379:ALA:HA	1.98	0.45
1:D:487:GLY:HA2	1:I:229:LYS:CG	2.45	0.45
1:F:171:ILE:HB	1:F:175:ARG:HG2	1.99	0.45
1:H:298:MET:HE1	1:H:327:VAL:HB	1.99	0.45
1:J:50:MET:SD	1:J:64:ILE:HG13	2.57	0.45
1:A:265:LEU:HD22	1:A:269:ILE:HG12	1.99	0.45
1:E:339:PRO:O	1:E:342:VAL:HG12	2.17	0.45
1:N:398:VAL:CG1	1:N:409:VAL:HG21	2.45	0.45
1:B:264:ASP:O	1:B:268:GLU:HB2	2.17	0.44
1:D:396:MET:HE3	1:D:396:MET:HB2	1.67	0.44
1:G:293:ILE:HG21	1:G:328:MET:HE3	1.98	0.44
1:J:214:ARG:HG2	1:J:218:GLN:OE1	2.17	0.44
1:N:481:ALA:HA	1:N:490:ASN:HD22	1.82	0.44
1:C:482:ASP:H	1:C:490:ASN:HD21	1.64	0.44
1:F:310:ARG:HG2	1:H:297:GLN:NE2	2.32	0.44
1:F:380:VAL:HG13	1:F:492:THR:HG22	2.00	0.44
1:G:112:ASP:HA	1:G:113:PRO:HD3	1.81	0.44
1:G:269:ILE:HG23	1:G:273:LYS:HB2	1.99	0.44
1:G:370:GLN:HG3	1:G:412:TYR:OH	2.16	0.44
1:J:309:THR:OG1	1:J:312:GLU:HG3	2.17	0.44
1:L:400:SER:HB2	1:L:405:SER:HB2	1.98	0.44
1:E:302:MET:HE1	1:E:345:TYR:HB3	1.99	0.44
1:F:396:MET:HE3	1:F:396:MET:HB2	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ILE:HG12	1:J:47:VAL:HB	1.98	0.44
1:A:92:GLY:H	1:A:174:ARG:HA	1.83	0.44
1:C:15:VAL:HB	1:C:351:LEU:HD22	1.99	0.44
1:L:221:ASP:HA	1:L:224:LYS:HE2	1.98	0.44
1:M:429:ARG:O	1:M:432:ASN:HB2	2.17	0.44
1:P:26:THR:HG21	1:P:49:ARG:NH1	2.31	0.44
1:D:405:SER:O	1:D:409:VAL:HG23	2.18	0.44
1:J:293:ILE:HG21	1:J:328:MET:HE3	2.00	0.44
1:B:296:THR:HG22	1:B:297:GLN:HG3	1.98	0.44
1:L:18:TYR:CD2	1:L:417:PRO:HG3	2.52	0.44
1:L:277:ALA:O	1:L:281:LEU:HG	2.17	0.44
1:P:479:ILE:HG12	1:P:492:THR:HG22	1.99	0.44
1:E:51:ASN:HA	1:E:83:ASP:HB3	2.00	0.44
1:G:380:VAL:HG13	1:G:492:THR:CG2	2.48	0.44
1:H:339:PRO:O	1:H:343:VAL:HG23	2.18	0.44
1:L:188:ALA:HB1	1:L:218:GLN:HG3	2.00	0.44
1:L:265:LEU:HD22	1:L:269:ILE:HG12	1.99	0.44
1:M:374:MET:HE3	1:M:379:ALA:CA	2.48	0.44
1:E:26:THR:CG2	1:E:49:ARG:HD3	2.42	0.44
1:F:204:GLY:HA3	8:F:711:HOH:O	2.18	0.44
1:F:240:GLU:HB2	1:F:264:ASP:CB	2.47	0.44
1:I:259:MET:HE2	1:I:328:MET:HE1	1.98	0.44
1:M:240:GLU:HB2	1:M:264:ASP:HB2	1.99	0.44
1:M:286:ASN:HB3	1:M:366:ILE:HD11	2.00	0.44
1:C:115:PHE:CE2	1:C:123:LYS:HD3	2.53	0.43
1:J:261:ALA:O	1:J:265:LEU:HB2	2.18	0.43
1:J:398[A]:VAL:HG11	1:J:409:VAL:CG2	2.36	0.43
1:L:214:ARG:HG2	1:L:218:GLN:OE1	2.18	0.43
1:N:23:ILE:HG21	1:N:343:VAL:HG13	1.99	0.43
1:O:482:ASP:HB3	1:O:491:GLN:NE2	2.33	0.43
1:A:51:ASN:ND2	6:A:1001:ATP:O3A	2.51	0.43
1:B:49:ARG:NH1	8:B:1882:HOH:O	2.48	0.43
1:E:149:ILE:H	1:E:167:ASN:HD21	1.66	0.43
1:F:380:VAL:HG21	1:F:490:ASN:HA	2.00	0.43
1:K:400:SER:HB2	1:K:405:SER:HB2	2.00	0.43
1:M:302:MET:HE3	1:M:342:VAL:HG23	2.00	0.43
1:M:339:PRO:O	1:M:342:VAL:HG12	2.18	0.43
1:E:234:MET:HE2	1:E:430:GLN:HG2	2.01	0.43
1:F:256:ASP:O	1:F:291:PRO:HD2	2.17	0.43
1:G:15:VAL:HB	1:G:351:LEU:HD22	1.99	0.43
1:I:198:GLN:OE1	1:I:198:GLN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:404:ARG:NH2	5:I:700:FDP:O6P	2.51	0.43
1:J:149:ILE:H	1:J:167:ASN:HD21	1.65	0.43
1:M:13:ASP:HA	1:M:14:PRO:HD3	1.89	0.43
1:F:296:THR:HG22	1:F:297:GLN:HG3	2.00	0.43
1:M:248:ILE:HG12	1:M:281:LEU:HD22	2.00	0.43
1:O:452:GLY:C	1:O:453:LYS:HG2	2.44	0.43
1:B:24:ILE:HG12	1:B:47:VAL:HB	2.00	0.43
1:B:339:PRO:O	1:B:342:VAL:HG12	2.18	0.43
1:H:302:MET:HE2	1:H:308:PRO:HB3	2.00	0.43
1:I:214:ARG:HB2	1:I:243:GLN:HG3	2.00	0.43
1:I:374:MET:HE3	1:I:378:GLU:HG2	1.99	0.43
1:K:293:ILE:HG12	1:K:326:CYS:HB2	2.00	0.43
1:L:396:MET:HE1	1:L:414:PRO:HB2	2.00	0.43
1:P:47:VAL:HG13	1:P:79:ALA:HB3	2.00	0.43
1:K:175:ARG:HD2	1:K:175:ARG:N	2.34	0.43
1:C:446:LYS:HG3	1:C:447:LEU:HG	2.01	0.43
1:I:298:MET:HE1	1:I:327:VAL:HB	2.01	0.43
1:L:112:ASP:HA	1:L:113:PRO:HD3	1.80	0.43
1:N:209:PHE:HD1	1:N:236:ILE:HB	1.84	0.43
1:P:241:ASN:HA	1:P:268:GLU:HG2	2.01	0.43
1:B:51:ASN:HA	1:B:83:ASP:HB3	2.01	0.43
1:B:79:ALA:HB2	1:B:429:ARG:O	2.18	0.43
5:D:700:FDP:O3P	5:D:700:FDP:O1	2.30	0.43
1:I:29:PRO:HA	8:I:637:HOH:O	2.18	0.43
1:J:214:ARG:HB2	1:J:243:GLN:HG3	2.01	0.43
1:J:325:ASP:HA	1:J:435:GLN:HB2	2.01	0.43
1:J:396:MET:HE1	1:J:414:PRO:HB3	2.00	0.43
1:L:216:ALA:HB1	1:L:254:GLU:HG3	1.99	0.43
1:A:143:ILE:HD13	1:A:177:VAL:HB	2.01	0.43
1:B:108:TYR:O	1:B:123:LYS:HA	2.19	0.43
1:E:26:THR:HG23	1:E:330:SER:HA	2.00	0.43
1:E:380:VAL:HG21	1:E:490:ASN:HA	2.01	0.43
1:B:242:HIS:CE1	1:D:12:PHE:HE1	2.37	0.43
1:B:298:MET:HE1	1:B:328:MET:N	2.27	0.43
1:D:302:MET:HE2	1:D:308:PRO:HB3	2.01	0.43
1:F:293:ILE:HG21	1:F:328:MET:HE3	2.00	0.43
1:G:390:GLU:HB3	1:H:374:MET:HE2	2.00	0.43
1:F:237:CYS:HB2	1:F:258:ILE:HD13	2.00	0.42
1:F:478:VAL:HG21	1:F:495:LEU:HD22	2.01	0.42
1:H:299:LEU:HD12	1:H:329:LEU:HD21	2.01	0.42
1:K:302:MET:HE2	1:K:308:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:380:VAL:HG13	1:P:492:THR:HG23	2.02	0.42
1:B:216:ALA:HB1	1:B:254:GLU:HG3	2.01	0.42
1:B:223:ARG:NH1	8:B:982:HOH:O	2.52	0.42
1:C:299:LEU:HD23	1:C:312:GLU:HB3	2.01	0.42
1:D:299:LEU:HD13	1:D:302:MET:HE3	2.00	0.42
1:D:374:MET:HE3	1:D:379:ALA:CA	2.48	0.42
1:G:175:ARG:NH1	6:G:1001:ATP:O3'	2.52	0.42
1:I:374:MET:CE	1:I:379:ALA:CA	2.94	0.42
1:K:402:THR:OG1	1:K:404:ARG:HB2	2.19	0.42
1:B:49:ARG:NH2	8:B:1882:HOH:O	2.27	0.42
1:B:285:CYS:HB3	1:B:290:LYS:O	2.19	0.42
1:G:259:MET:HG3	1:G:293:ILE:HB	2.00	0.42
1:K:302:MET:HE1	1:K:345:TYR:CB	2.49	0.42
1:A:10:SER:HB3	1:A:13:ASP:OD1	2.20	0.42
1:B:425:LEU:HD13	1:B:441:PHE:CG	2.54	0.42
1:I:367:LYS:HD3	1:J:390:GLU:OE2	2.20	0.42
1:L:363:PHE:HB2	1:L:412:TYR:O	2.19	0.42
1:L:452:GLY:C	1:L:453:LYS:HG2	2.45	0.42
1:M:261:ALA:HB1	4:M:510:OXL:C1	2.49	0.42
1:B:87:PRO:HB2	8:B:868:HOH:O	2.18	0.42
1:C:237:CYS:HB2	1:C:258:ILE:HD13	2.01	0.42
1:C:298:MET:HE3	1:C:328:MET:H	1.84	0.42
1:L:302:MET:CE	1:L:342:VAL:HA	2.49	0.42
1:F:91:THR:O	1:F:174:ARG:HA	2.20	0.42
1:G:396:MET:HB2	1:G:396:MET:HE3	1.60	0.42
1:L:111:THR:CG2	1:L:129:GLN:HA	2.50	0.42
1:N:359:GLU:HB3	1:N:389:TYR:OH	2.19	0.42
1:P:41:ILE:HG21	1:P:76:VAL:HG21	2.01	0.42
1:B:299:LEU:HD13	1:B:302:MET:CE	2.50	0.42
1:C:24:ILE:HG12	1:C:47:VAL:HB	2.01	0.42
1:E:248:ILE:HG12	1:E:281:LEU:HD22	2.01	0.42
1:G:89:ILE:HG22	1:G:177:VAL:HG13	2.01	0.42
1:I:17:ASN:HB3	8:I:798:HOH:O	2.19	0.42
1:K:54:HIS:HE1	6:K:1001:ATP:O2B	2.02	0.42
1:E:240:GLU:HB3	1:E:261:ALA:HB3	2.01	0.42
1:E:256:ASP:O	1:E:291:PRO:HD2	2.20	0.42
1:G:471:GLN:HE21	1:G:471:GLN:HB2	1.69	0.42
1:J:399:LEU:HG	1:J:480:HIS:HB3	2.02	0.42
1:L:17:ASN:C	1:L:17:ASN:HD22	2.27	0.42
1:M:175:ARG:HE	1:M:175:ARG:CA	2.32	0.42
1:O:240:GLU:HB2	1:O:264:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:MET:HE3	1:A:379:ALA:CA	2.43	0.42
1:E:173:ASP:O	1:E:175:ARG:NH1	2.52	0.42
1:H:20:ALA:HB1	1:H:435:GLN:HG2	2.02	0.42
1:N:144:ASP:N	1:N:176:GLY:O	2.52	0.42
1:D:171:ILE:HB	1:D:175:ARG:HG2	2.02	0.42
1:G:258:ILE:HB	1:G:285:CYS:SG	2.59	0.42
1:B:307:ARG:HB2	1:B:308:PRO:HD2	2.02	0.41
1:K:144:ASP:HB2	1:K:175:ARG:HG3	2.03	0.41
1:K:171:ILE:HB	1:K:175:ARG:HG2	2.02	0.41
1:A:481:ALA:HA	1:A:490:ASN:HD22	1.85	0.41
1:B:429:ARG:O	1:B:432:ASN:HB2	2.19	0.41
1:D:89:ILE:HG12	1:D:128:TYR:HB2	2.02	0.41
1:D:299:LEU:HD23	1:D:312:GLU:HB3	2.02	0.41
1:H:377:ASP:HB3	1:H:488:TYR:HB2	2.02	0.41
1:K:302:MET:HE1	1:K:345:TYR:HB3	2.02	0.41
1:L:374:MET:CE	1:L:379:ALA:CA	2.94	0.41
1:C:143:ILE:HD13	1:C:177:VAL:HB	2.02	0.41
1:D:298:MET:HE3	1:D:346:MET:HE1	2.01	0.41
6:D:1001:ATP:H5'1	6:D:1001:ATP:C8	2.48	0.41
1:F:109:VAL:HG23	1:F:161:LEU:HB2	2.01	0.41
1:H:89:ILE:HG23	1:H:128:TYR:HB2	2.02	0.41
1:H:366:ILE:HD13	1:H:411:LYS:O	2.20	0.41
1:K:79:ALA:HB2	1:K:429:ARG:O	2.20	0.41
1:A:298:MET:CE	1:A:328:MET:H	2.34	0.41
1:G:380:VAL:HG13	1:G:492:THR:HG23	2.02	0.41
1:H:50:MET:SD	1:H:64:ILE:HG13	2.60	0.41
1:I:237:CYS:SG	1:I:255:SER:HB3	2.60	0.41
1:J:130[B]:ASN:H	1:J:130[B]:ASN:HD22	1.68	0.41
1:L:396:MET:HE2	1:L:416:CYS:SG	2.60	0.41
1:M:472:THR:HG23	1:M:498:GLU:HA	2.02	0.41
1:N:87:PRO:HD2	1:N:212:PHE:HB2	2.03	0.41
1:P:179:LEU:HA	1:P:180:PRO:HD3	1.89	0.41
1:A:282:ILE:HA	1:A:292:VAL:HG21	2.02	0.41
1:A:298:MET:HE1	1:A:327:VAL:HB	2.02	0.41
1:G:26:THR:HG22	1:G:49:ARG:HB3	2.03	0.41
1:J:86:GLY:O	1:J:88:GLU:N	2.53	0.41
1:O:298:MET:HG2	1:O:315:ASP:OD2	2.20	0.41
1:B:435:GLN:NE2	8:B:1233:HOH:O	2.41	0.41
1:C:372:ILE:HG23	1:C:373:PRO:HA	2.03	0.41
1:H:24:ILE:HG12	1:H:47:VAL:HB	2.02	0.41
1:I:2:GLN:NE2	8:I:683:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:HIS:ND1	1:I:269:ILE:HG22	2.35	0.41
1:N:265:LEU:O	1:N:269:ILE:HG22	2.21	0.41
1:B:11:ILE:O	1:D:273:LYS:HD2	2.21	0.41
1:E:302:MET:HA	1:E:305:ASN:O	2.21	0.41
1:H:237:CYS:HB2	1:H:258:ILE:HD13	2.03	0.41
1:L:451:GLU:O	1:L:453:LYS:HE2	2.20	0.41
1:M:240:GLU:HB3	1:M:261:ALA:HB3	2.02	0.41
1:N:172:SER:HB2	1:N:175:ARG:HH11	1.85	0.41
1:O:470:VAL:HB	1:O:497:VAL:HG21	2.03	0.41
1:E:374:MET:HE1	1:E:379:ALA:HA	2.02	0.41
1:F:15:VAL:HB	1:F:351:LEU:HD22	2.02	0.41
1:G:209:PHE:HD1	1:G:236:ILE:HB	1.85	0.41
1:H:263:GLY:CA	1:H:296:THR:HG21	2.51	0.41
1:H:399:LEU:HG	1:H:480:HIS:HB3	2.03	0.41
1:K:179:LEU:O	1:K:182:CYS:HB2	2.20	0.41
1:M:146:GLY:O	1:O:307:ARG:HD2	2.21	0.41
1:N:26:THR:HA	1:N:49:ARG:HB3	2.01	0.41
1:O:211:SER:HA	1:O:238:LYS:HB2	2.02	0.41
1:A:399:LEU:HG	1:A:480:HIS:HB3	2.02	0.41
1:D:377:ASP:HB3	1:D:488:TYR:CD1	2.56	0.41
1:G:26:THR:CG2	1:G:49:ARG:HD3	2.42	0.41
1:G:490:ASN:H	1:G:490:ASN:HD22	1.69	0.41
1:I:452:GLY:C	1:I:453:LYS:HG2	2.46	0.41
1:K:79:ALA:HB1	1:K:207:MET:HE3	2.01	0.41
1:K:87:PRO:HD2	1:K:212:PHE:HB2	2.03	0.41
1:K:294:CYS:O	1:K:298:MET:CE	2.69	0.41
1:L:56:SER:H	1:L:59:TYR:HB3	1.85	0.41
1:N:85:LYS:HE2	1:N:192:LYS:HD3	2.03	0.41
1:C:293:ILE:HG12	1:C:326:CYS:HB2	2.03	0.41
1:D:262:ARG:NH2	1:D:298:MET:HG2	2.36	0.41
5:D:700:FDP:O3P	5:D:700:FDP:C1	2.69	0.41
1:G:397:VAL:HB	1:G:478:VAL:HG22	2.02	0.41
1:J:148:LEU:HA	1:J:167:ASN:HD21	1.84	0.41
1:K:108:TYR:O	1:K:123:LYS:HA	2.21	0.41
1:M:112:ASP:HA	1:M:113:PRO:HD3	1.87	0.41
1:M:362:PHE:CD2	1:M:413:ARG:HG3	2.56	0.41
1:O:229:LYS:HE2	1:O:229:LYS:HA	2.03	0.41
1:P:13:ASP:HA	1:P:14:PRO:HD3	1.94	0.41
1:B:248:ILE:O	1:B:252:ILE:HG13	2.20	0.40
1:D:26:THR:HG22	1:D:49:ARG:HD3	2.03	0.40
1:D:299:LEU:HD13	1:D:302:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:SER:HB2	1:E:405:SER:HB2	2.03	0.40
1:F:310:ARG:H	1:H:297:GLN:NE2	2.15	0.40
1:I:114:ALA:O	1:I:118:LYS:HE2	2.20	0.40
1:J:474:ASP:O	1:J:497:VAL:HG13	2.20	0.40
1:K:390:GLU:HB3	1:L:374:MET:HE2	2.02	0.40
1:L:299:LEU:HD12	1:L:329:LEU:HD21	2.02	0.40
1:L:374:MET:HE3	1:L:379:ALA:HA	1.96	0.40
1:N:298:MET:CE	1:N:328:MET:H	2.34	0.40
1:N:396:MET:HE1	1:N:414:PRO:CB	2.51	0.40
1:O:237:CYS:SG	1:O:255:SER:HB3	2.61	0.40
1:P:24:ILE:HG21	1:P:328:MET:HE2	2.03	0.40
1:B:34:VAL:O	1:B:38:LYS:HG3	2.21	0.40
1:C:56:SER:H	1:C:59:TYR:HB3	1.86	0.40
1:C:213:ILE:HA	1:C:218:GLN:OE1	2.20	0.40
1:D:115:PHE:CE2	1:D:123:LYS:HD3	2.56	0.40
6:D:1001:ATP:O1G	6:D:1001:ATP:O1A	2.40	0.40
1:F:24:ILE:HG12	1:F:47:VAL:HB	2.03	0.40
1:F:396:MET:CE	1:F:414:PRO:HG3	2.48	0.40
1:G:396:MET:HE1	1:G:414:PRO:HB2	2.01	0.40
1:H:260:VAL:HG22	1:H:281:LEU:HD12	2.02	0.40
1:K:263:GLY:HA3	1:K:296:THR:HG21	2.02	0.40
1:M:136:ARG:HB3	1:M:137:PRO:CD	2.51	0.40
1:O:261:ALA:O	1:O:265:LEU:HB2	2.21	0.40
1:P:26:THR:HG22	1:P:49:ARG:HD3	2.03	0.40
1:P:378:GLU:HA	1:P:408:LEU:HD21	2.02	0.40
1:E:26:THR:CG2	1:E:49:ARG:HH11	2.34	0.40
1:C:24:ILE:HG21	1:C:328:MET:HE2	2.03	0.40
1:H:402:THR:HG22	1:H:424:ARG:NH2	2.36	0.40
1:H:17:ASN:HD22	1:H:17:ASN:H	1.67	0.40
1:J:175:ARG:NH2	8:J:634:HOH:O	2.54	0.40
1:J:188:ALA:HB1	1:J:218:GLN:HG3	2.04	0.40
1:N:302:MET:HE1	1:N:345:TYR:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/499 (100%)	481 (97%)	14 (3%)	3 (1%)	21	27
1	B	496/499 (99%)	486 (98%)	8 (2%)	2 (0%)	30	38
1	C	498/499 (100%)	482 (97%)	15 (3%)	1 (0%)	43	55
1	D	497/499 (100%)	483 (97%)	14 (3%)	0	100	100
1	E	497/499 (100%)	477 (96%)	19 (4%)	1 (0%)	43	55
1	F	496/499 (99%)	480 (97%)	14 (3%)	2 (0%)	30	38
1	G	496/499 (99%)	465 (94%)	27 (5%)	4 (1%)	16	20
1	H	498/499 (100%)	477 (96%)	20 (4%)	1 (0%)	43	55
1	I	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	43	55
1	J	499/499 (100%)	483 (97%)	15 (3%)	1 (0%)	43	55
1	K	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	43	55
1	L	496/499 (99%)	477 (96%)	18 (4%)	1 (0%)	43	55
1	M	496/499 (99%)	472 (95%)	20 (4%)	4 (1%)	16	20
1	N	497/499 (100%)	476 (96%)	20 (4%)	1 (0%)	43	55
1	O	496/499 (99%)	466 (94%)	27 (5%)	3 (1%)	21	27
1	P	496/499 (99%)	469 (95%)	25 (5%)	2 (0%)	30	38
All	All	7952/7984 (100%)	7646 (96%)	278 (4%)	28 (0%)	30	38

All (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
1	P	137	PRO
1	B	296	THR
1	F	183	ASP
1	F	377	ASP
1	G	482	ASP
1	M	174	ARG
1	A	296	THR

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Mol	Chain	Res	Type
1	E	296	THR
1	G	174	ARG
1	G	296	THR
1	K	296	THR
1	L	296	THR
1	M	296	THR
1	N	296	THR
1	B	183	ASP
1	C	296	THR
1	H	296	THR
1	M	183	ASP
1	P	296	THR
1	M	97	GLY
1	A	44	GLY
1	O	137	PRO
1	G	44	GLY

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%)	401 (96%)	17 (4%)	27	41
1	B	416/417 (100%)	394 (95%)	22 (5%)	20	30
1	C	418/417 (100%)	401 (96%)	17 (4%)	27	41
1	D	417/417 (100%)	395 (95%)	22 (5%)	20	30
1	E	417/417 (100%)	393 (94%)	24 (6%)	18	26
1	F	416/417 (100%)	398 (96%)	18 (4%)	26	39
1	G	416/417 (100%)	393 (94%)	23 (6%)	19	28
1	H	418/417 (100%)	397 (95%)	21 (5%)	22	33
1	I	418/417 (100%)	389 (93%)	29 (7%)	14	20
1	J	419/417 (100%)	397 (95%)	22 (5%)	20	30
1	K	418/417 (100%)	391 (94%)	27 (6%)	15	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	416/417 (100%)	399 (96%)	17 (4%)	27	41
1	M	416/417 (100%)	395 (95%)	21 (5%)	22	33
1	N	417/417 (100%)	399 (96%)	18 (4%)	26	39
1	O	416/417 (100%)	401 (96%)	15 (4%)	31	47
1	P	416/417 (100%)	403 (97%)	13 (3%)	35	52
All	All	6672/6672 (100%)	6346 (95%)	326 (5%)	22	34

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	ASN
1	A	40	LEU
1	A	84	THR
1	A	175	ARG
1	A	177	VAL
1	A	265	LEU
1	A	304	TYR
1	A	314	SER
1	A	351	LEU
1	A	367	LYS
1	A	368	LYS
1	A	396	MET
1	A	454	GLU
1	A	471	GLN
1	A	490	ASN
1	A	495	LEU
1	B	17	ASN
1	B	26	THR
1	B	34	VAL
1	B	40	LEU
1	B	106	THR
1	B	130	ASN
1	B	143	ILE
1	B	177	VAL
1	B	179	LEU
1	B	229	LYS
1	B	240	GLU
1	B	265	LEU
1	B	267	VAL

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Mol	Chain	Res	Type
1	B	307	ARG
1	B	367	LYS
1	B	368	LYS
1	B	398	VAL
1	B	425	LEU
1	B	454	GLU
1	B	471	GLN
1	B	490	ASN
1	B	493	ARG
1	C	17	ASN
1	C	40	LEU
1	C	106	THR
1	C	175	ARG
1	C	177	VAL
1	C	179	LEU
1	C	189	VAL
1	C	265	LEU
1	C	298	MET
1	C	351	LEU
1	C	367	LYS
1	C	451[A]	GLU
1	C	451[B]	GLU
1	C	490	ASN
1	C	493	ARG
1	C	495	LEU
1	C	497	VAL
1	D	3	LEU
1	D	17	ASN
1	D	26	THR
1	D	40	LEU
1	D	106	THR
1	D	143	ILE
1	D	174	ARG
1	D	175	ARG
1	D	177	VAL
1	D	229	LYS
1	D	265	LEU
1	D	281	LEU
1	D	304	TYR
1	D	351	LEU
1	D	367	LYS
1	D	368	LYS

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Mol	Chain	Res	Type
1	D	391	THR
1	D	398	VAL
1	D	404	ARG
1	D	451	GLU
1	D	471	GLN
1	D	490	ASN
1	E	3	LEU
1	E	17	ASN
1	E	26	THR
1	E	34	VAL
1	E	40	LEU
1	E	175	ARG
1	E	177	VAL
1	E	189	VAL
1	E	224	LYS
1	E	265	LEU
1	E	267	VAL
1	E	269	ILE
1	E	304	TYR
1	E	307	ARG
1	E	345	TYR
1	E	351	LEU
1	E	367	LYS
1	E	368	LYS
1	E	391	THR
1	E	404	ARG
1	E	465	LYS
1	E	490	ASN
1	E	493	ARG
1	E	495	LEU
1	F	17	ASN
1	F	111	THR
1	F	153	GLN
1	F	175	ARG
1	F	177	VAL
1	F	213	ILE
1	F	214	ARG
1	F	267	VAL
1	F	351	LEU
1	F	367	LYS
1	F	368	LYS
1	F	396	MET

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Mol	Chain	Res	Type
1	F	398	VAL
1	F	454	GLU
1	F	490	ASN
1	F	492	THR
1	F	493	ARG
1	F	497	VAL
1	G	3	LEU
1	G	17	ASN
1	G	157	ASP
1	G	177	VAL
1	G	265	LEU
1	G	267	VAL
1	G	269	ILE
1	G	298	MET
1	G	345	TYR
1	G	351	LEU
1	G	367	LYS
1	G	368	LYS
1	G	391	THR
1	G	396	MET
1	G	409	VAL
1	G	434	THR
1	G	435	GLN
1	G	451	GLU
1	G	454	GLU
1	G	471	GLN
1	G	490	ASN
1	G	495	LEU
1	G	497	VAL
1	H	3	LEU
1	H	17	ASN
1	H	26	THR
1	H	40	LEU
1	H	84	THR
1	H	175	ARG
1	H	177	VAL
1	H	179	LEU
1	H	265	LEU
1	H	269	ILE
1	H	304	TYR
1	H	345	TYR
1	H	351	LEU

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Mol	Chain	Res	Type
1	H	367	LYS
1	H	368	LYS
1	H	396	MET
1	H	435	GLN
1	H	471	GLN
1	H	490	ASN
1	H	495	LEU
1	H	497	VAL
1	I	3	LEU
1	I	17	ASN
1	I	26	THR
1	I	31	THR
1	I	34	VAL
1	I	40	LEU
1	I	106	THR
1	I	111	THR
1	I	158	GLU
1	I	175	ARG
1	I	177	VAL
1	I	189	VAL
1	I	229	LYS
1	I	242	HIS
1	I	265	LEU
1	I	268	GLU
1	I	335	LYS
1	I	345	TYR
1	I	351	LEU
1	I	367	LYS
1	I	368	LYS
1	I	398[A]	VAL
1	I	398[B]	VAL
1	I	425	LEU
1	I	451	GLU
1	I	471	GLN
1	I	492	THR
1	I	495	LEU
1	I	497	VAL
1	J	3	LEU
1	J	17	ASN
1	J	26	THR
1	J	34	VAL
1	J	106	THR

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Mol	Chain	Res	Type
1	J	111	THR
1	J	121	LYS
1	J	134	VAL
1	J	175	ARG
1	J	177	VAL
1	J	179	LEU
1	J	195	VAL
1	J	265	LEU
1	J	304	TYR
1	J	351	LEU
1	J	367	LYS
1	J	368	LYS
1	J	424	ARG
1	J	425	LEU
1	J	454	GLU
1	J	492	THR
1	J	497	VAL
1	K	3	LEU
1	K	17	ASN
1	K	34	VAL
1	K	40	LEU
1	K	95	VAL
1	K	134	VAL
1	K	175	ARG
1	K	177	VAL
1	K	189	VAL
1	K	240	GLU
1	K	243	GLN
1	K	265	LEU
1	K	267	VAL
1	K	304	TYR
1	K	345	TYR
1	K	362	PHE
1	K	367	LYS
1	K	368	LYS
1	K	382	SER
1	K	391	THR
1	K	404	ARG
1	K	425	LEU
1	K	451	GLU
1	K	454	GLU
1	K	471	GLN

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Mol	Chain	Res	Type
1	K	495	LEU
1	K	497	VAL
1	L	3	LEU
1	L	17	ASN
1	L	34	VAL
1	L	35	GLU
1	L	40	LEU
1	L	111	THR
1	L	175	ARG
1	L	177	VAL
1	L	265	LEU
1	L	314	SER
1	L	345	TYR
1	L	355	SER
1	L	367	LYS
1	L	396	MET
1	L	425	LEU
1	L	493	ARG
1	L	497	VAL
1	M	3	LEU
1	M	17	ASN
1	M	26	THR
1	M	40	LEU
1	M	84	THR
1	M	167	ASN
1	M	175	ARG
1	M	177	VAL
1	M	189	VAL
1	M	265	LEU
1	M	269	ILE
1	M	367	LYS
1	M	368	LYS
1	M	391	THR
1	M	424	ARG
1	M	425	LEU
1	M	451	GLU
1	M	454	GLU
1	M	465	LYS
1	M	471	GLN
1	M	490	ASN
1	N	3	LEU
1	N	17	ASN

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Mol	Chain	Res	Type
1	N	175	ARG
1	N	177	VAL
1	N	231	ARG
1	N	265	LEU
1	N	307	ARG
1	N	359	GLU
1	N	367	LYS
1	N	368	LYS
1	N	391	THR
1	N	396	MET
1	N	398	VAL
1	N	404	ARG
1	N	454	GLU
1	N	465	LYS
1	N	484	LYS
1	N	490	ASN
1	O	3	LEU
1	O	17	ASN
1	O	153	GLN
1	O	175	ARG
1	O	177	VAL
1	O	265	LEU
1	O	269	ILE
1	O	296	THR
1	O	367	LYS
1	O	380	VAL
1	O	396	MET
1	O	424	ARG
1	O	435	GLN
1	O	451	GLU
1	O	490	ASN
1	P	3	LEU
1	P	17	ASN
1	P	84	THR
1	P	175	ARG
1	P	177	VAL
1	P	265	LEU
1	P	269	ILE
1	P	304	TYR
1	P	327	VAL
1	P	367	LYS
1	P	380	VAL

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Mol	Chain	Res	Type
1	P	474	ASP
1	P	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (209) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	65	ASN
1	A	167	ASN
1	A	178	ASN
1	A	203	GLN
1	A	286	ASN
1	A	297	GLN
1	A	322	ASN
1	A	386	ASN
1	A	471	GLN
1	A	490	ASN
1	B	5	HIS
1	B	17	ASN
1	B	42	GLN
1	B	93	GLN
1	B	139	ASN
1	B	155	HIS
1	B	167	ASN
1	B	242	HIS
1	B	243	GLN
1	B	297	GLN
1	B	305	ASN
1	B	318	ASN
1	B	322	ASN
1	B	344	GLN
1	B	386	ASN
1	B	490	ASN
1	B	491	GLN
1	C	17	ASN
1	C	54	HIS
1	C	77	ASN
1	C	93	GLN
1	C	139	ASN
1	C	243	GLN
1	C	286	ASN
1	C	297	GLN

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Mol	Chain	Res	Type
1	C	322	ASN
1	C	386	ASN
1	C	490	ASN
1	D	5	HIS
1	D	17	ASN
1	D	42	GLN
1	D	139	ASN
1	D	167	ASN
1	D	178	ASN
1	D	344	GLN
1	D	386	ASN
1	D	435	GLN
1	D	490	ASN
1	E	5	HIS
1	E	17	ASN
1	E	77	ASN
1	E	129	GLN
1	E	151	GLN
1	E	167	ASN
1	E	178	ASN
1	E	242	HIS
1	E	286	ASN
1	E	297	GLN
1	E	318	ASN
1	E	340	ASN
1	E	344	GLN
1	E	386	ASN
1	E	483	HIS
1	E	490	ASN
1	F	5	HIS
1	F	6	ASN
1	F	17	ASN
1	F	42	GLN
1	F	167	ASN
1	F	278	GLN
1	F	286	ASN
1	F	297	GLN
1	F	322	ASN
1	F	344	GLN
1	F	386	ASN
1	F	490	ASN
1	G	2	GLN

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Mol	Chain	Res	Type
1	G	51	ASN
1	G	57	HIS
1	G	93	GLN
1	G	129	GLN
1	G	139	ASN
1	G	167	ASN
1	G	286	ASN
1	G	297	GLN
1	G	305	ASN
1	G	322	ASN
1	G	340	ASN
1	G	344	GLN
1	G	371	HIS
1	G	386	ASN
1	G	401	ASN
1	G	471	GLN
1	G	490	ASN
1	H	5	HIS
1	H	17	ASN
1	H	93	GLN
1	H	151	GLN
1	H	167	ASN
1	H	286	ASN
1	H	297	GLN
1	H	344	GLN
1	H	364	ASN
1	H	386	ASN
1	H	401	ASN
1	H	490	ASN
1	H	491	GLN
1	I	5	HIS
1	I	6	ASN
1	I	17	ASN
1	I	32	GLN
1	I	93	GLN
1	I	167	ASN
1	I	286	ASN
1	I	297	GLN
1	I	305	ASN
1	I	344	GLN
1	I	401	ASN
1	I	435	GLN

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Mol	Chain	Res	Type
1	J	17	ASN
1	J	54	HIS
1	J	69	GLN
1	J	151	GLN
1	J	155	HIS
1	J	167	ASN
1	J	246	GLN
1	J	297	GLN
1	J	305	ASN
1	J	401	ASN
1	J	471	GLN
1	K	2	GLN
1	K	17	ASN
1	K	54	HIS
1	K	93	GLN
1	K	130	ASN
1	K	167	ASN
1	K	243	GLN
1	K	286	ASN
1	K	305	ASN
1	K	322	ASN
1	K	340	ASN
1	K	435	GLN
1	K	471	GLN
1	L	5	HIS
1	L	17	ASN
1	L	42	GLN
1	L	54	HIS
1	L	69	GLN
1	L	155	HIS
1	L	167	ASN
1	L	242	HIS
1	L	243	GLN
1	L	305	ASN
1	L	318	ASN
1	L	344	GLN
1	M	2	GLN
1	M	5	HIS
1	M	17	ASN
1	M	130	ASN
1	M	167	ASN
1	M	178	ASN

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Mol	Chain	Res	Type
1	M	278	GLN
1	M	286	ASN
1	M	297	GLN
1	M	305	ASN
1	M	322	ASN
1	M	340	ASN
1	M	386	ASN
1	M	401	ASN
1	M	490	ASN
1	N	5	HIS
1	N	17	ASN
1	N	42	GLN
1	N	51	ASN
1	N	54	HIS
1	N	139	ASN
1	N	155	HIS
1	N	167	ASN
1	N	198	GLN
1	N	242	HIS
1	N	243	GLN
1	N	286	ASN
1	N	305	ASN
1	N	344	GLN
1	N	386	ASN
1	N	401	ASN
1	N	471	GLN
1	N	490	ASN
1	O	6	ASN
1	O	17	ASN
1	O	42	GLN
1	O	167	ASN
1	O	278	GLN
1	O	286	ASN
1	O	322	ASN
1	O	386	ASN
1	O	401	ASN
1	O	480	HIS
1	O	490	ASN
1	O	491	GLN
1	P	5	HIS
1	P	17	ASN
1	P	178	ASN

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Mol	Chain	Res	Type
1	P	286	ASN
1	P	318	ASN
1	P	322	ASN
1	P	386	ASN
1	P	491	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
6	ATP	N	1001	3,2	32,33,33	1.59	7 (21%)	48,52,52	1.77	9 (18%)
5	FDP	F	700	-	19,20,20	1.19	2 (10%)	29,32,32	1.42	4 (13%)
6	ATP	E	1001	3,2	32,33,33	1.54	7 (21%)	48,52,52	1.77	9 (18%)
6	ATP	P	1001	3,2	32,33,33	1.50	6 (18%)	48,52,52	1.77	9 (18%)
6	ATP	K	1001	3,2	32,33,33	1.59	7 (21%)	48,52,52	1.72	9 (18%)
4	OXL	M	510	2	5,5,5	1.15	0	6,6,6	1.78	2 (33%)
6	ATP	J	1001	3,2	32,33,33	1.54	7 (21%)	48,52,52	1.82	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OXL	E	510	2	5,5,5	1.99	2 (40%)	6,6,6	1.51	2 (33%)
6	ATP	B	1001	3,2	32,33,33	1.50	7 (21%)	48,52,52	1.75	10 (20%)
4	OXL	L	510	2	5,5,5	0.77	0	6,6,6	2.14	4 (66%)
5	FDP	A	700	-	19,20,20	0.91	0	29,32,32	1.37	5 (17%)
5	FDP	O	700	-	19,20,20	1.05	0	29,32,32	1.02	1 (3%)
6	ATP	I	1001	3,2	32,33,33	1.52	5 (15%)	48,52,52	1.79	10 (20%)
6	ATP	G	1001	2	32,33,33	1.49	6 (18%)	48,52,52	1.70	8 (16%)
7	GOL	E	499	-	5,5,5	0.40	0	5,5,5	0.33	0
6	ATP	H	1001	3,2	32,33,33	1.53	7 (21%)	48,52,52	1.69	10 (20%)
5	FDP	B	700	-	19,20,20	1.53	3 (15%)	29,32,32	1.62	6 (20%)
6	ATP	A	1001	3,2	32,33,33	1.54	7 (21%)	48,52,52	1.71	7 (14%)
6	ATP	C	1001	3,2	32,33,33	1.60	6 (18%)	48,52,52	1.76	11 (22%)
7	GOL	J	499	-	5,5,5	0.37	0	5,5,5	0.35	0
5	FDP	M	700	-	19,20,20	0.75	0	29,32,32	1.15	3 (10%)
5	FDP	J	700	-	19,20,20	1.08	2 (10%)	29,32,32	1.40	5 (17%)
5	FDP	H	700	-	19,20,20	0.94	2 (10%)	29,32,32	1.44	4 (13%)
4	OXL	B	510	2	5,5,5	1.13	1 (20%)	6,6,6	2.36	3 (50%)
7	GOL	G	499	-	5,5,5	0.38	0	5,5,5	0.28	0
7	GOL	O	499	-	5,5,5	0.39	0	5,5,5	0.25	0
4	OXL	D	510	2	5,5,5	1.28	0	6,6,6	1.93	3 (50%)
6	ATP	L	1001	3,2	32,33,33	1.54	6 (18%)	48,52,52	1.69	10 (20%)
5	FDP	C	700	-	19,20,20	0.92	0	29,32,32	1.57	5 (17%)
6	ATP	M	1001	3,2	32,33,33	1.54	7 (21%)	48,52,52	1.70	10 (20%)
4	OXL	P	510	2	5,5,5	1.03	0	6,6,6	1.88	2 (33%)
4	OXL	K	510	2	5,5,5	2.28	2 (40%)	6,6,6	1.64	2 (33%)
5	FDP	D	700	-	19,20,20	1.14	1 (5%)	29,32,32	1.43	3 (10%)
4	OXL	F	510	2	5,5,5	1.12	0	6,6,6	1.87	2 (33%)
4	OXL	N	510	2	5,5,5	1.55	1 (20%)	6,6,6	1.61	2 (33%)
5	FDP	K	700	-	19,20,20	1.16	3 (15%)	29,32,32	1.51	8 (27%)
5	FDP	L	700	-	19,20,20	1.06	2 (10%)	29,32,32	1.48	4 (13%)
5	FDP	P	700	-	19,20,20	1.21	3 (15%)	29,32,32	0.84	1 (3%)
6	ATP	F	1001	3,2	32,33,33	1.61	7 (21%)	48,52,52	1.75	9 (18%)
5	FDP	E	700	-	19,20,20	1.23	2 (10%)	29,32,32	1.13	2 (6%)
4	OXL	I	510	2	5,5,5	2.38	2 (40%)	6,6,6	1.67	1 (16%)
7	GOL	I	499	-	5,5,5	0.37	0	5,5,5	0.31	0
5	FDP	N	700	-	19,20,20	1.16	2 (10%)	29,32,32	1.21	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	I	501	-	5,5,5	0.42	0	5,5,5	0.35	0
4	OXL	H	510	2	5,5,5	0.98	0	6,6,6	1.98	2 (33%)
5	FDP	I	700	-	19,20,20	1.63	3 (15%)	29,32,32	1.52	4 (13%)
4	OXL	J	510	2	5,5,5	1.29	1 (20%)	6,6,6	2.11	2 (33%)
4	OXL	A	510	2	5,5,5	1.44	1 (20%)	6,6,6	1.76	2 (33%)
4	OXL	C	510	2	5,5,5	1.53	1 (20%)	6,6,6	1.81	2 (33%)
4	OXL	G	510	2	5,5,5	1.39	1 (20%)	6,6,6	1.85	2 (33%)
6	ATP	D	1001	3,2	32,33,33	1.58	6 (18%)	48,52,52	1.76	11 (22%)
5	FDP	G	700	-	19,20,20	1.28	2 (10%)	29,32,32	1.34	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	N	1001	3,2	-	5/22/38/38	0/3/3/3
5	FDP	F	700	-	-	7/12/34/34	0/1/1/1
6	ATP	E	1001	3,2	-	4/22/38/38	0/3/3/3
6	ATP	P	1001	3,2	-	3/22/38/38	0/3/3/3
6	ATP	K	1001	3,2	-	3/22/38/38	0/3/3/3
4	OXL	M	510	2	-	0/4/4/4	-
6	ATP	J	1001	3,2	-	2/22/38/38	0/3/3/3
4	OXL	E	510	2	-	4/4/4/4	-
6	ATP	B	1001	3,2	-	3/22/38/38	0/3/3/3
4	OXL	L	510	2	-	0/4/4/4	-
5	FDP	A	700	-	-	3/12/34/34	0/1/1/1
5	FDP	O	700	-	-	8/12/34/34	0/1/1/1
6	ATP	I	1001	3,2	-	3/22/38/38	0/3/3/3
6	ATP	G	1001	2	-	5/22/38/38	0/3/3/3
7	GOL	E	499	-	-	2/4/4/4	-
6	ATP	H	1001	3,2	-	9/22/38/38	0/3/3/3
5	FDP	B	700	-	-	1/12/34/34	0/1/1/1
6	ATP	A	1001	3,2	-	7/22/38/38	0/3/3/3
6	ATP	C	1001	3,2	-	2/22/38/38	0/3/3/3
7	GOL	J	499	-	-	4/4/4/4	-
5	FDP	M	700	-	-	3/12/34/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FDP	J	700	-	-	1/12/34/34	0/1/1/1
5	FDP	H	700	-	-	2/12/34/34	0/1/1/1
4	OXL	B	510	2	-	4/4/4/4	-
7	GOL	G	499	-	-	0/4/4/4	-
7	GOL	O	499	-	-	4/4/4/4	-
4	OXL	D	510	2	-	0/4/4/4	-
6	ATP	L	1001	3,2	-	8/22/38/38	0/3/3/3
5	FDP	C	700	-	-	1/12/34/34	0/1/1/1
6	ATP	M	1001	3,2	-	4/22/38/38	0/3/3/3
4	OXL	P	510	2	-	0/4/4/4	-
4	OXL	K	510	2	-	0/4/4/4	-
5	FDP	D	700	-	-	1/12/34/34	0/1/1/1
4	OXL	F	510	2	-	0/4/4/4	-
4	OXL	N	510	2	-	4/4/4/4	-
5	FDP	K	700	-	-	0/12/34/34	0/1/1/1
5	FDP	L	700	-	-	2/12/34/34	0/1/1/1
5	FDP	P	700	-	-	7/12/34/34	0/1/1/1
6	ATP	F	1001	3,2	-	2/22/38/38	0/3/3/3
5	FDP	E	700	-	-	3/12/34/34	0/1/1/1
4	OXL	I	510	2	-	4/4/4/4	-
7	GOL	I	499	-	-	2/4/4/4	-
5	FDP	N	700	-	-	5/12/34/34	0/1/1/1
7	GOL	I	501	-	-	4/4/4/4	-
4	OXL	H	510	2	-	0/4/4/4	-
5	FDP	I	700	-	-	1/12/34/34	0/1/1/1
4	OXL	J	510	2	-	4/4/4/4	-
4	OXL	A	510	2	-	0/4/4/4	-
4	OXL	C	510	2	-	0/4/4/4	-
4	OXL	G	510	2	-	4/4/4/4	-
6	ATP	D	1001	3,2	-	6/22/38/38	0/3/3/3
5	FDP	G	700	-	-	0/12/34/34	0/1/1/1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1001	ATP	C5-C4	5.17	1.48	1.39
6	C	1001	ATP	C5-C4	5.14	1.48	1.39
6	M	1001	ATP	C5-C4	5.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	ATP	C5-C4	5.11	1.48	1.39
6	N	1001	ATP	C5-C4	5.08	1.48	1.39
6	D	1001	ATP	C5-C4	5.04	1.48	1.39
6	G	1001	ATP	C5-C4	5.00	1.48	1.39
6	F	1001	ATP	C5-C4	4.95	1.47	1.39
6	H	1001	ATP	C5-C4	4.95	1.47	1.39
6	E	1001	ATP	C5-C4	4.94	1.47	1.39
6	P	1001	ATP	C5-C4	4.92	1.47	1.39
6	I	1001	ATP	C5-C4	4.88	1.47	1.39
6	B	1001	ATP	C5-C4	4.76	1.47	1.39
6	J	1001	ATP	C5-C4	4.76	1.47	1.39
5	B	700	FDP	P2-O6	-4.63	1.45	1.60
6	K	1001	ATP	C5-C4	4.62	1.47	1.39
4	I	510	OXL	O3-C1	-4.54	1.18	1.30
5	I	700	FDP	P1-O2P	-3.97	1.40	1.54
6	K	1001	ATP	PB-O3B	3.93	1.63	1.59
6	B	1001	ATP	PB-O3B	3.42	1.63	1.59
4	K	510	OXL	O2-C2	3.41	1.31	1.22
6	C	1001	ATP	PB-O3A	3.30	1.63	1.59
5	I	700	FDP	O3-C3	-3.19	1.36	1.42
6	I	1001	ATP	PB-O3B	3.19	1.62	1.59
4	K	510	OXL	O4-C2	-3.13	1.22	1.30
5	E	700	FDP	P2-O6	-3.07	1.50	1.60
6	D	1001	ATP	PB-O3B	3.04	1.62	1.59
6	F	1001	ATP	PA-O3A	3.03	1.62	1.59
6	F	1001	ATP	PB-O3A	3.02	1.62	1.59
6	L	1001	ATP	C5-C6	3.01	1.49	1.41
6	N	1001	ATP	C5-C6	2.99	1.49	1.41
6	D	1001	ATP	C5-C6	2.95	1.49	1.41
6	F	1001	ATP	C5-C6	2.94	1.49	1.41
6	M	1001	ATP	C5-C6	2.94	1.49	1.41
5	G	700	FDP	O5-C2	2.92	1.48	1.42
6	A	1001	ATP	C5-C6	2.91	1.49	1.41
6	E	1001	ATP	C5-C6	2.90	1.49	1.41
5	I	700	FDP	P2-O6	-2.89	1.51	1.60
6	I	1001	ATP	C5-C6	2.88	1.49	1.41
5	D	700	FDP	O5-C5	2.88	1.50	1.43
6	G	1001	ATP	C5-C6	2.87	1.49	1.41
6	P	1001	ATP	C5-C6	2.87	1.49	1.41
6	J	1001	ATP	C5-C6	2.87	1.49	1.41
6	C	1001	ATP	C5-C6	2.86	1.49	1.41
6	N	1001	ATP	PA-O3A	2.86	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	ATP	PA-O3A	2.85	1.62	1.59
6	K	1001	ATP	C5-C6	2.85	1.48	1.41
4	E	510	OXL	O3-C1	-2.85	1.22	1.30
5	E	700	FDP	O5-C2	2.85	1.48	1.42
6	H	1001	ATP	C5-C6	2.84	1.48	1.41
6	K	1001	ATP	PB-O3A	2.84	1.62	1.59
4	E	510	OXL	O4-C2	-2.81	1.22	1.30
6	J	1001	ATP	PB-O3A	2.74	1.62	1.59
6	N	1001	ATP	PB-O3A	2.71	1.62	1.59
4	C	510	OXL	O2-C2	2.70	1.29	1.22
6	E	1001	ATP	PB-O3A	2.69	1.62	1.59
6	E	1001	ATP	PA-O3A	2.69	1.62	1.59
6	D	1001	ATP	PA-O3A	2.68	1.62	1.59
6	H	1001	ATP	PB-O3A	2.66	1.62	1.59
4	I	510	OXL	O1-C1	2.61	1.29	1.22
6	N	1001	ATP	PB-O3B	2.60	1.62	1.59
6	J	1001	ATP	C8-N7	2.60	1.36	1.31
5	F	700	FDP	P1-O2	2.59	1.64	1.59
6	B	1001	ATP	C5-C6	2.58	1.48	1.41
6	G	1001	ATP	PB-O3B	2.58	1.62	1.59
6	I	1001	ATP	C8-N7	2.58	1.36	1.31
6	J	1001	ATP	PA-O3A	2.55	1.62	1.59
6	H	1001	ATP	PA-O3A	2.51	1.62	1.59
6	A	1001	ATP	PB-O3B	2.51	1.62	1.59
6	M	1001	ATP	PB-O3A	2.50	1.62	1.59
6	L	1001	ATP	PB-O3A	2.50	1.62	1.59
6	C	1001	ATP	C8-N7	2.48	1.36	1.31
6	L	1001	ATP	PB-O3B	2.47	1.62	1.59
6	D	1001	ATP	C8-N7	2.44	1.36	1.31
6	M	1001	ATP	PA-O3A	2.43	1.62	1.59
6	N	1001	ATP	C8-N7	2.41	1.36	1.31
6	E	1001	ATP	C8-N7	2.41	1.36	1.31
6	C	1001	ATP	C5-N7	-2.41	1.34	1.39
5	L	700	FDP	P2-O6	-2.40	1.52	1.60
5	P	700	FDP	P1-O3P	2.40	1.63	1.54
6	P	1001	ATP	PB-O3A	2.39	1.62	1.59
4	N	510	OXL	O4-C2	-2.39	1.24	1.30
6	B	1001	ATP	C8-N7	2.38	1.36	1.31
6	F	1001	ATP	C5-N7	-2.38	1.34	1.39
6	P	1001	ATP	PA-O3A	2.37	1.62	1.59
6	A	1001	ATP	C8-N7	2.37	1.36	1.31
6	K	1001	ATP	PA-O3A	2.37	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	510	OXL	O3-C1	-2.35	1.24	1.30
6	P	1001	ATP	C8-N7	2.35	1.36	1.31
6	H	1001	ATP	PB-O3B	2.34	1.62	1.59
6	M	1001	ATP	C8-N7	2.33	1.36	1.31
6	M	1001	ATP	PB-O3B	2.33	1.62	1.59
6	K	1001	ATP	C8-N7	2.33	1.36	1.31
6	L	1001	ATP	C8-N7	2.32	1.36	1.31
5	J	700	FDP	O4-C4	-2.31	1.37	1.43
6	J	1001	ATP	C5-N7	-2.30	1.34	1.39
5	J	700	FDP	P2-O5P	-2.29	1.46	1.54
5	K	700	FDP	O5-C2	2.28	1.47	1.42
6	G	1001	ATP	C8-N7	2.28	1.36	1.31
6	A	1001	ATP	PA-O3A	2.27	1.62	1.59
6	F	1001	ATP	PB-O3B	2.27	1.62	1.59
6	A	1001	ATP	C5-N7	-2.27	1.34	1.39
6	D	1001	ATP	C5-N7	-2.27	1.34	1.39
6	H	1001	ATP	C8-N7	2.27	1.36	1.31
5	B	700	FDP	P1-O2	2.26	1.63	1.59
6	F	1001	ATP	C8-N7	2.25	1.36	1.31
6	P	1001	ATP	C5-N7	-2.24	1.35	1.39
4	G	510	OXL	O3-C1	-2.23	1.24	1.30
6	M	1001	ATP	C5-N7	-2.22	1.35	1.39
5	H	700	FDP	P1-O2	2.21	1.63	1.59
5	K	700	FDP	P1-O2P	-2.21	1.46	1.54
5	N	700	FDP	P2-O5P	2.20	1.63	1.54
5	F	700	FDP	O5-C2	-2.19	1.37	1.42
6	B	1001	ATP	PB-O3A	2.19	1.61	1.59
6	G	1001	ATP	C5-N7	-2.19	1.35	1.39
6	H	1001	ATP	C5-N7	-2.19	1.35	1.39
4	B	510	OXL	O3-C1	-2.18	1.24	1.30
5	G	700	FDP	P2-O6P	2.18	1.62	1.54
6	B	1001	ATP	C5-N7	-2.16	1.35	1.39
6	A	1001	ATP	PB-O3A	2.15	1.61	1.59
6	E	1001	ATP	C5-N7	-2.13	1.35	1.39
5	B	700	FDP	P1-O3P	-2.13	1.46	1.54
6	N	1001	ATP	C5-N7	-2.13	1.35	1.39
6	I	1001	ATP	C5-N7	-2.12	1.35	1.39
6	E	1001	ATP	PB-O3B	2.12	1.61	1.59
6	J	1001	ATP	PB-O3B	2.11	1.61	1.59
6	K	1001	ATP	C5-N7	-2.10	1.35	1.39
5	H	700	FDP	P2-O5P	2.08	1.62	1.54
5	K	700	FDP	P1-O2	2.07	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1001	ATP	PB-O3A	2.07	1.61	1.59
5	N	700	FDP	P1-O2	2.07	1.63	1.59
6	B	1001	ATP	PA-O3A	2.06	1.61	1.59
4	A	510	OXL	O3-C1	-2.06	1.25	1.30
5	P	700	FDP	O5-C2	2.05	1.46	1.42
5	P	700	FDP	P1-O2P	2.05	1.62	1.54
6	L	1001	ATP	C5-N7	-2.03	1.35	1.39
5	L	700	FDP	O5-C2	2.02	1.46	1.42

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1001	ATP	C5-C4-N3	-6.21	118.17	126.72
6	F	1001	ATP	C5-C4-N3	-6.08	118.35	126.72
6	P	1001	ATP	C5-C4-N3	-6.00	118.46	126.72
6	A	1001	ATP	C5-C4-N3	-5.97	118.50	126.72
6	C	1001	ATP	C5-C4-N3	-5.91	118.58	126.72
6	N	1001	ATP	C5-C4-N3	-5.89	118.61	126.72
6	E	1001	ATP	C5-C4-N3	-5.81	118.72	126.72
6	H	1001	ATP	C5-C4-N3	-5.78	118.76	126.72
6	M	1001	ATP	C5-C4-N3	-5.71	118.85	126.72
6	J	1001	ATP	C5-C4-N3	-5.70	118.86	126.72
6	K	1001	ATP	C5-C4-N3	-5.70	118.86	126.72
6	G	1001	ATP	C5-C4-N3	-5.69	118.88	126.72
6	D	1001	ATP	C5-C4-N3	-5.60	119.01	126.72
6	B	1001	ATP	C5-C4-N3	-5.57	119.05	126.72
6	L	1001	ATP	C5-C4-N3	-5.54	119.09	126.72
6	F	1001	ATP	N3-C4-N9	4.84	135.39	127.17
6	P	1001	ATP	N3-C4-N9	4.78	135.30	127.17
6	I	1001	ATP	N3-C4-N9	4.75	135.24	127.17
6	A	1001	ATP	N3-C4-N9	4.69	135.14	127.17
6	E	1001	ATP	N3-C4-N9	4.69	135.14	127.17
6	N	1001	ATP	N3-C4-N9	4.68	135.12	127.17
6	G	1001	ATP	N3-C4-N9	4.60	134.99	127.17
6	C	1001	ATP	N3-C4-N9	4.60	134.99	127.17
6	B	1001	ATP	N3-C4-N9	4.59	134.97	127.17
6	M	1001	ATP	N3-C4-N9	4.58	134.95	127.17
6	K	1001	ATP	N3-C4-N9	4.56	134.93	127.17
6	H	1001	ATP	N3-C4-N9	4.54	134.88	127.17
6	L	1001	ATP	N3-C4-N9	4.44	134.72	127.17
6	J	1001	ATP	N3-C4-N9	4.39	134.63	127.17
6	D	1001	ATP	N3-C4-N9	4.28	134.44	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FDP	O2-C2-C3	4.06	120.92	108.28
5	I	700	FDP	O2-C2-C3	4.00	120.74	108.28
5	B	700	FDP	O2-C2-C3	3.98	120.67	108.28
6	B	1001	ATP	N3-C2-N1	-3.97	122.57	128.58
6	I	1001	ATP	C2-N3-C4	3.95	121.47	111.83
6	E	1001	ATP	C2-N3-C4	3.94	121.46	111.83
5	C	700	FDP	O6-P2-O4P	3.91	117.01	106.44
5	L	700	FDP	O2-C2-C3	3.90	120.44	108.28
6	F	1001	ATP	C2-N3-C4	3.90	121.36	111.83
5	L	700	FDP	O2-P1-O1P	3.90	123.24	109.33
6	P	1001	ATP	C2-N3-C4	3.90	121.35	111.83
6	B	1001	ATP	C2-N3-C4	3.87	121.27	111.83
6	J	1001	ATP	C2-N3-C4	3.85	121.24	111.83
4	B	510	OXL	O4-C2-C1	3.85	120.29	112.83
6	N	1001	ATP	C2-N3-C4	3.84	121.20	111.83
5	G	700	FDP	C6-C5-C4	-3.81	101.50	115.21
6	K	1001	ATP	C2-N3-C4	3.80	121.11	111.83
6	G	1001	ATP	C2-N3-C4	3.79	121.08	111.83
5	I	700	FDP	O5-C2-C3	-3.78	97.83	105.42
6	A	1001	ATP	C2-N3-C4	3.77	121.05	111.83
6	H	1001	ATP	C2-N3-C4	3.73	120.95	111.83
6	M	1001	ATP	C2-N3-C4	3.73	120.94	111.83
6	E	1001	ATP	N3-C2-N1	-3.72	122.95	128.58
5	H	700	FDP	C6-C5-C4	-3.70	101.88	115.21
6	L	1001	ATP	C2-N3-C4	3.70	120.87	111.83
6	J	1001	ATP	N3-C2-N1	-3.63	123.09	128.58
4	D	510	OXL	O4-C2-C1	3.63	119.86	112.83
6	C	1001	ATP	C2-N3-C4	3.63	120.69	111.83
6	D	1001	ATP	C2-N3-C4	3.57	120.55	111.83
5	B	700	FDP	C6-C5-C4	-3.56	102.39	115.21
6	G	1001	ATP	N3-C2-N1	-3.55	123.20	128.58
5	F	700	FDP	O2-C2-C3	3.54	119.30	108.28
6	L	1001	ATP	N3-C2-N1	-3.53	123.23	128.58
6	C	1001	ATP	C4-C5-N7	-3.53	106.55	110.58
6	P	1001	ATP	N3-C2-N1	-3.52	123.25	128.58
6	K	1001	ATP	N3-C2-N1	-3.50	123.29	128.58
6	N	1001	ATP	C4-C5-N7	-3.49	106.59	110.58
6	J	1001	ATP	C4-C5-N7	-3.48	106.60	110.58
6	N	1001	ATP	N3-C2-N1	-3.46	123.35	128.58
6	I	1001	ATP	C4-C5-N7	-3.45	106.64	110.58
6	M	1001	ATP	N3-C2-N1	-3.42	123.41	128.58
6	I	1001	ATP	N3-C2-N1	-3.42	123.41	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1001	ATP	N3-C2-N1	-3.41	123.42	128.58
6	D	1001	ATP	C4-C5-N7	-3.39	106.71	110.58
6	F	1001	ATP	C4-C5-N7	-3.37	106.73	110.58
4	J	510	OXL	O3-C1-C2	3.36	119.35	112.83
6	M	1001	ATP	C4-C5-N7	-3.34	106.77	110.58
6	H	1001	ATP	N3-C2-N1	-3.32	123.55	128.58
5	B	700	FDP	O5-C2-C3	-3.31	98.77	105.42
6	P	1001	ATP	C4-C5-N7	-3.30	106.81	110.58
6	E	1001	ATP	C4-C5-N7	-3.28	106.83	110.58
6	A	1001	ATP	N3-C2-N1	-3.28	123.62	128.58
5	J	700	FDP	O2-C2-C3	3.28	118.48	108.28
5	F	700	FDP	O6P-P2-O6	-3.27	98.14	106.67
6	H	1001	ATP	C4-C5-N7	-3.26	106.86	110.58
4	C	510	OXL	O3-C1-C2	3.24	119.12	112.83
5	F	700	FDP	O5-C2-C3	-3.23	98.93	105.42
4	H	510	OXL	O4-C2-C1	3.23	119.09	112.83
6	A	1001	ATP	C4-C5-N7	-3.21	106.91	110.58
6	D	1001	ATP	N3-C2-N1	-3.21	123.73	128.58
6	C	1001	ATP	N3-C2-N1	-3.20	123.74	128.58
5	J	700	FDP	O6-P2-O4P	3.19	115.06	106.44
4	J	510	OXL	O4-C2-C1	3.17	118.98	112.83
6	K	1001	ATP	C4-C5-N7	-3.17	106.96	110.58
6	G	1001	ATP	C4-C5-N7	-3.15	106.98	110.58
4	P	510	OXL	O4-C2-C1	3.14	118.92	112.83
5	K	700	FDP	C6-C5-C4	-3.13	103.96	115.21
5	D	700	FDP	O2-P1-O1P	3.08	120.30	109.33
4	L	510	OXL	O3-C1-C2	3.07	118.78	112.83
6	L	1001	ATP	C4-C5-N7	-3.06	107.08	110.58
4	A	510	OXL	O3-C1-C2	3.05	118.75	112.83
4	L	510	OXL	O4-C2-C1	3.05	118.75	112.83
4	I	510	OXL	O4-C2-C1	3.04	118.73	112.83
4	F	510	OXL	O3-C1-C2	3.03	118.72	112.83
4	B	510	OXL	O3-C1-C2	3.01	118.66	112.83
5	K	700	FDP	O2-C2-C3	3.00	117.63	108.28
5	H	700	FDP	O3P-P1-O1P	2.99	122.49	110.83
6	J	1001	ATP	C2'-C1'-N9	-2.96	105.96	113.30
4	G	510	OXL	O4-C2-C1	2.95	118.55	112.83
5	D	700	FDP	O3P-P1-O2	-2.95	94.36	105.85
5	L	700	FDP	C6-C5-C4	-2.95	104.61	115.21
6	K	1001	ATP	C2'-C1'-N9	-2.88	106.14	113.30
6	B	1001	ATP	C4-C5-N7	-2.83	107.35	110.58
4	F	510	OXL	O4-C2-C1	2.81	118.28	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	510	OXL	O3-C1-C2	2.80	118.26	112.83
6	D	1001	ATP	C2'-C1'-N9	-2.79	106.37	113.30
4	K	510	OXL	O3-C1-C2	2.78	118.22	112.83
5	C	700	FDP	O5P-P2-O6	-2.78	99.42	106.67
6	D	1001	ATP	O4'-C1'-N9	2.76	113.39	108.09
5	M	700	FDP	O6-P2-O4P	2.76	113.90	106.44
4	H	510	OXL	O3-C1-C2	2.75	118.16	112.83
5	J	700	FDP	C6-C5-C4	-2.74	105.34	115.21
5	A	700	FDP	C6-C5-C4	-2.70	105.48	115.21
5	L	700	FDP	O5-C2-C3	-2.70	100.00	105.42
5	N	700	FDP	O6-P2-O4P	2.69	113.70	106.44
6	C	1001	ATP	C2'-C1'-N9	-2.66	106.70	113.30
5	B	700	FDP	O3P-P1-O2	-2.66	95.49	105.85
4	E	510	OXL	O4-C2-C1	2.65	117.98	112.83
4	M	510	OXL	O4-C2-C1	2.65	117.97	112.83
6	J	1001	ATP	C5-N7-C8	2.63	107.58	103.45
6	B	1001	ATP	C2'-C1'-N9	-2.62	106.78	113.30
6	J	1001	ATP	O4'-C1'-N9	2.62	113.12	108.09
4	P	510	OXL	O3-C1-C2	2.60	117.88	112.83
6	K	1001	ATP	C4-N9-C8	2.60	108.47	105.74
6	I	1001	ATP	C2'-C1'-N9	-2.59	106.87	113.30
4	N	510	OXL	O4-C2-C1	2.58	117.84	112.83
4	N	510	OXL	O3-C1-C2	2.57	117.82	112.83
4	G	510	OXL	O3-C1-C2	2.57	117.81	112.83
4	B	510	OXL	O2-C2-C1	-2.57	115.29	120.63
6	N	1001	ATP	C5-N7-C8	2.55	107.45	103.45
6	I	1001	ATP	C5-N7-C8	2.54	107.44	103.45
6	J	1001	ATP	C4-N9-C8	2.52	108.38	105.74
6	E	1001	ATP	C2'-C1'-N9	-2.51	107.07	113.30
5	C	700	FDP	O6P-P2-O4P	2.51	120.61	110.83
6	F	1001	ATP	C5-N7-C8	2.50	107.38	103.45
5	E	700	FDP	O5-C2-C3	-2.49	100.42	105.42
6	E	1001	ATP	C5-N7-C8	2.49	107.36	103.45
5	B	700	FDP	O6-P2-O4P	2.49	113.16	106.44
5	K	700	FDP	C2-C3-C4	-2.49	96.65	102.19
5	A	700	FDP	O6-P2-O4P	2.48	113.15	106.44
6	M	1001	ATP	C5-N7-C8	2.48	107.34	103.45
6	B	1001	ATP	C4-N9-C8	2.47	108.34	105.74
5	D	700	FDP	C6-C5-C4	-2.47	106.33	115.21
6	P	1001	ATP	C3'-C2'-C1'	2.47	106.13	101.46
6	C	1001	ATP	C5-N7-C8	2.46	107.32	103.45
5	O	700	FDP	C5-C4-C3	-2.45	94.46	102.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	1001	ATP	C4-N9-C8	2.44	108.30	105.74
6	F	1001	ATP	C2'-C1'-N9	-2.43	107.25	113.30
6	E	1001	ATP	C4-N9-C8	2.43	108.29	105.74
6	P	1001	ATP	C5-N7-C8	2.43	107.27	103.45
5	B	700	FDP	O2-P1-O1P	2.41	117.92	109.33
4	A	510	OXL	O4-C2-C1	2.38	117.45	112.83
6	D	1001	ATP	C5-N7-C8	2.37	107.17	103.45
4	K	510	OXL	O1-C1-C2	-2.36	115.71	120.63
5	G	700	FDP	O6-P2-O4P	2.35	112.80	106.44
6	B	1001	ATP	C2-N1-C6	2.35	122.59	118.73
6	H	1001	ATP	C5-N7-C8	2.33	107.11	103.45
6	K	1001	ATP	C5-N7-C8	2.33	107.11	103.45
6	N	1001	ATP	C3'-C2'-C1'	2.32	105.86	101.46
5	K	700	FDP	O4-C4-C5	-2.32	104.42	111.08
4	C	510	OXL	O1-C1-C2	-2.32	115.80	120.63
6	M	1001	ATP	C4-N9-C8	2.31	108.17	105.74
6	G	1001	ATP	C4-N9-C8	2.31	108.16	105.74
5	F	700	FDP	O6-P2-O4P	2.29	112.62	106.44
5	E	700	FDP	O6-P2-O4P	2.28	112.60	106.44
5	H	700	FDP	O2-C2-C3	2.28	115.37	108.28
6	G	1001	ATP	C5-N7-C8	2.27	107.03	103.45
6	J	1001	ATP	C6-C5-N7	2.27	136.47	132.09
5	M	700	FDP	C6-C5-C4	-2.26	107.07	115.21
6	P	1001	ATP	C4-N9-C8	2.24	108.09	105.74
6	L	1001	ATP	O4'-C1'-N9	2.24	112.38	108.09
5	K	700	FDP	O6P-P2-O4P	2.23	119.53	110.83
5	J	700	FDP	O5-C2-C3	-2.23	100.94	105.42
6	I	1001	ATP	O3G-PG-O2G	2.23	116.17	107.80
6	A	1001	ATP	C5-N7-C8	2.22	106.94	103.45
6	N	1001	ATP	C6-C5-N7	2.21	136.35	132.09
6	E	1001	ATP	C6-C5-N7	2.21	136.35	132.09
6	K	1001	ATP	C6-C5-N7	2.21	136.35	132.09
5	I	700	FDP	O3P-P1-O2	2.21	114.45	105.85
6	F	1001	ATP	C4-N9-C8	2.20	108.05	105.74
5	C	700	FDP	C6-C5-C4	-2.17	107.41	115.21
6	L	1001	ATP	C5-N7-C8	2.16	106.84	103.45
6	L	1001	ATP	C4-N9-C8	2.15	108.00	105.74
6	M	1001	ATP	C6-C5-N7	2.15	136.23	132.09
6	C	1001	ATP	O3G-PG-O2G	2.14	115.83	107.80
4	E	510	OXL	O3-C1-C2	2.14	116.98	112.83
6	L	1001	ATP	C6-C5-N7	2.13	136.19	132.09
5	M	700	FDP	O2-C2-C1	2.12	115.72	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1001	ATP	C2-N1-C6	2.12	122.21	118.73
6	J	1001	ATP	N9-C8-N7	-2.11	110.94	113.94
5	K	700	FDP	C1-C2-C3	-2.11	108.62	114.83
5	H	700	FDP	O6-P2-O4P	2.11	112.14	106.44
6	D	1001	ATP	C6-C5-N7	2.10	136.14	132.09
4	D	510	OXL	O2-C2-C1	-2.10	116.25	120.63
6	H	1001	ATP	C4-N9-C8	2.10	107.94	105.74
4	L	510	OXL	O2-C2-C1	-2.10	116.25	120.63
6	B	1001	ATP	C5-N7-C8	2.10	106.75	103.45
5	P	700	FDP	O6-P2-O4P	2.10	112.11	106.44
5	J	700	FDP	C1-C2-C3	-2.10	108.67	114.83
5	A	700	FDP	O3P-P1-O2	2.09	114.00	105.85
6	G	1001	ATP	C6-C5-N7	2.09	136.12	132.09
5	I	700	FDP	O6P-P2-O6	2.08	112.11	106.67
6	C	1001	ATP	C4-N9-C8	2.08	107.93	105.74
5	A	700	FDP	O3P-P1-O2P	-2.08	100.00	107.80
6	H	1001	ATP	O4'-C1'-N9	2.08	112.08	108.09
6	P	1001	ATP	C6-C5-N7	2.07	136.08	132.09
5	K	700	FDP	O6-P2-O4P	2.07	112.02	106.44
6	M	1001	ATP	C2'-C1'-N9	-2.07	108.17	113.30
4	D	510	OXL	O3-C1-C2	2.06	116.83	112.83
6	B	1001	ATP	C6-C5-N7	2.06	136.06	132.09
6	H	1001	ATP	C6-C5-N7	2.06	136.06	132.09
6	C	1001	ATP	O2A-PA-O1A	2.05	122.00	112.44
5	C	700	FDP	O6P-P2-O6	-2.05	101.33	106.67
6	H	1001	ATP	C2'-C1'-N9	-2.05	108.22	113.30
5	G	700	FDP	O5P-P2-O6	2.05	112.00	106.67
6	I	1001	ATP	C4-N9-C8	2.04	107.88	105.74
6	M	1001	ATP	C2-N1-C6	2.04	122.08	118.73
5	K	700	FDP	O5-C5-C6	2.04	114.29	109.50
6	D	1001	ATP	O3G-PG-O2G	2.03	115.42	107.80
6	C	1001	ATP	C6-C5-N7	2.03	136.00	132.09
6	I	1001	ATP	O2A-PA-O1A	2.03	121.87	112.44
5	N	700	FDP	O2-P1-O1P	2.02	116.54	109.33
5	G	700	FDP	O5-C5-C6	2.02	114.25	109.50
6	F	1001	ATP	C6-C5-N7	2.02	135.98	132.09
6	D	1001	ATP	C2-N1-C6	2.01	122.04	118.73
6	A	1001	ATP	C4-N9-C8	2.01	107.85	105.74
4	L	510	OXL	O1-C1-C2	-2.01	116.45	120.63

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	FDP	O1-C1-C2-O2
5	A	700	FDP	O1-C1-C2-C3
5	A	700	FDP	O1-C1-C2-O5
5	N	700	FDP	O1-C1-C2-C3
5	N	700	FDP	C6-O6-P2-O4P
5	O	700	FDP	O1-C1-C2-O2
5	O	700	FDP	O1-C1-C2-C3
5	O	700	FDP	O1-C1-C2-O5
5	O	700	FDP	C6-O6-P2-O4P
5	O	700	FDP	C6-O6-P2-O5P
5	O	700	FDP	C6-O6-P2-O6P
5	P	700	FDP	O1-C1-C2-C3
6	A	1001	ATP	C5'-O5'-PA-O1A
6	A	1001	ATP	C5'-O5'-PA-O2A
6	A	1001	ATP	C5'-O5'-PA-O3A
6	D	1001	ATP	PB-O3B-PG-O2G
6	D	1001	ATP	C5'-O5'-PA-O1A
6	D	1001	ATP	C5'-O5'-PA-O2A
6	D	1001	ATP	C5'-O5'-PA-O3A
6	E	1001	ATP	PB-O3B-PG-O3G
6	G	1001	ATP	C5'-O5'-PA-O1A
6	G	1001	ATP	C5'-O5'-PA-O3A
6	H	1001	ATP	C5'-O5'-PA-O1A
6	H	1001	ATP	C5'-O5'-PA-O2A
6	H	1001	ATP	C5'-O5'-PA-O3A
6	I	1001	ATP	PB-O3B-PG-O3G
6	L	1001	ATP	C5'-O5'-PA-O1A
6	L	1001	ATP	C5'-O5'-PA-O2A
6	L	1001	ATP	C5'-O5'-PA-O3A
6	M	1001	ATP	PB-O3B-PG-O3G
6	P	1001	ATP	O4'-C4'-C5'-O5'
7	I	499	GOL	O1-C1-C2-C3
7	I	501	GOL	C1-C2-C3-O3
7	J	499	GOL	C1-C2-C3-O3
7	O	499	GOL	O1-C1-C2-C3
7	O	499	GOL	C1-C2-C3-O3
5	O	700	FDP	C4-C5-C6-O6
7	I	501	GOL	O2-C2-C3-O3
7	J	499	GOL	O2-C2-C3-O3
5	P	700	FDP	C4-C5-C6-O6
5	N	700	FDP	O1-C1-C2-O2
5	P	700	FDP	O1-C1-C2-O2
5	F	700	FDP	O1-C1-C2-O5

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Mol	Chain	Res	Type	Atoms
7	E	499	GOL	O1-C1-C2-C3
7	I	501	GOL	O1-C1-C2-C3
7	J	499	GOL	O1-C1-C2-C3
7	I	499	GOL	O1-C1-C2-O2
7	O	499	GOL	O1-C1-C2-O2
7	O	499	GOL	O2-C2-C3-O3
5	O	700	FDP	O5-C5-C6-O6
6	P	1001	ATP	C3'-C4'-C5'-O5'
5	C	700	FDP	O1-C1-C2-C3
5	I	700	FDP	O1-C1-C2-C3
5	N	700	FDP	O1-C1-C2-O5
7	J	499	GOL	O1-C1-C2-O2
6	L	1001	ATP	O4'-C4'-C5'-O5'
5	F	700	FDP	C6-O6-P2-O4P
5	F	700	FDP	O1-C1-C2-O2
5	M	700	FDP	O1-C1-C2-O5
7	I	501	GOL	O1-C1-C2-O2
5	P	700	FDP	O5-C5-C6-O6
5	E	700	FDP	O1-C1-C2-O5
6	H	1001	ATP	O4'-C4'-C5'-O5'
5	N	700	FDP	C6-O6-P2-O6P
4	B	510	OXL	O3-C1-C2-O4
4	E	510	OXL	O3-C1-C2-O4
4	G	510	OXL	O3-C1-C2-O4
4	I	510	OXL	O3-C1-C2-O4
4	J	510	OXL	O3-C1-C2-O4
4	N	510	OXL	O3-C1-C2-O4
6	H	1001	ATP	PB-O3B-PG-O1G
6	L	1001	ATP	PB-O3B-PG-O1G
6	B	1001	ATP	PB-O3B-PG-O3G
6	J	1001	ATP	PB-O3B-PG-O3G
6	K	1001	ATP	PB-O3B-PG-O3G
6	A	1001	ATP	PA-O3A-PB-O1B
6	C	1001	ATP	PB-O3A-PA-O1A
6	D	1001	ATP	PA-O3A-PB-O1B
6	G	1001	ATP	PA-O3A-PB-O2B
6	M	1001	ATP	PB-O3A-PA-O1A
4	B	510	OXL	O1-C1-C2-O2
4	E	510	OXL	O1-C1-C2-O2
4	G	510	OXL	O1-C1-C2-O2
4	I	510	OXL	O1-C1-C2-O2
4	J	510	OXL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	N	510	OXL	O1-C1-C2-O2
5	P	700	FDP	O1-C1-C2-O5
6	N	1001	ATP	O4'-C4'-C5'-O5'
6	G	1001	ATP	C5'-O5'-PA-O2A
5	H	700	FDP	C6-O6-P2-O4P
5	F	700	FDP	C4-C5-C6-O6
6	A	1001	ATP	O4'-C4'-C5'-O5'
6	I	1001	ATP	PB-O3A-PA-O1A
5	M	700	FDP	O1-C1-C2-O2
5	F	700	FDP	O5-C5-C6-O6
4	B	510	OXL	O3-C1-C2-O2
4	E	510	OXL	O1-C1-C2-O4
4	E	510	OXL	O3-C1-C2-O2
4	G	510	OXL	O1-C1-C2-O4
4	I	510	OXL	O1-C1-C2-O4
4	J	510	OXL	O1-C1-C2-O4
4	J	510	OXL	O3-C1-C2-O2
4	N	510	OXL	O1-C1-C2-O4
4	N	510	OXL	O3-C1-C2-O2
5	P	700	FDP	C2-O2-P1-O3P
6	B	1001	ATP	PA-O3A-PB-O1B
6	G	1001	ATP	PA-O3A-PB-O1B
6	J	1001	ATP	PB-O3A-PA-O1A
5	H	700	FDP	O1-C1-C2-C3
5	M	700	FDP	O1-C1-C2-C3
5	P	700	FDP	C2-O2-P1-O1P
4	B	510	OXL	O1-C1-C2-O4
4	G	510	OXL	O3-C1-C2-O2
4	I	510	OXL	O3-C1-C2-O2
7	E	499	GOL	O1-C1-C2-O2
6	N	1001	ATP	C3'-C4'-C5'-O5'
5	E	700	FDP	C6-O6-P2-O4P
5	F	700	FDP	C6-O6-P2-O6P
6	A	1001	ATP	PB-O3B-PG-O1G
6	A	1001	ATP	PB-O3B-PG-O2G
6	H	1001	ATP	PB-O3B-PG-O2G
6	H	1001	ATP	PB-O3B-PG-O3G
6	L	1001	ATP	PB-O3B-PG-O2G
6	L	1001	ATP	PB-O3B-PG-O3G
6	C	1001	ATP	PB-O3A-PA-O2A
6	E	1001	ATP	PB-O3A-PA-O1A
6	F	1001	ATP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	N	1001	ATP	PA-O3A-PB-O1B
6	N	1001	ATP	PB-O3A-PA-O2A
5	L	700	FDP	C2-O2-P1-O3P
5	B	700	FDP	O1-C1-C2-C3
5	D	700	FDP	O1-C1-C2-C3
5	F	700	FDP	O1-C1-C2-C3
5	J	700	FDP	O1-C1-C2-C3
5	L	700	FDP	O1-C1-C2-C3
5	E	700	FDP	O1-C1-C2-O2
6	B	1001	ATP	PA-O3A-PB-O2B
6	D	1001	ATP	PA-O3A-PB-O2B
6	E	1001	ATP	PA-O3A-PB-O2B
6	E	1001	ATP	PB-O3A-PA-O2A
6	F	1001	ATP	PB-O3A-PA-O1A
6	H	1001	ATP	PA-O3A-PB-O1B
6	H	1001	ATP	PA-O3A-PB-O2B
6	I	1001	ATP	PB-O3A-PA-O2A
6	K	1001	ATP	PA-O3A-PB-O2B
6	K	1001	ATP	PB-O3A-PA-O2A
6	L	1001	ATP	PA-O3A-PB-O2B
6	M	1001	ATP	PA-O3A-PB-O2B
6	M	1001	ATP	PB-O3A-PA-O2A
6	N	1001	ATP	PA-O3A-PB-O2B
6	P	1001	ATP	PG-O3B-PB-O2B

There are no ring outliers.

17 monomers are involved in 25 short contacts:

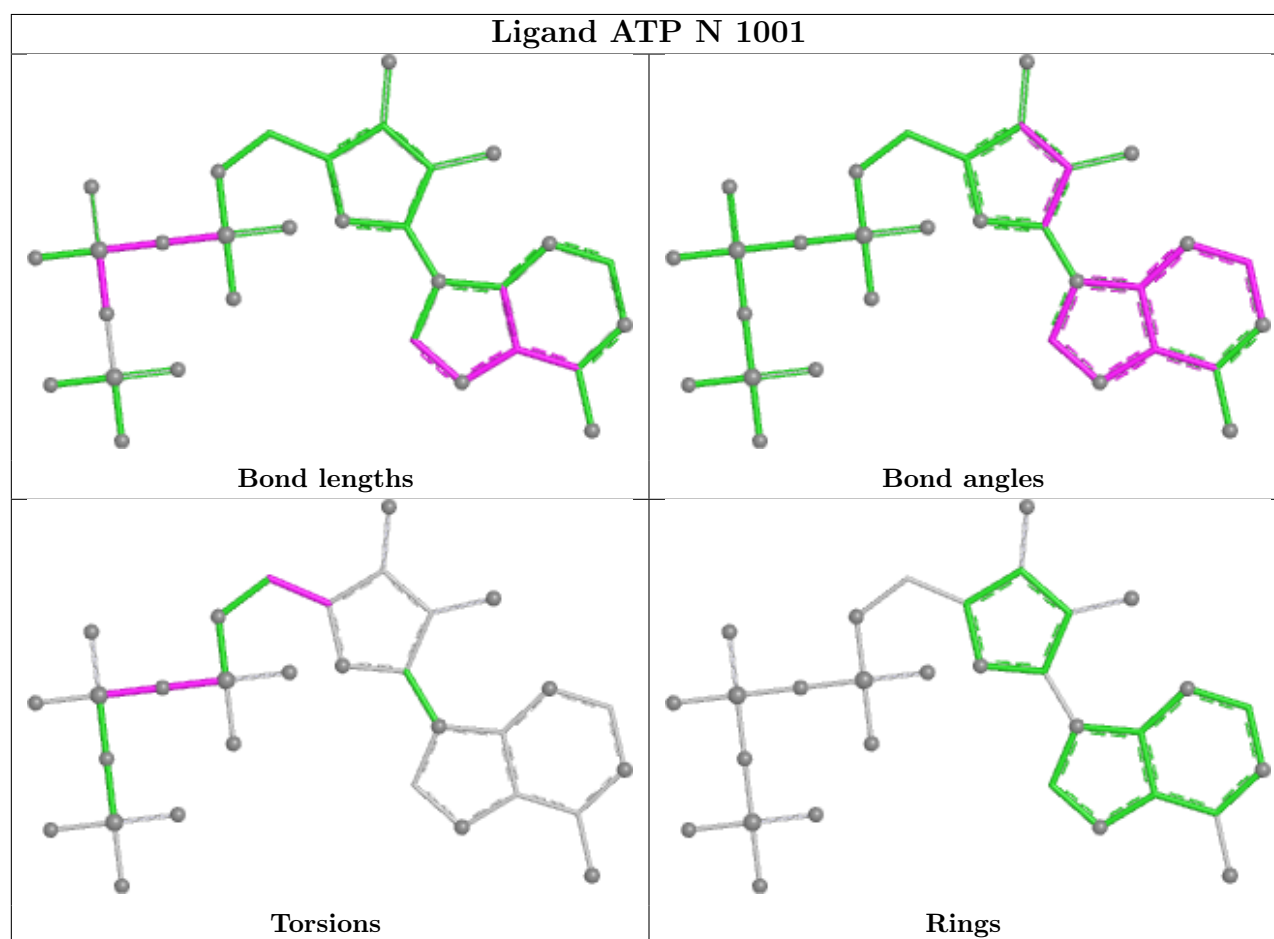
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1001	ATP	1	0
6	K	1001	ATP	2	0
4	M	510	OXL	1	0
5	O	700	FDP	1	0
6	G	1001	ATP	1	0
6	H	1001	ATP	1	0
6	A	1001	ATP	2	0
6	C	1001	ATP	3	0
7	J	499	GOL	1	0
5	D	700	FDP	2	0
5	P	700	FDP	1	0
6	F	1001	ATP	1	0
7	I	499	GOL	1	0

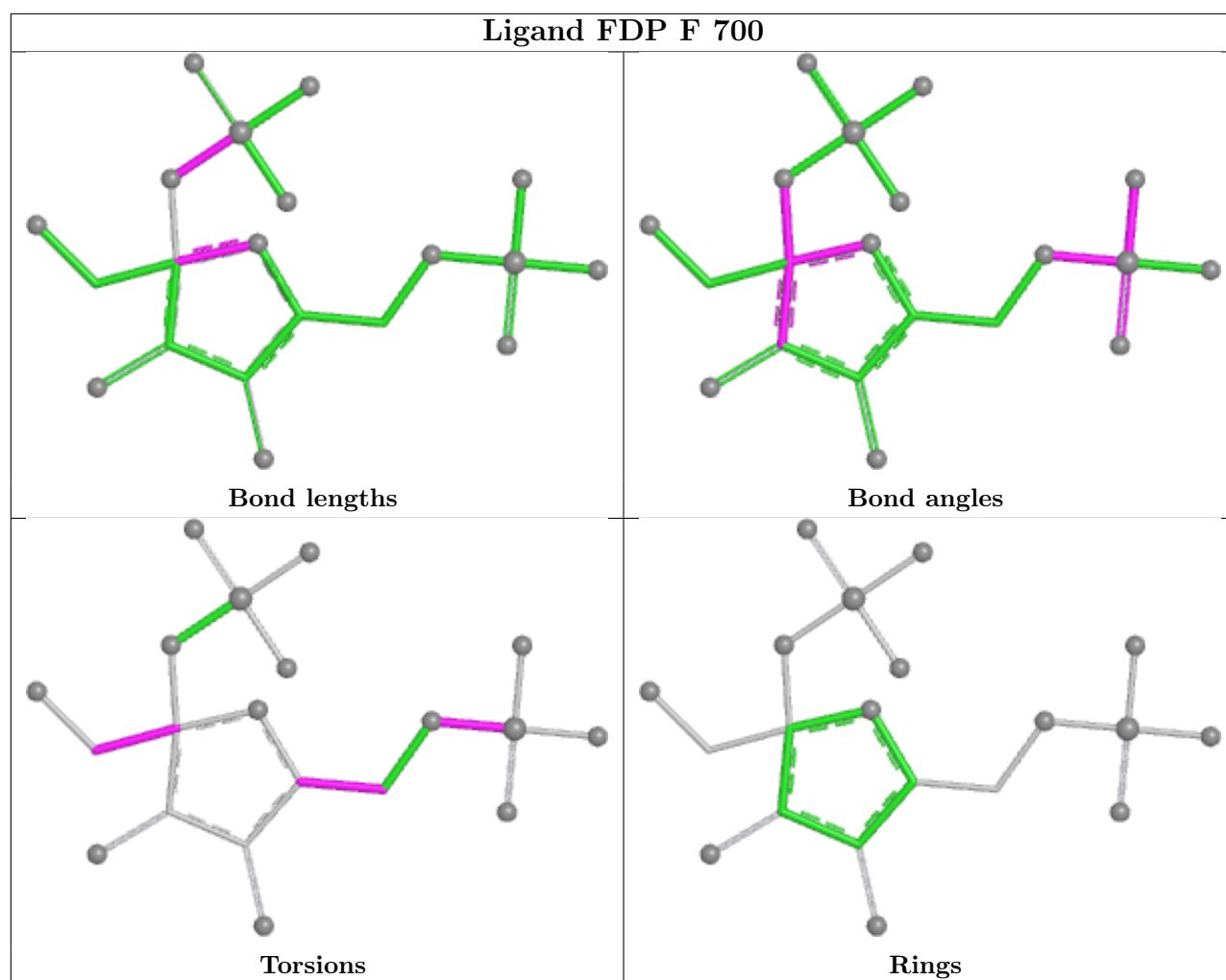
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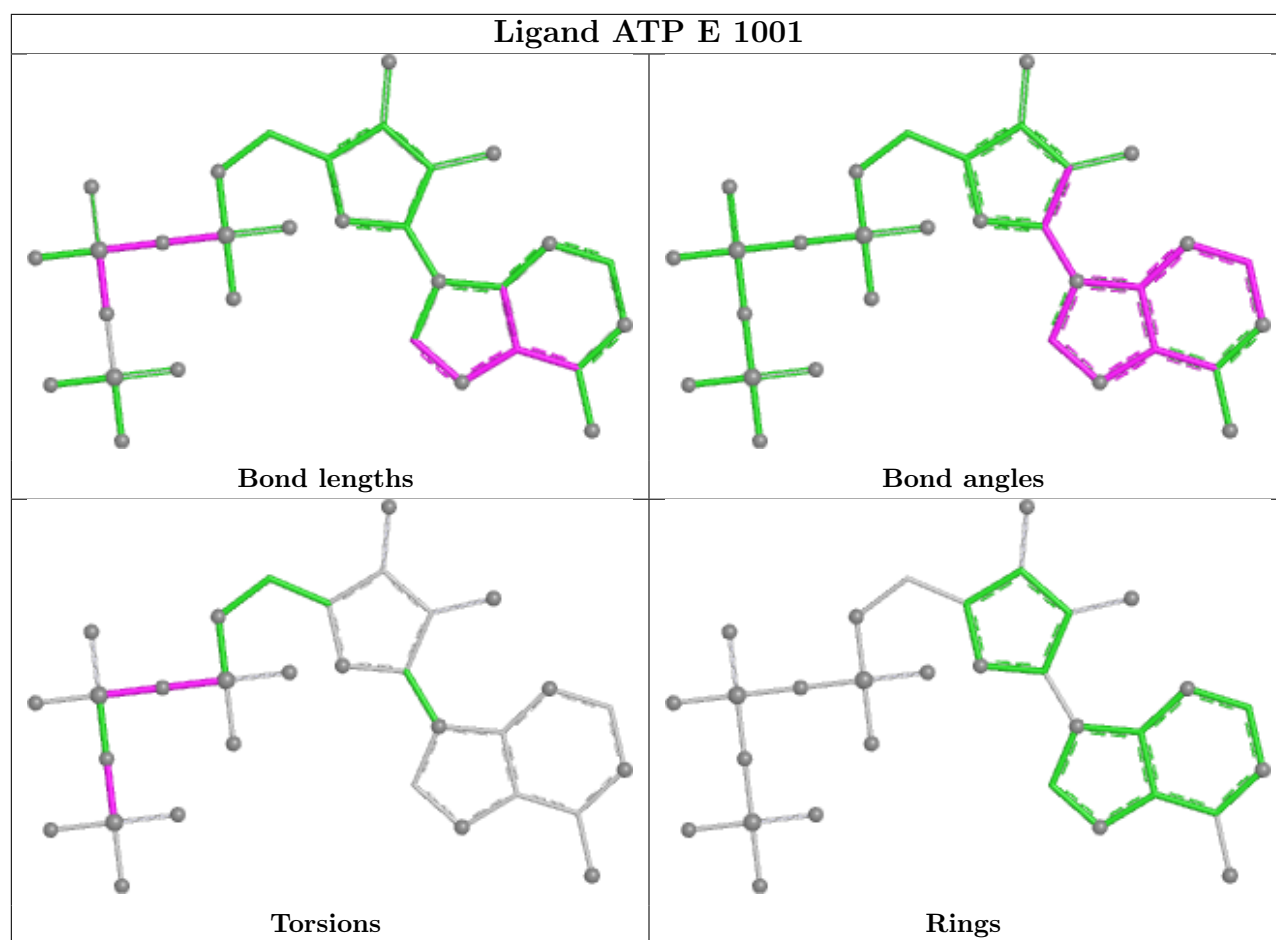
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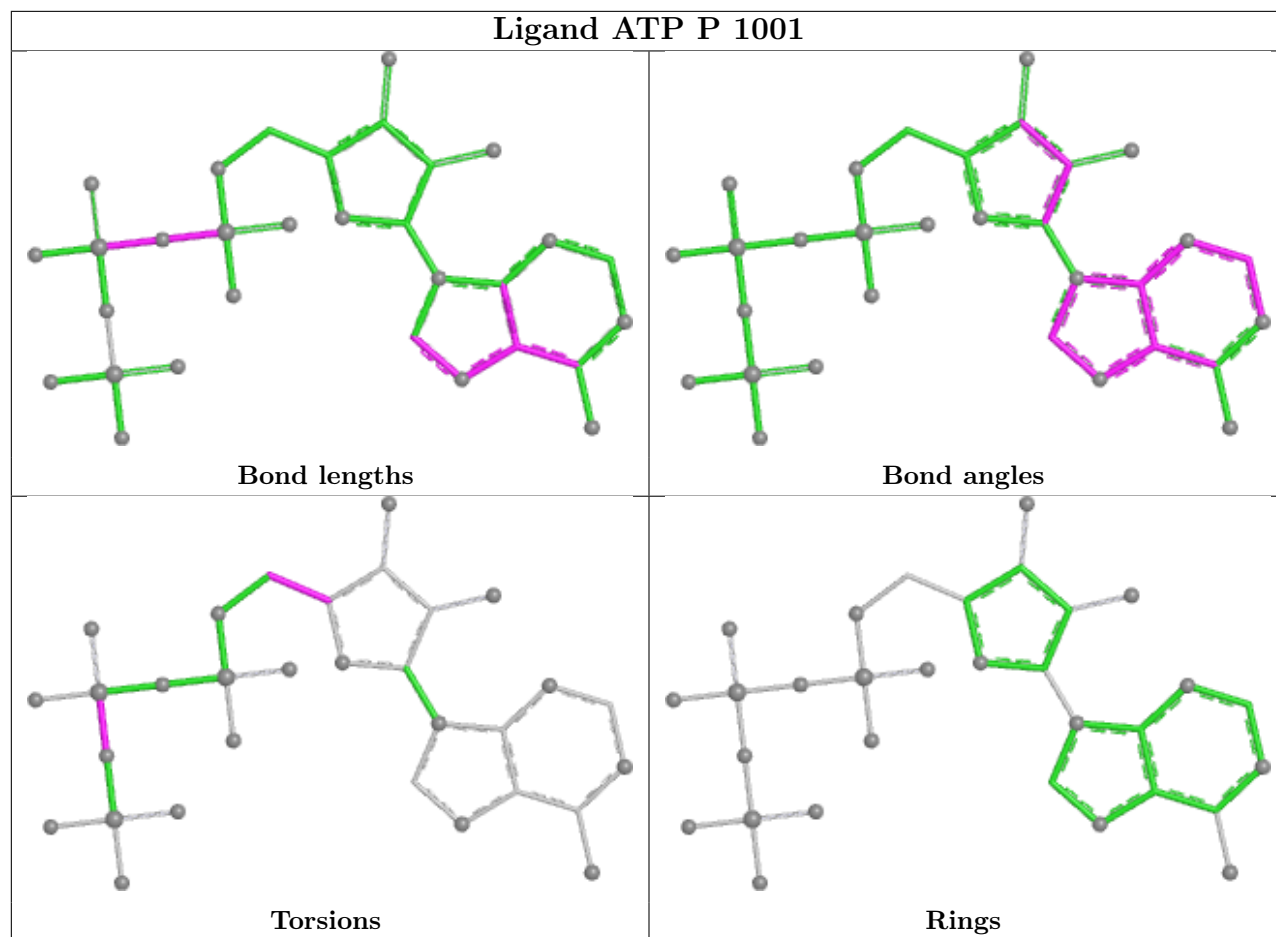
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	700	FDP	2	0
5	I	700	FDP	1	0
6	D	1001	ATP	3	0
5	G	700	FDP	1	0

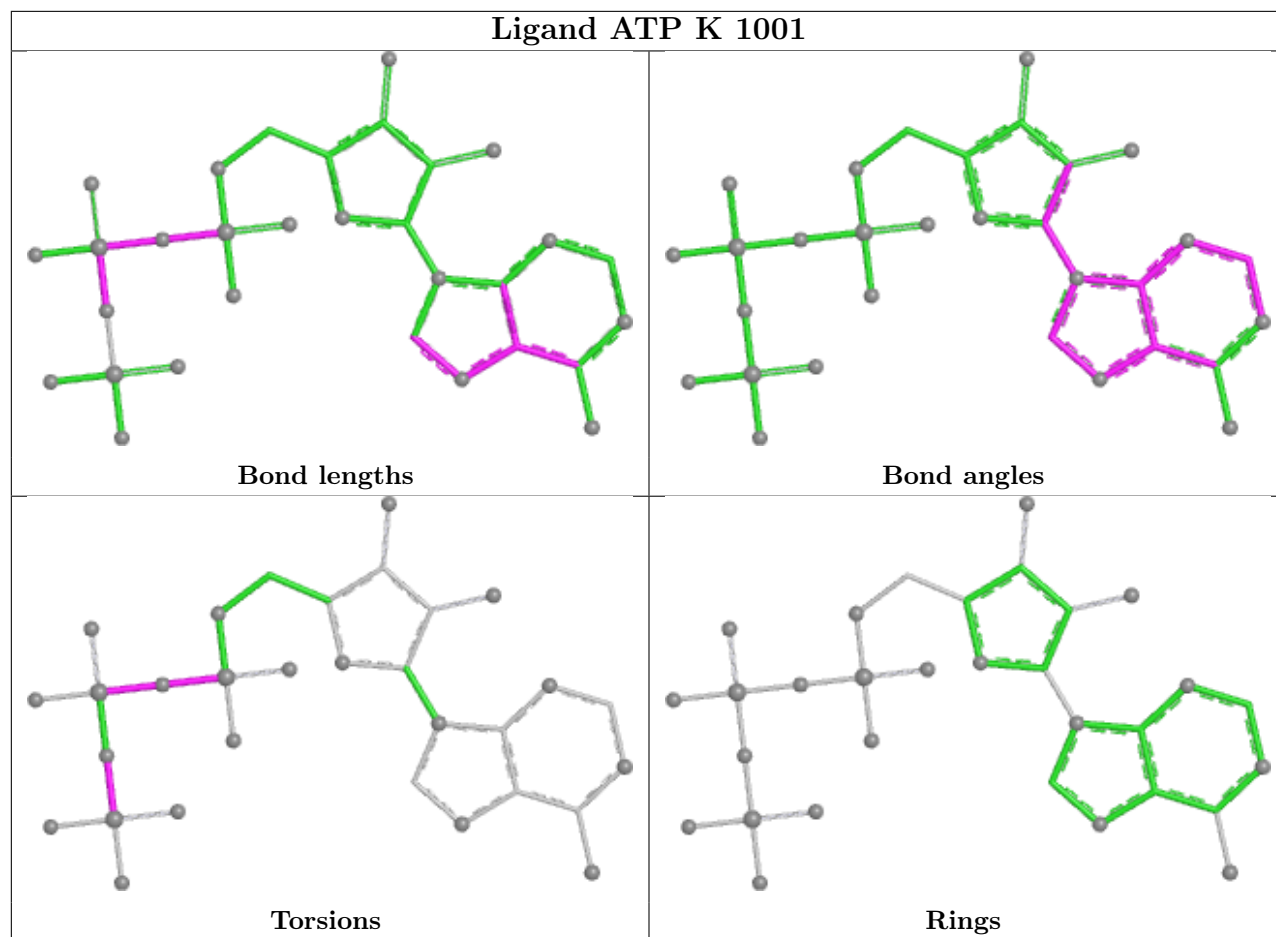
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

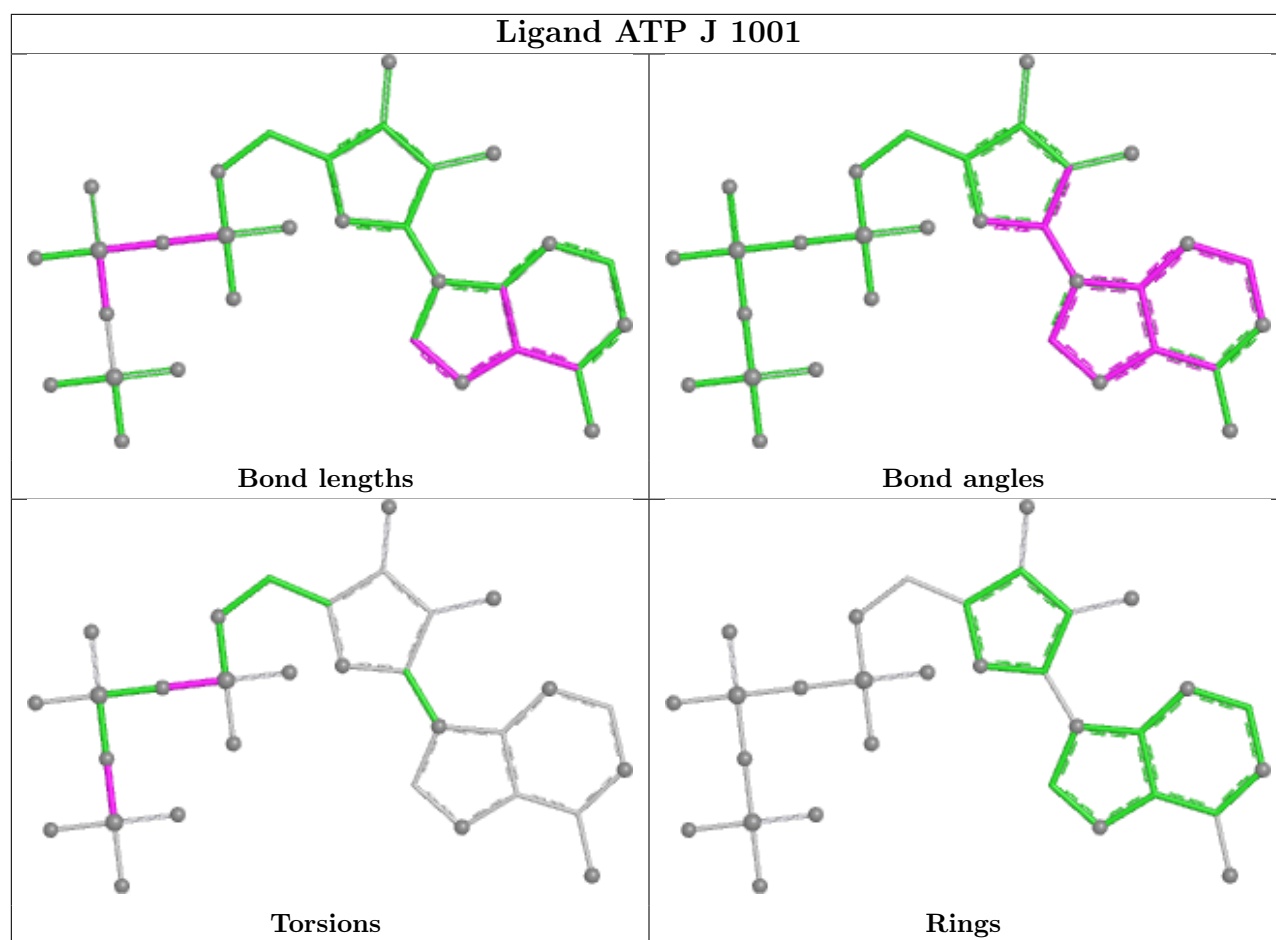


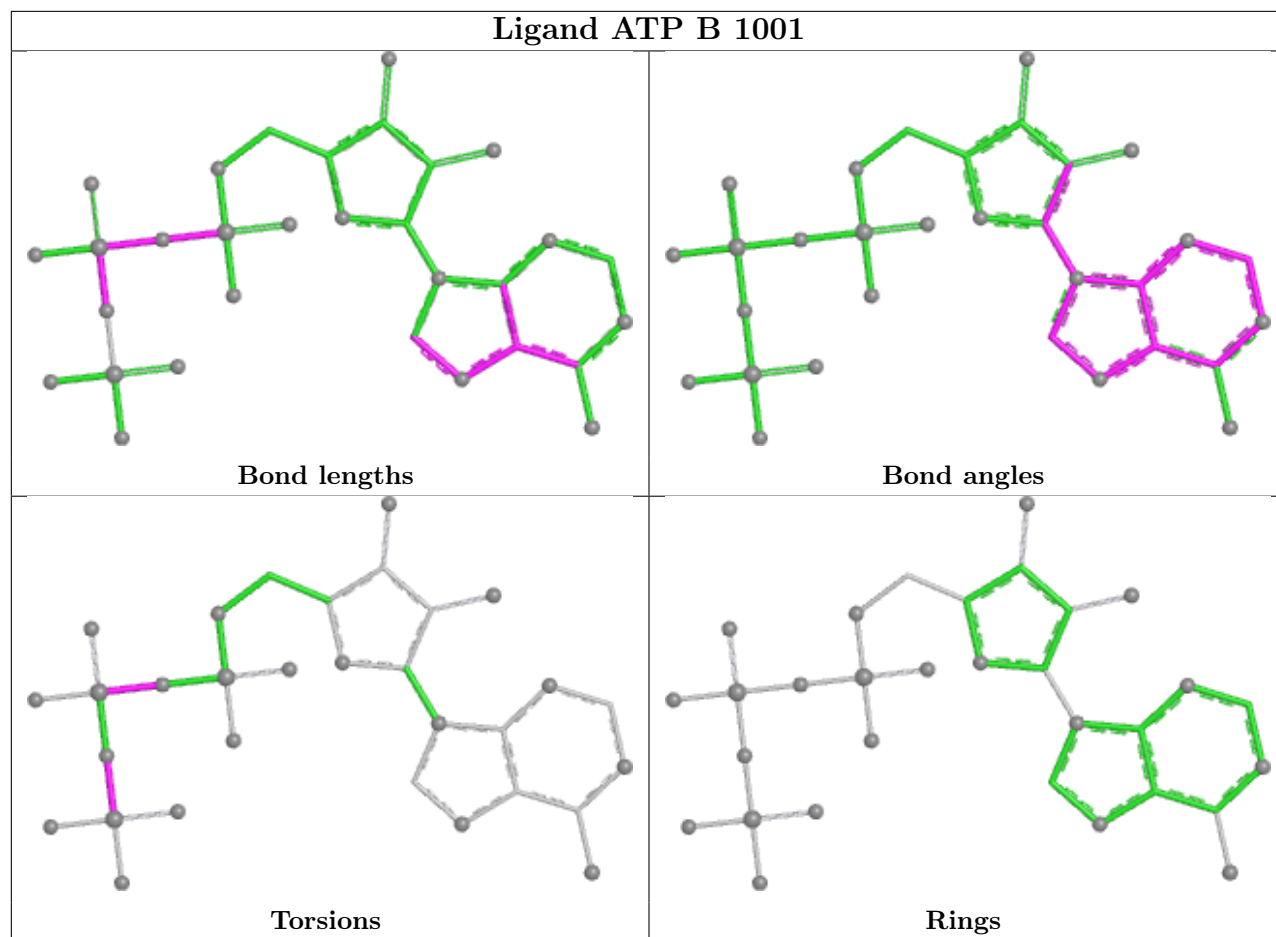


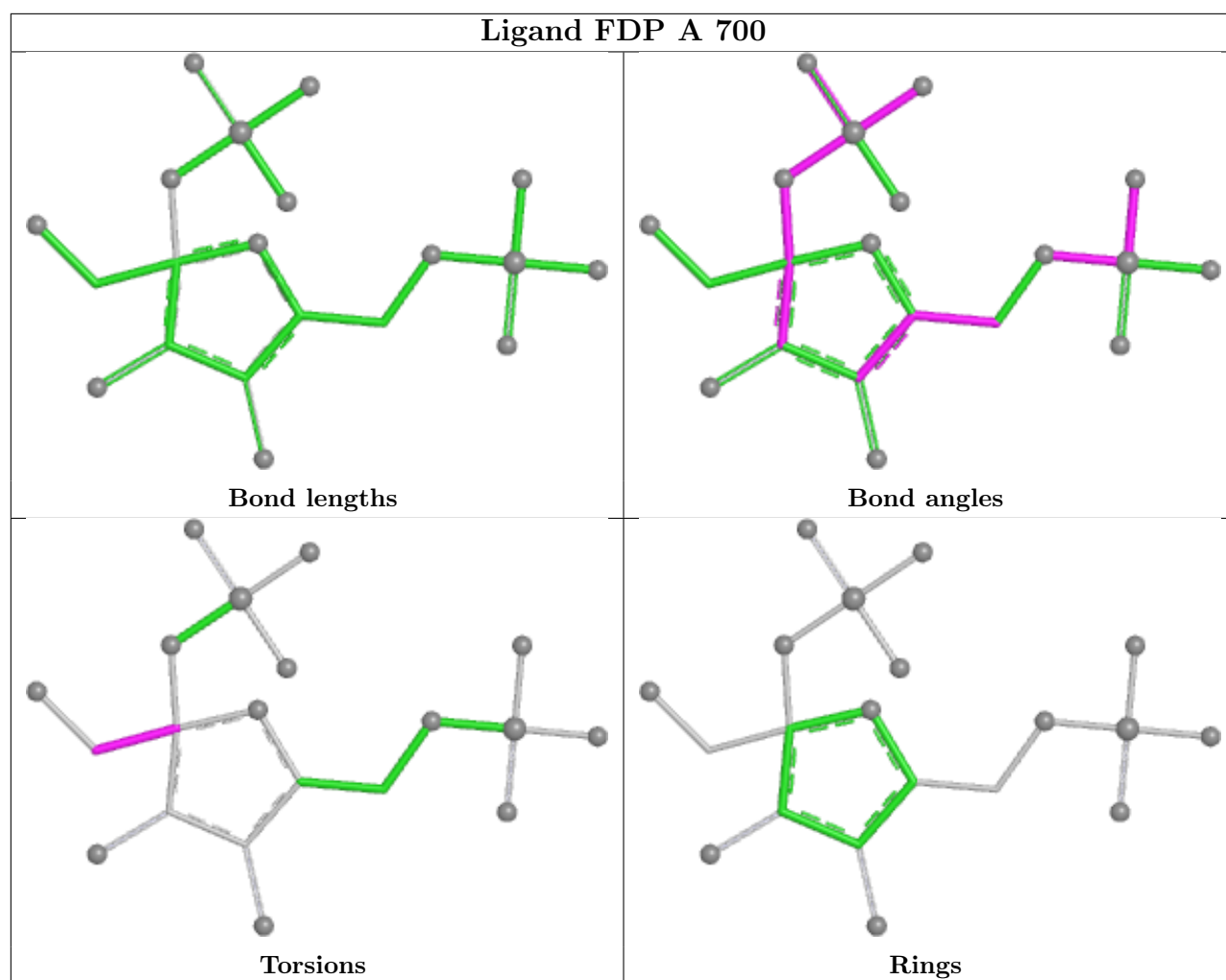


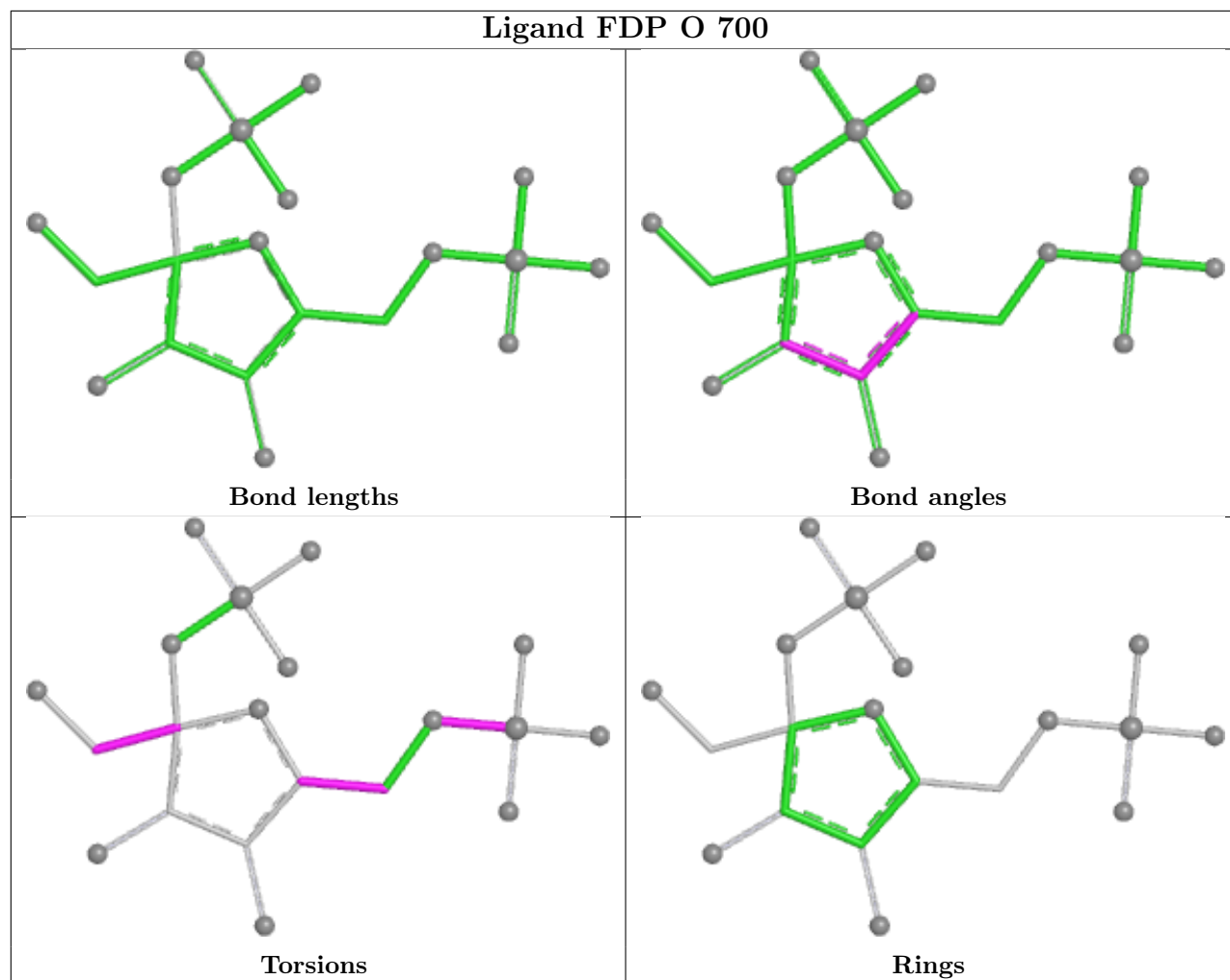


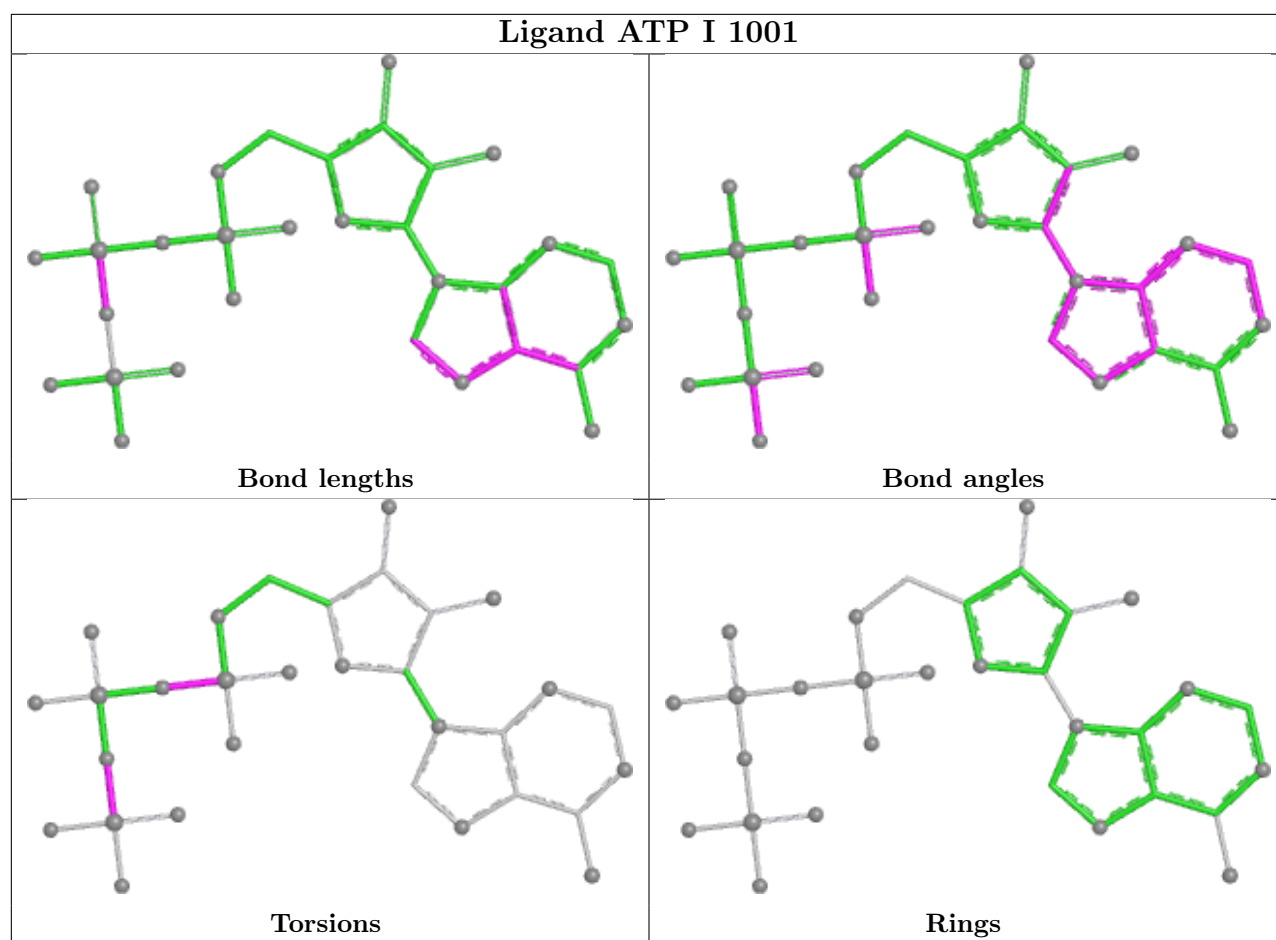


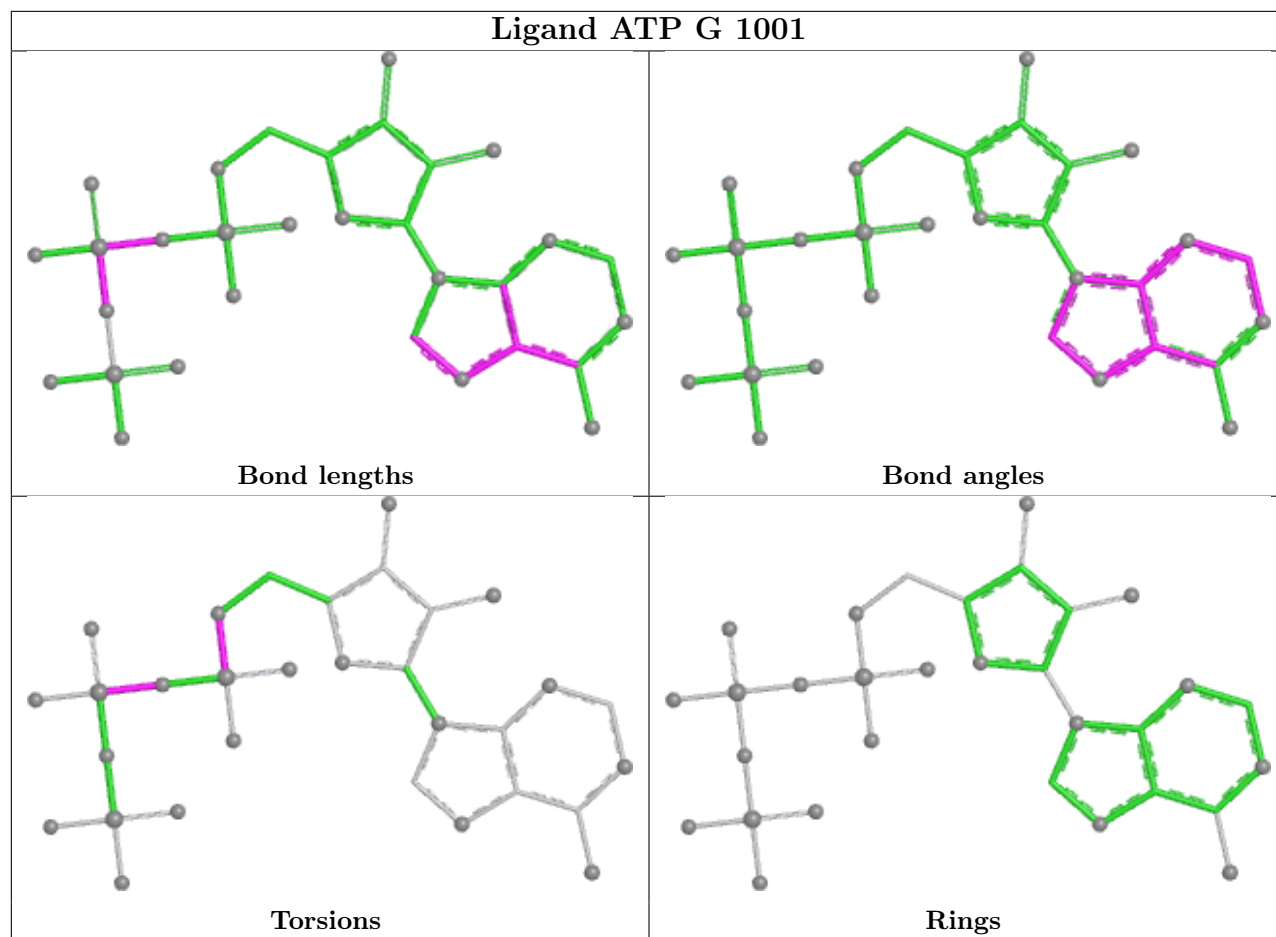


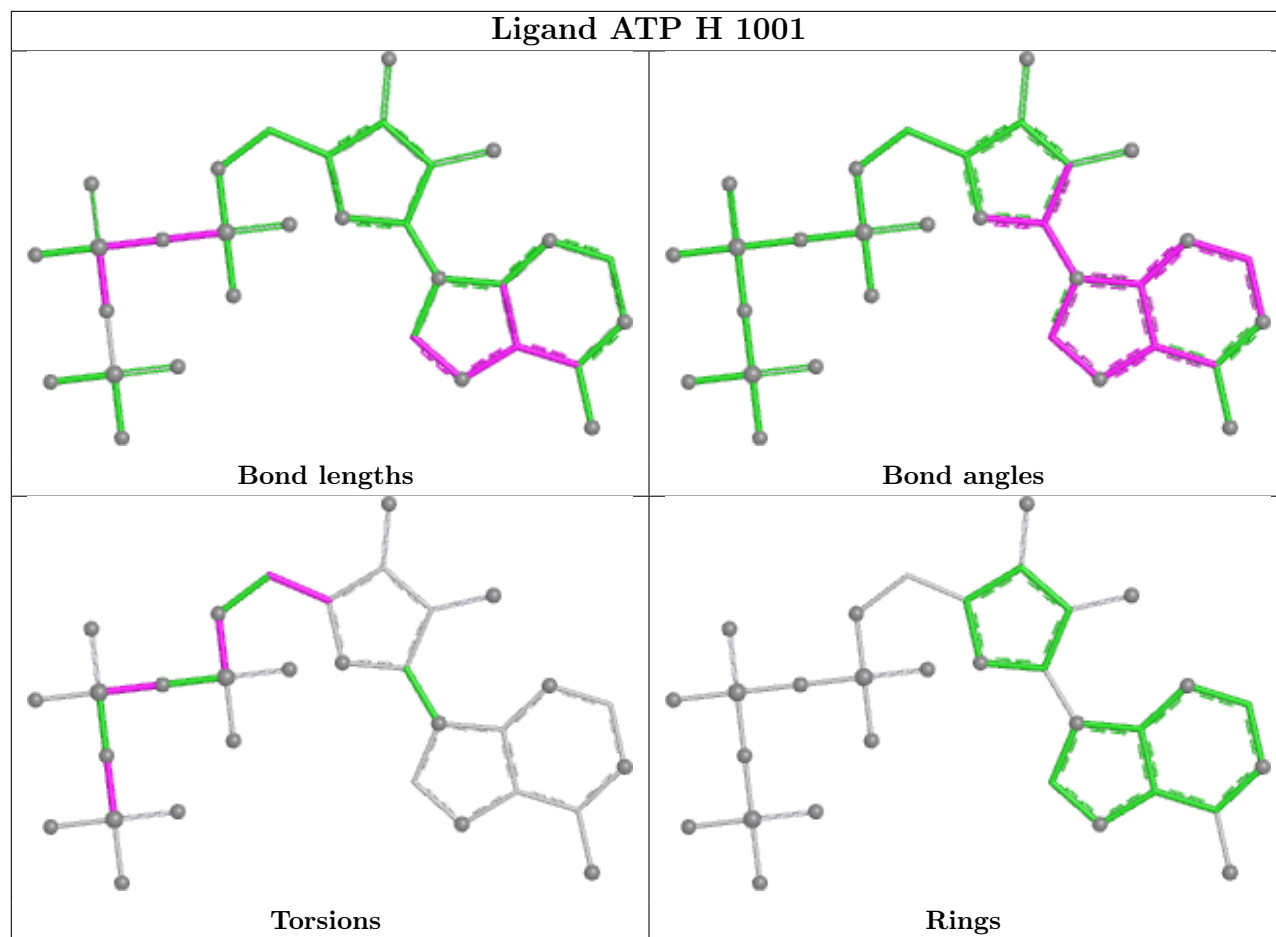


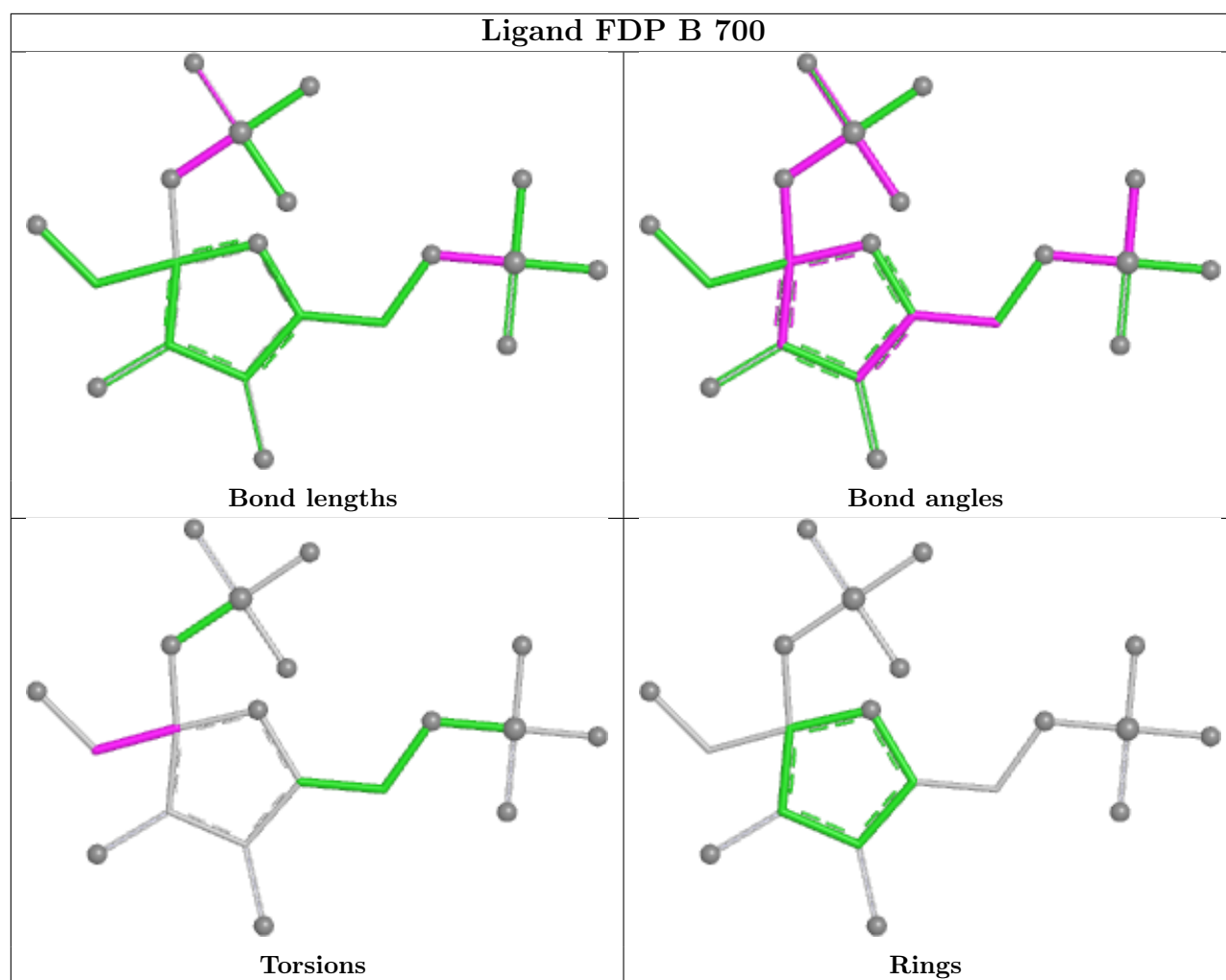


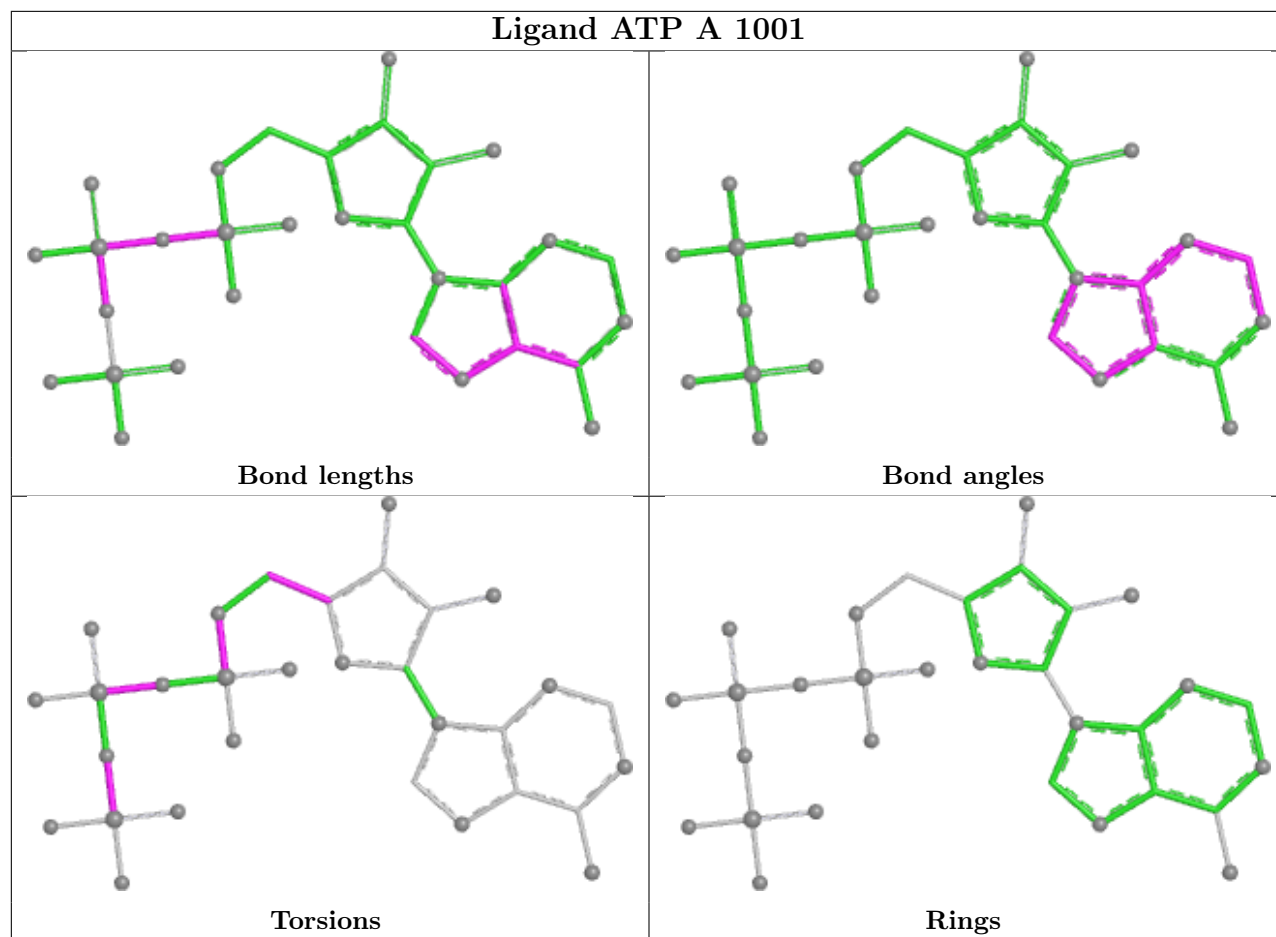


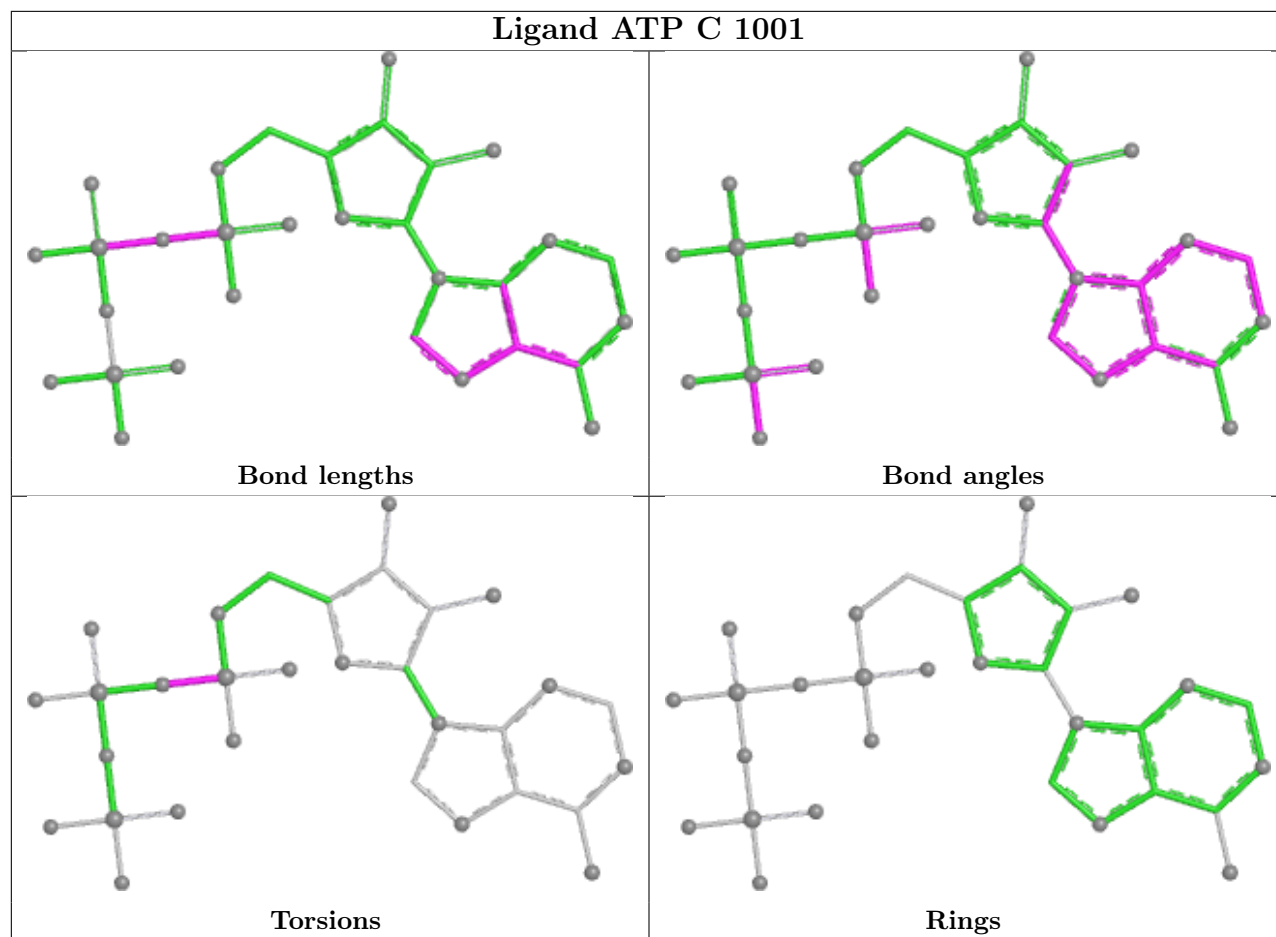


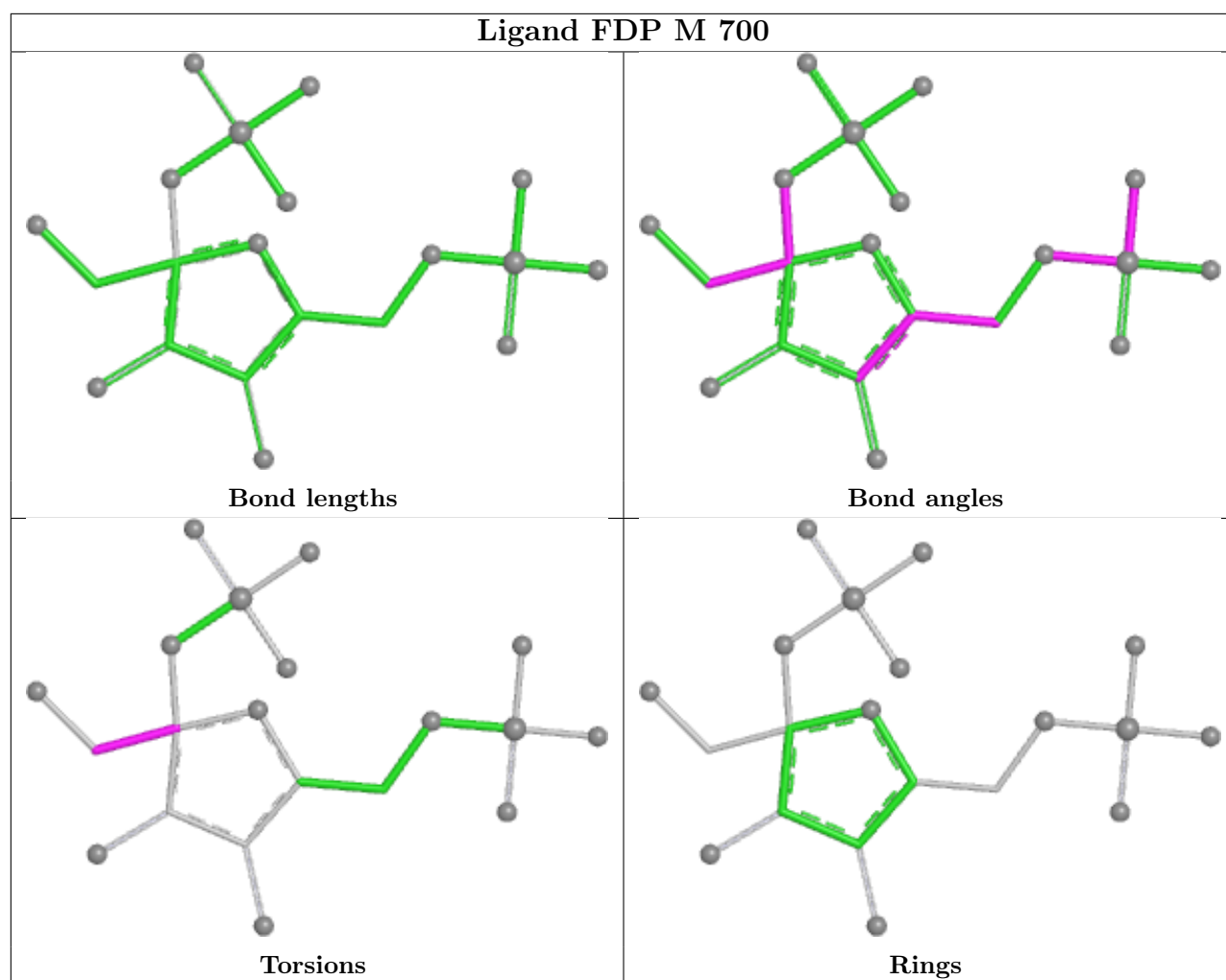




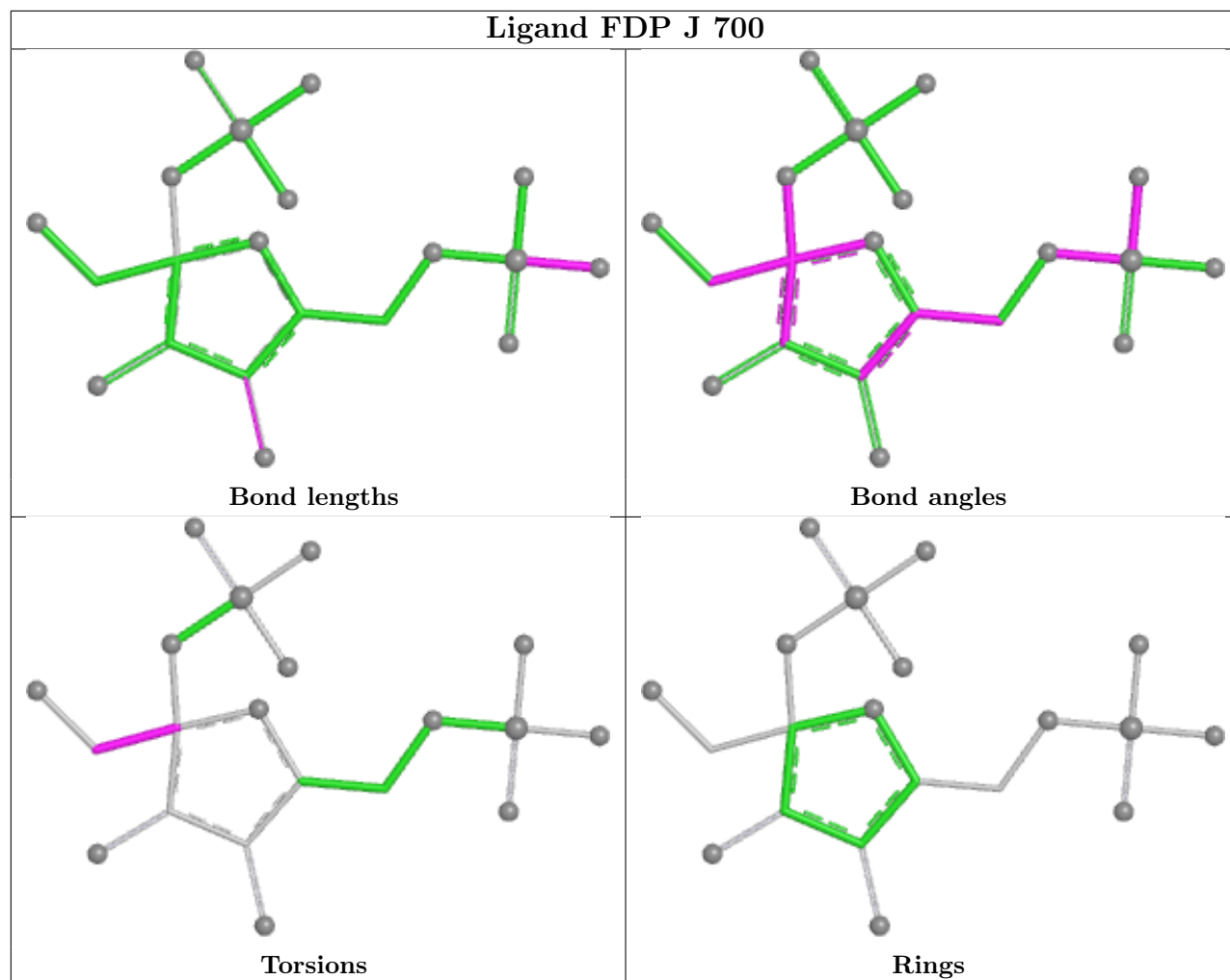


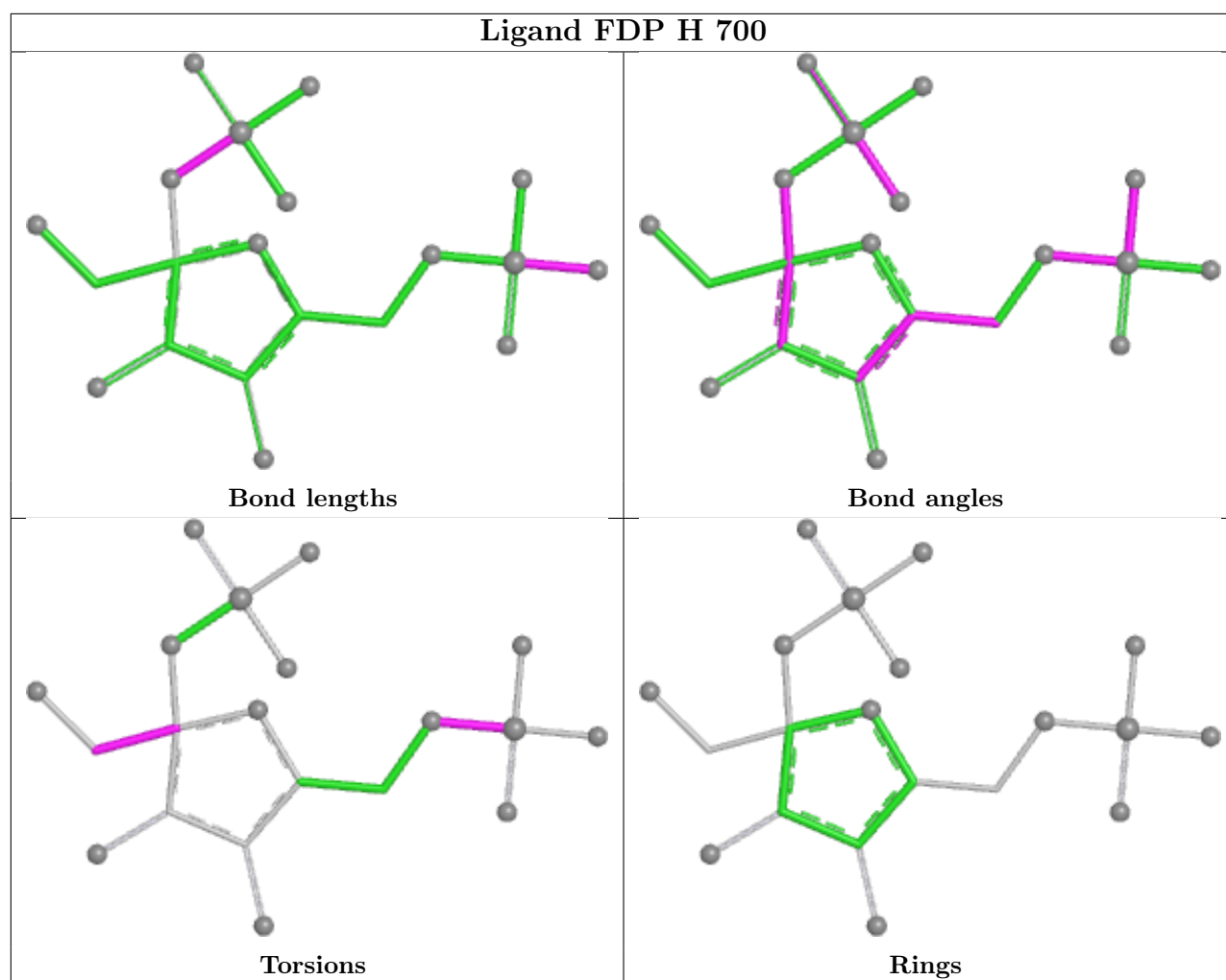


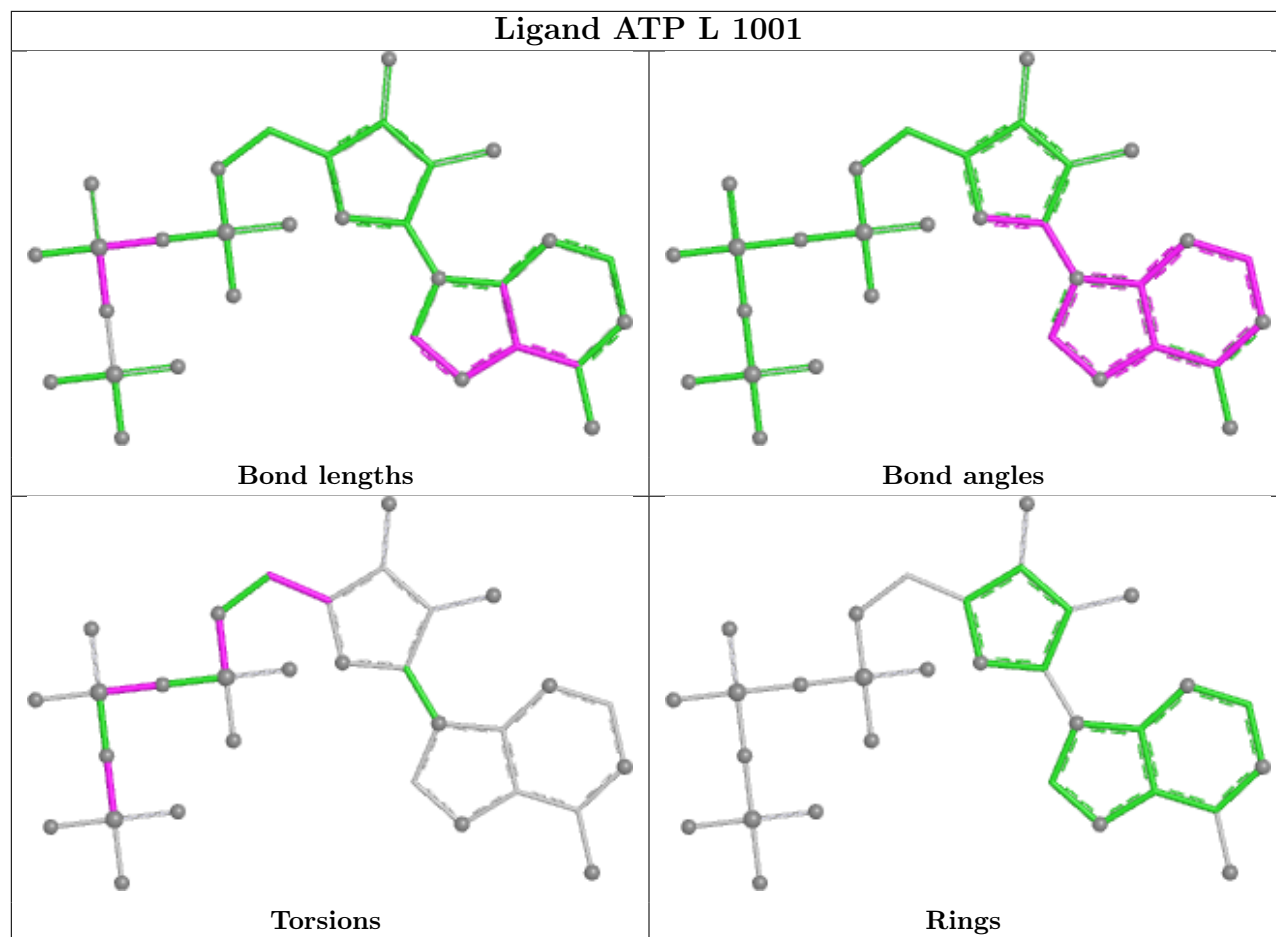


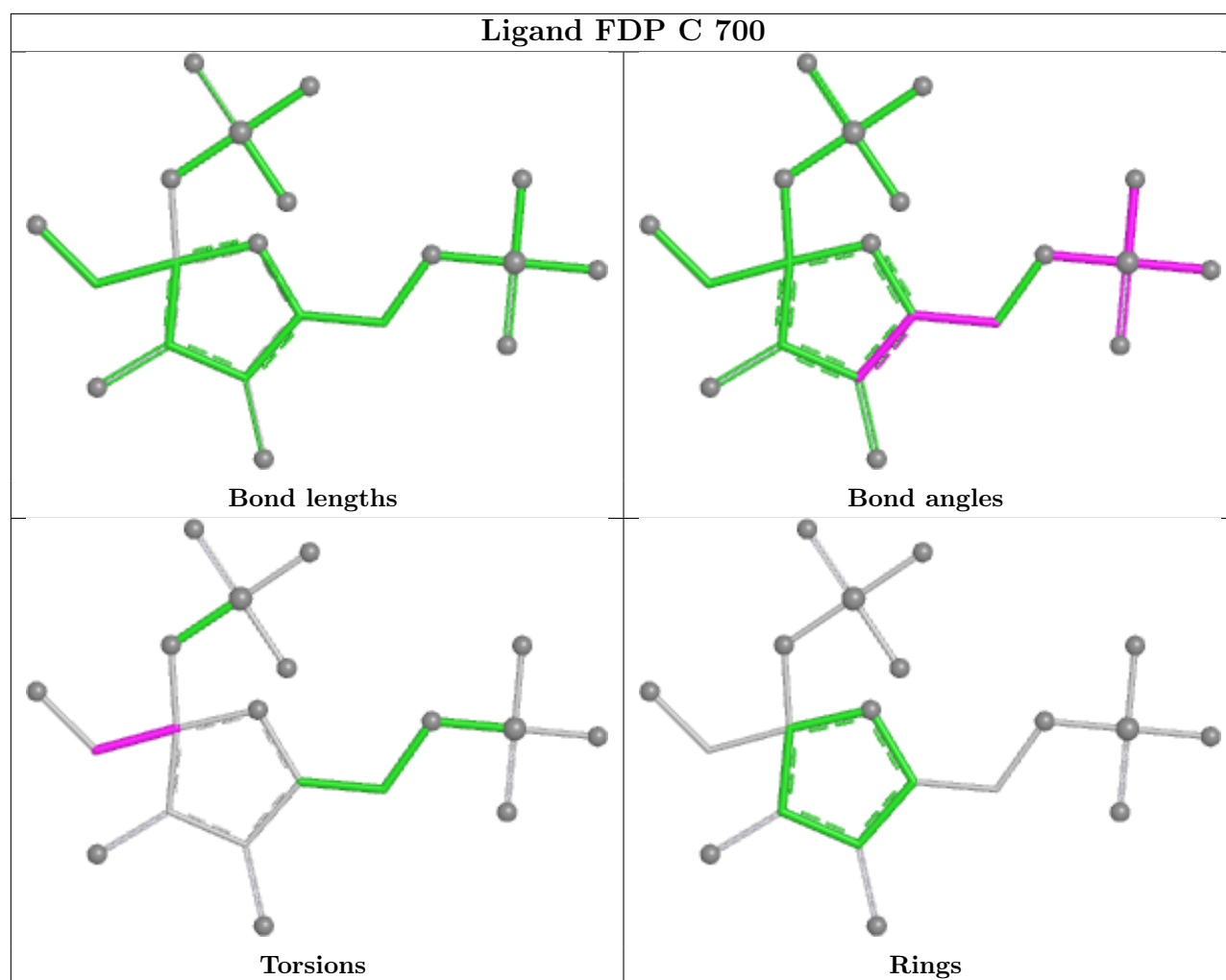


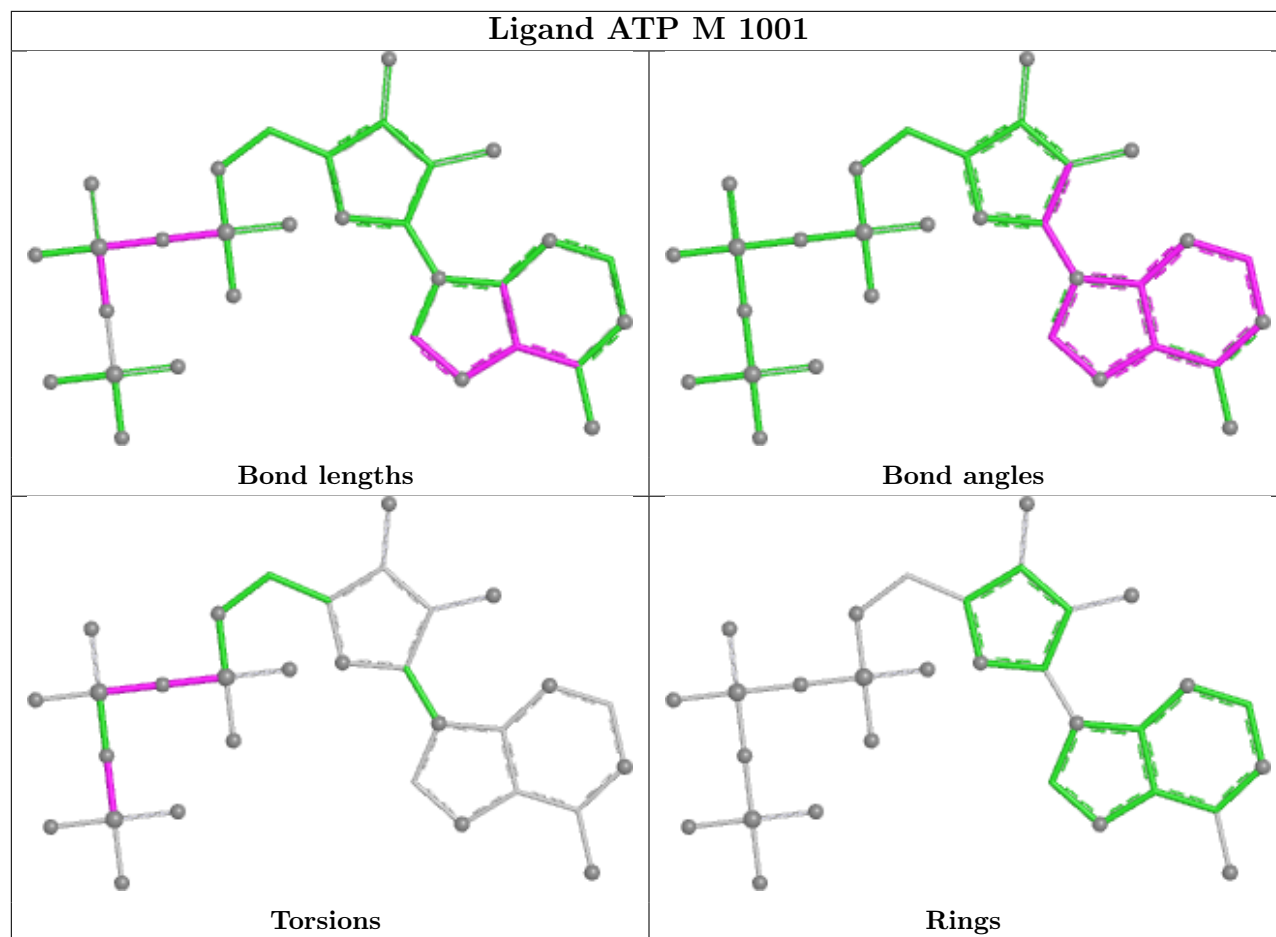
Ligand FDP J 700

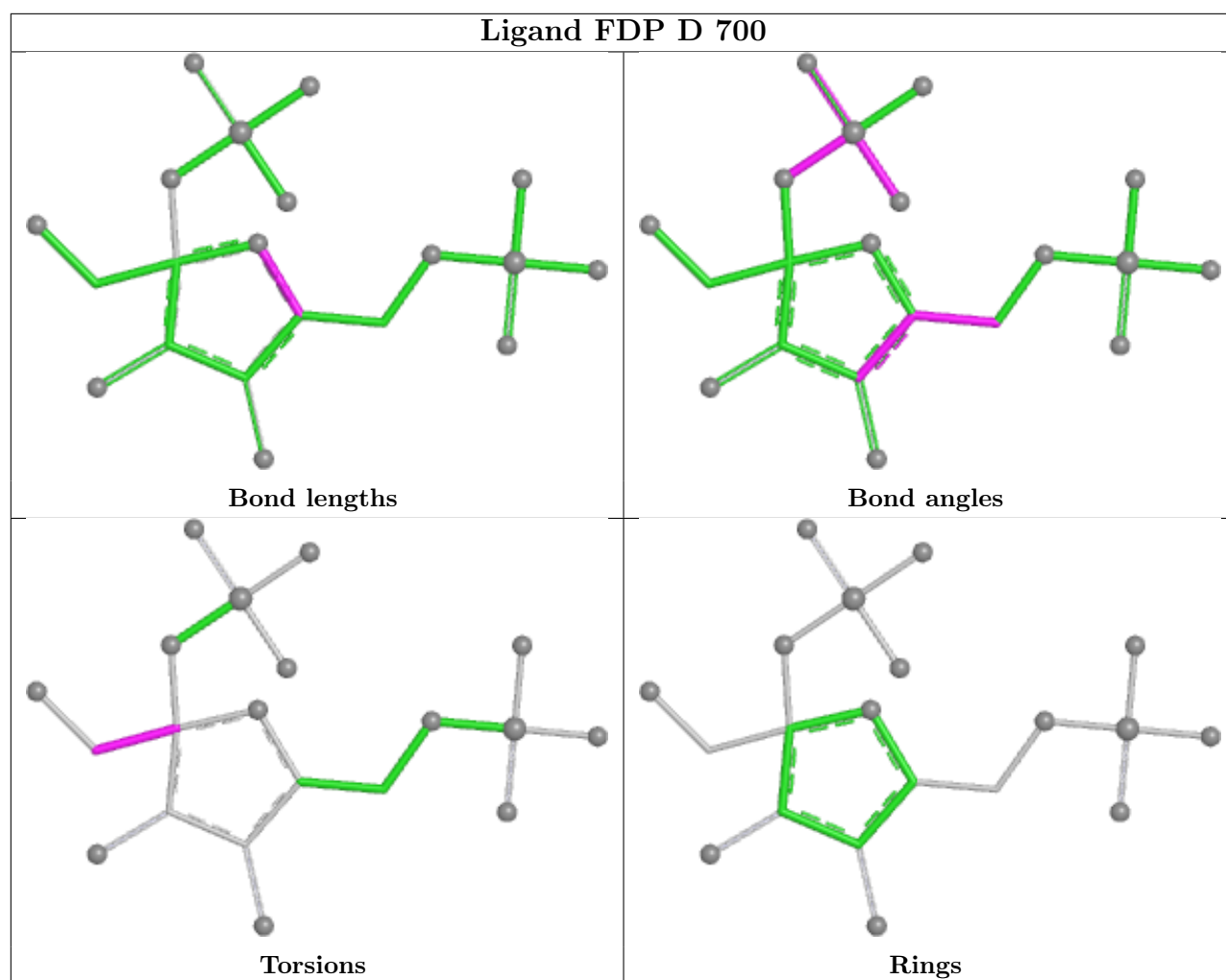


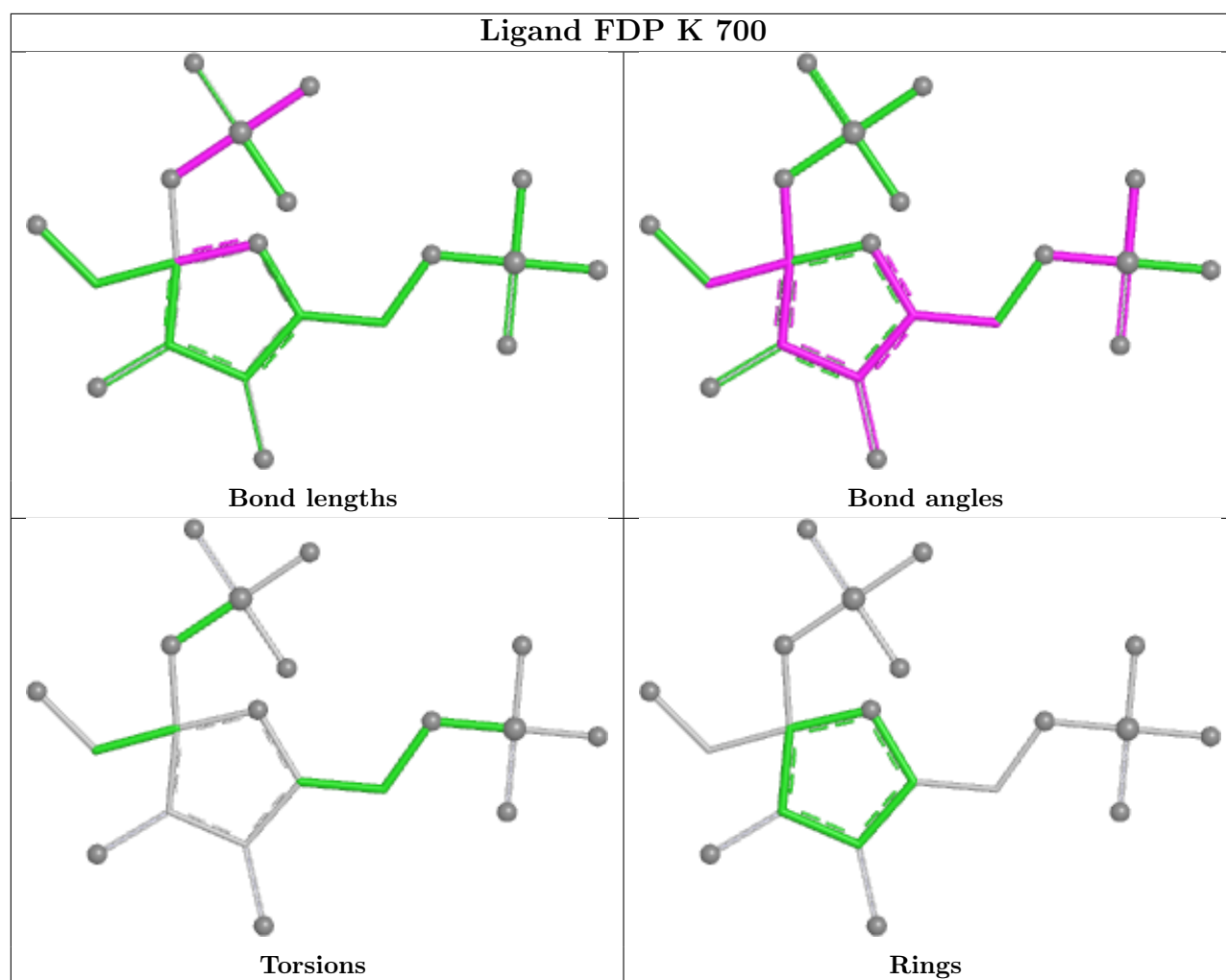




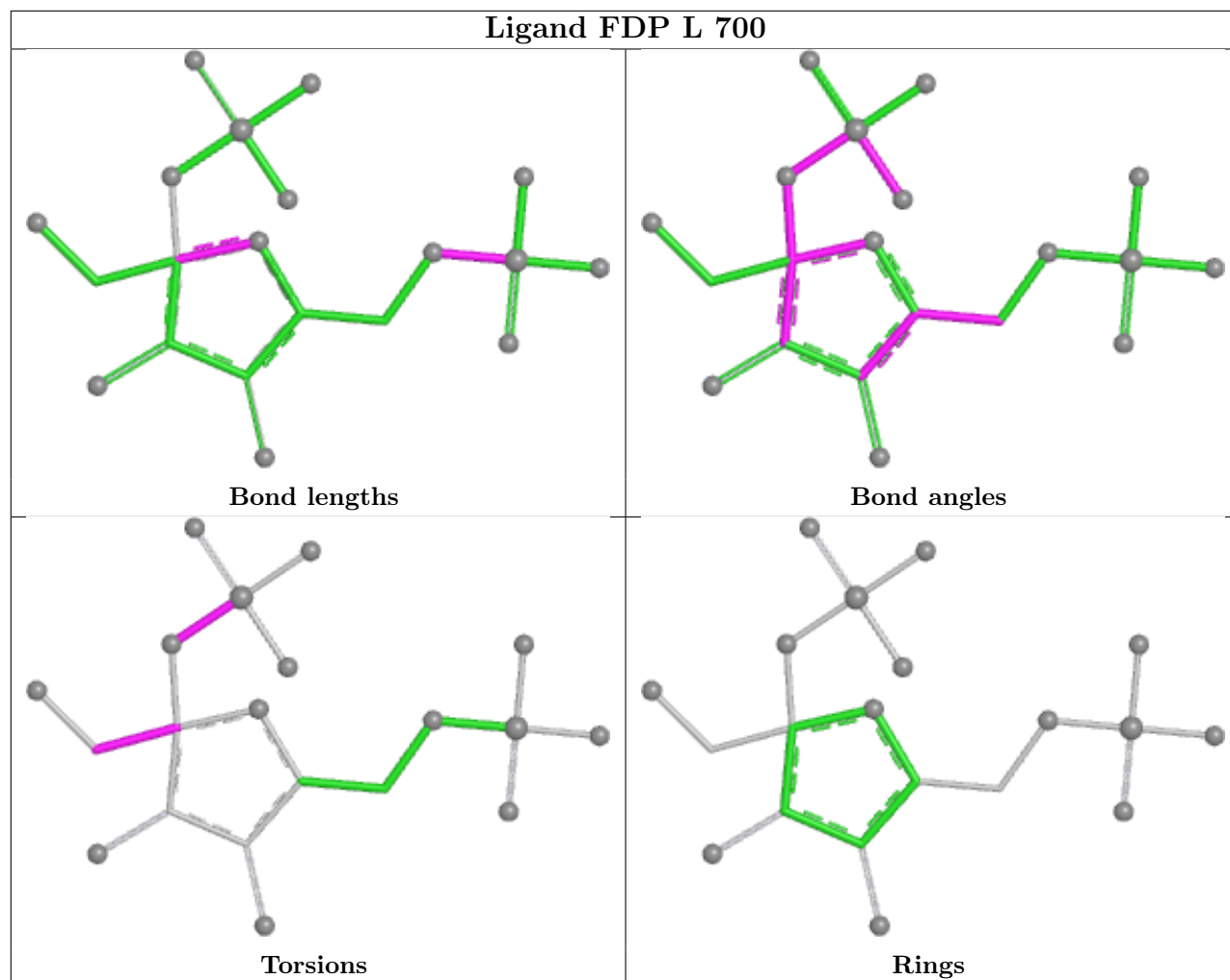




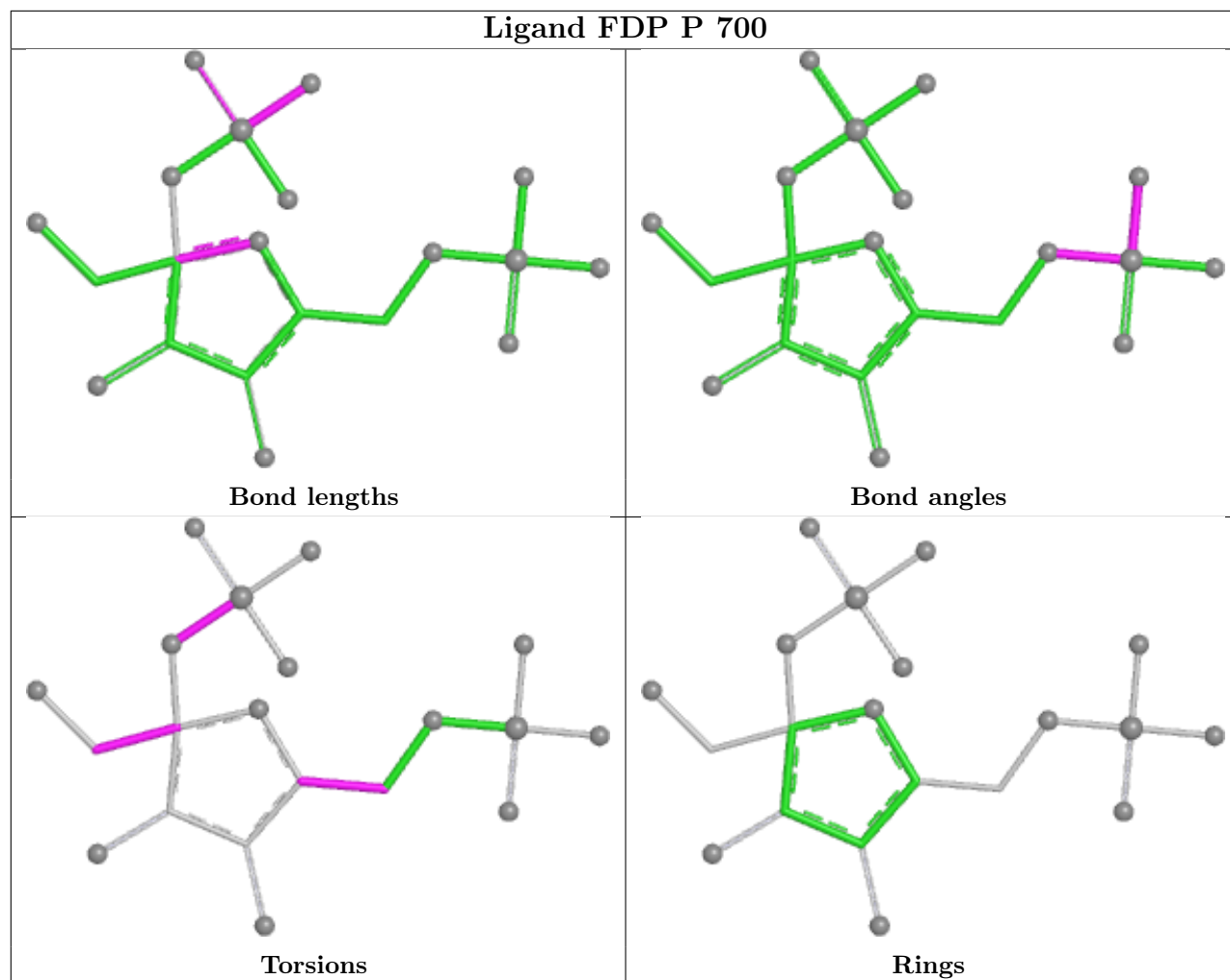


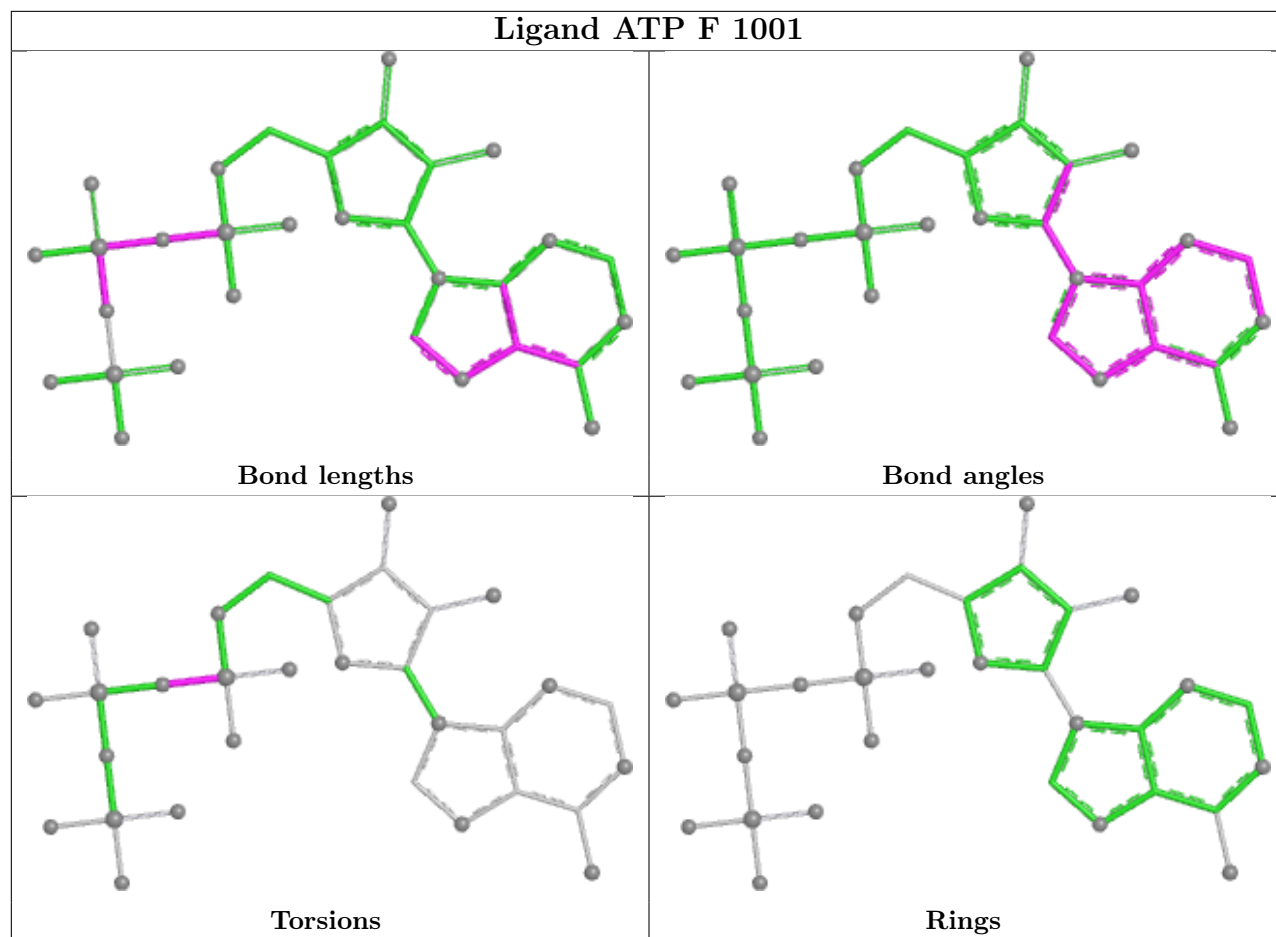


Ligand FDP L 700

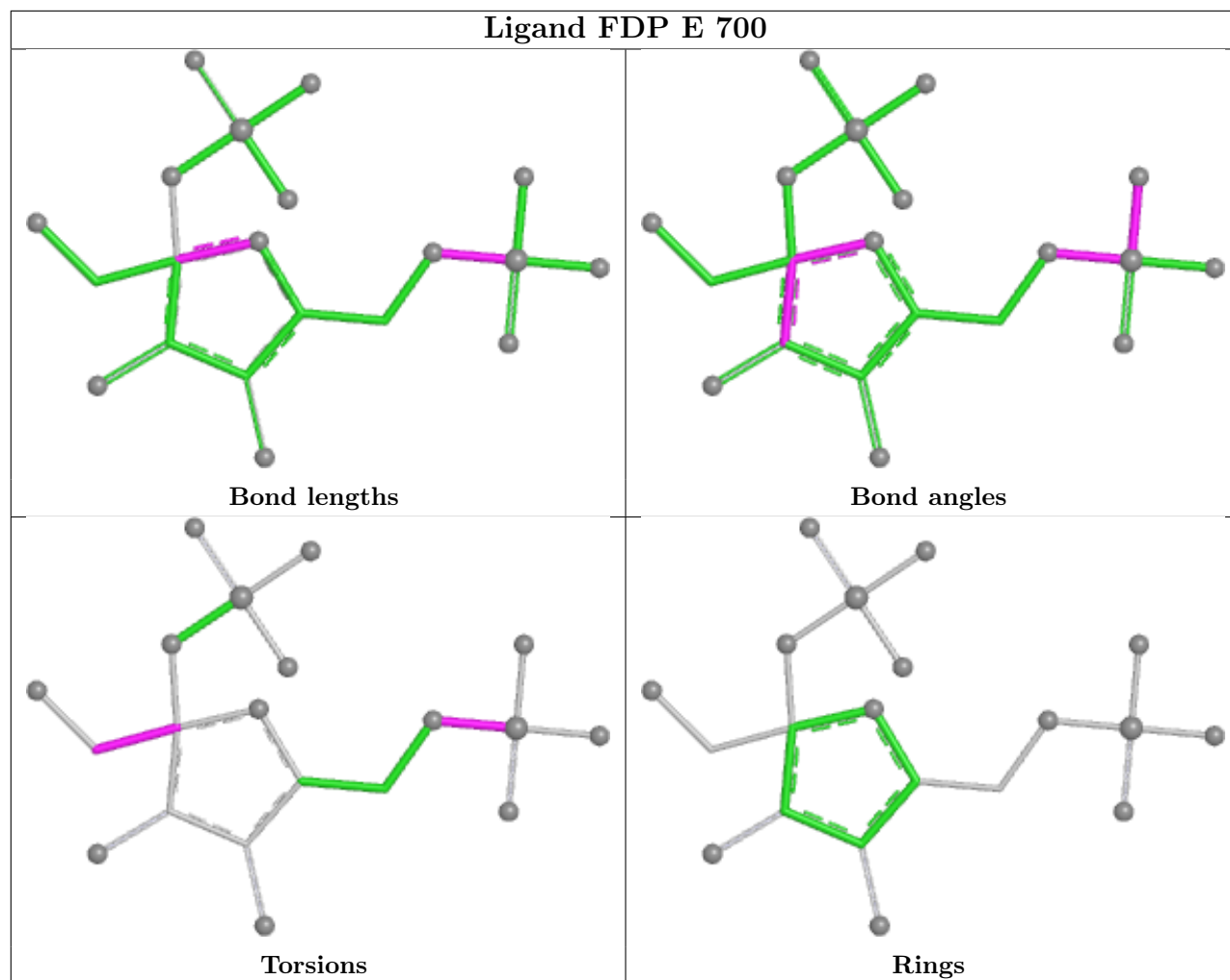


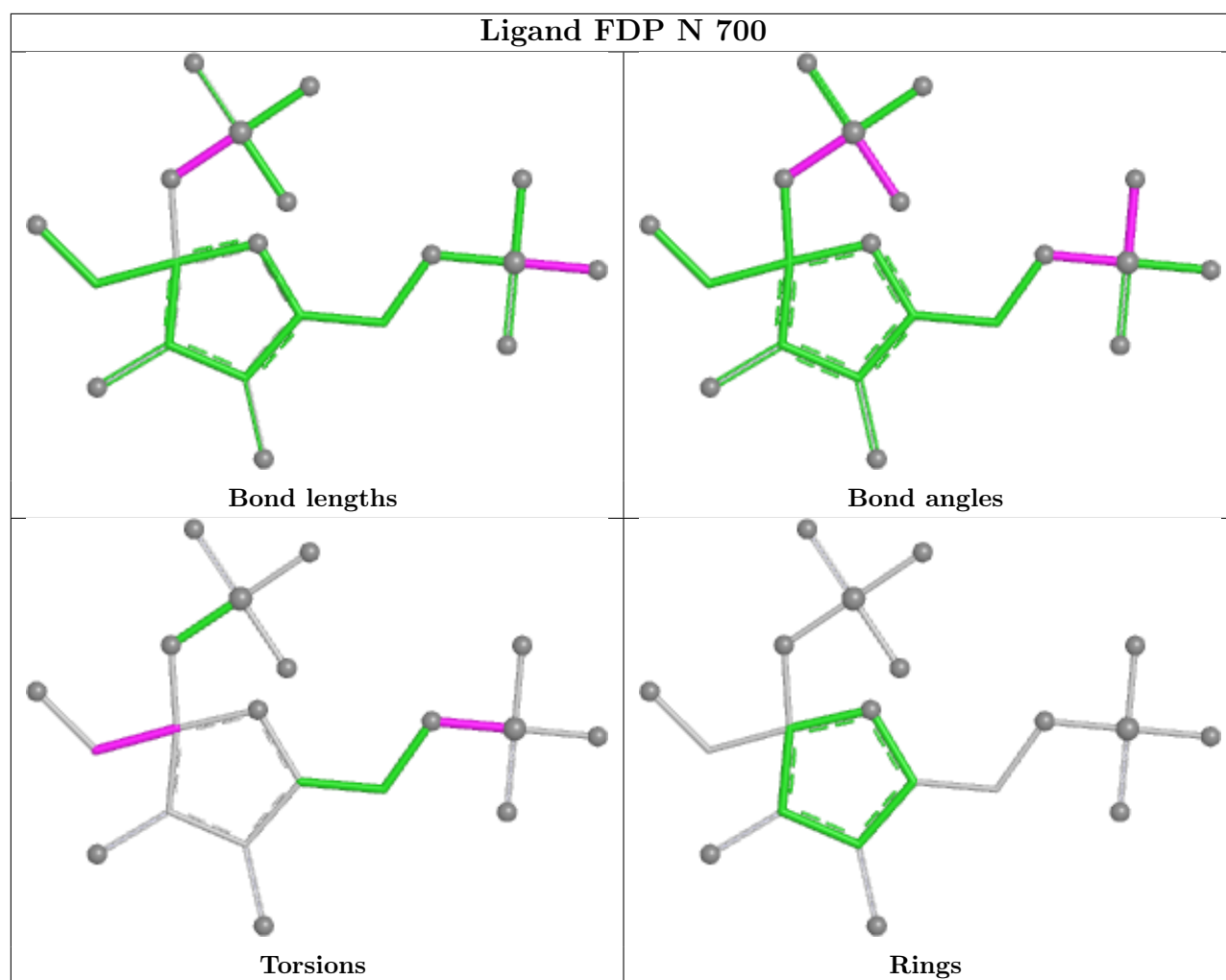
Ligand FDP P 700



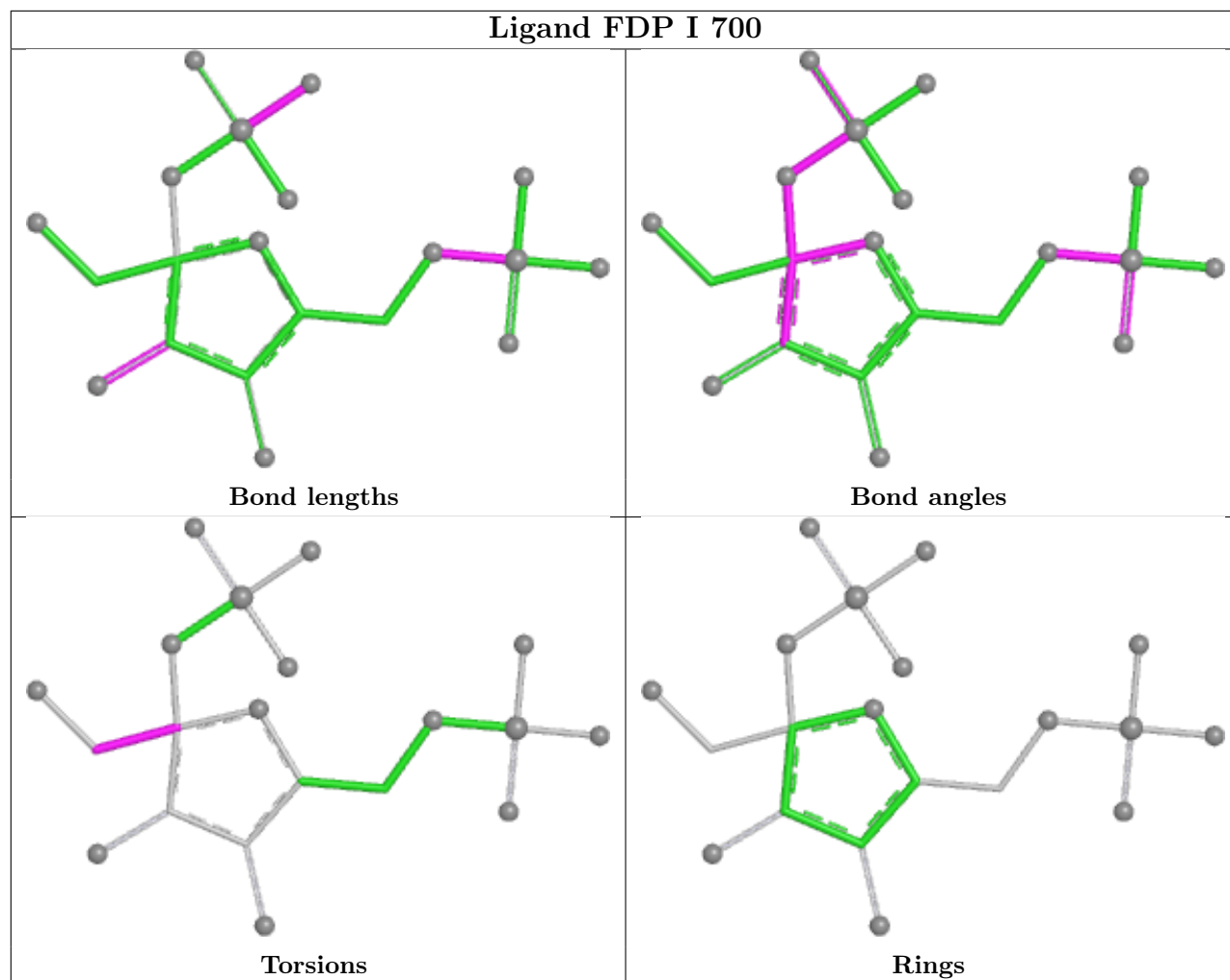


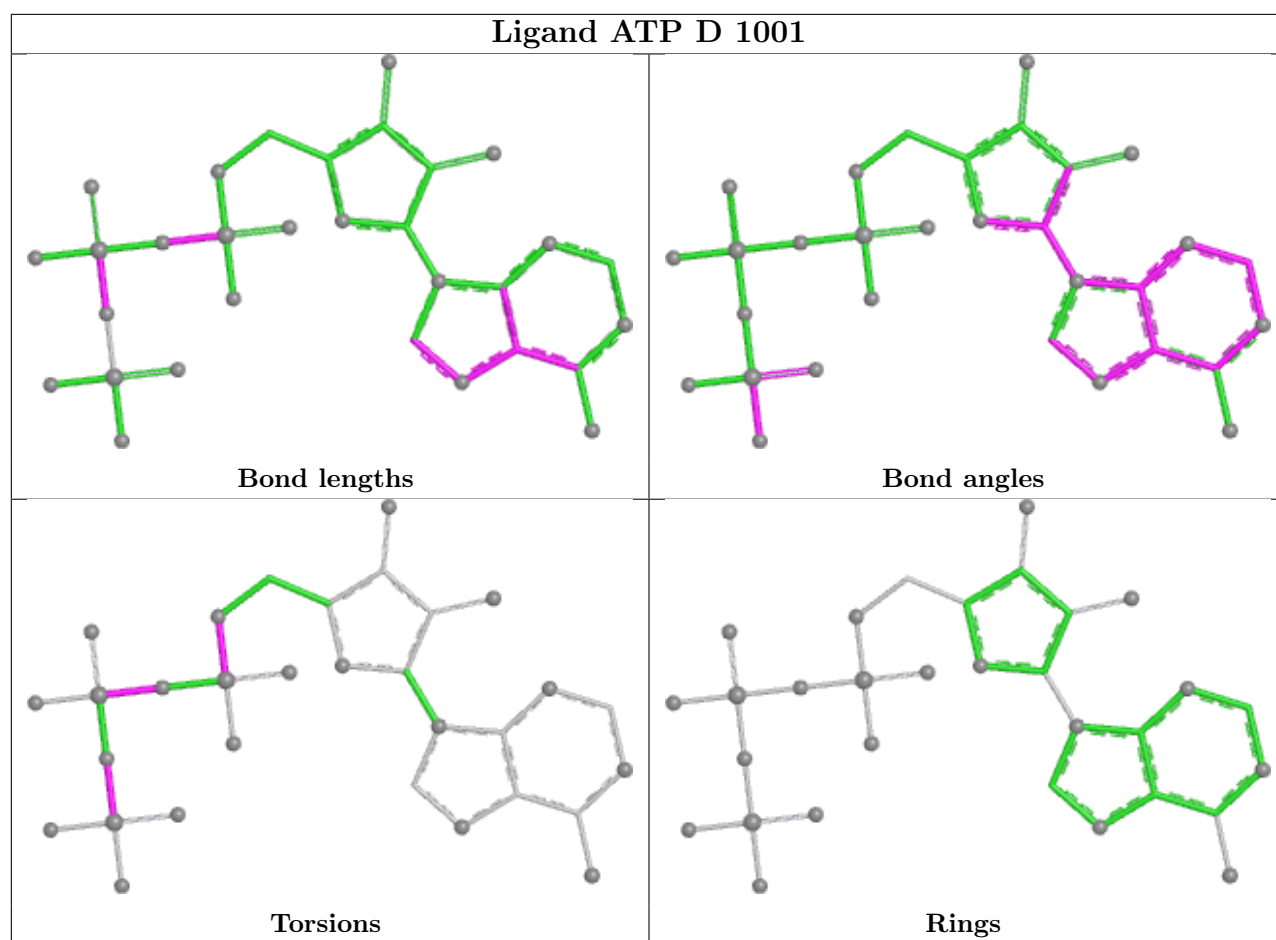
Ligand FDP E 700

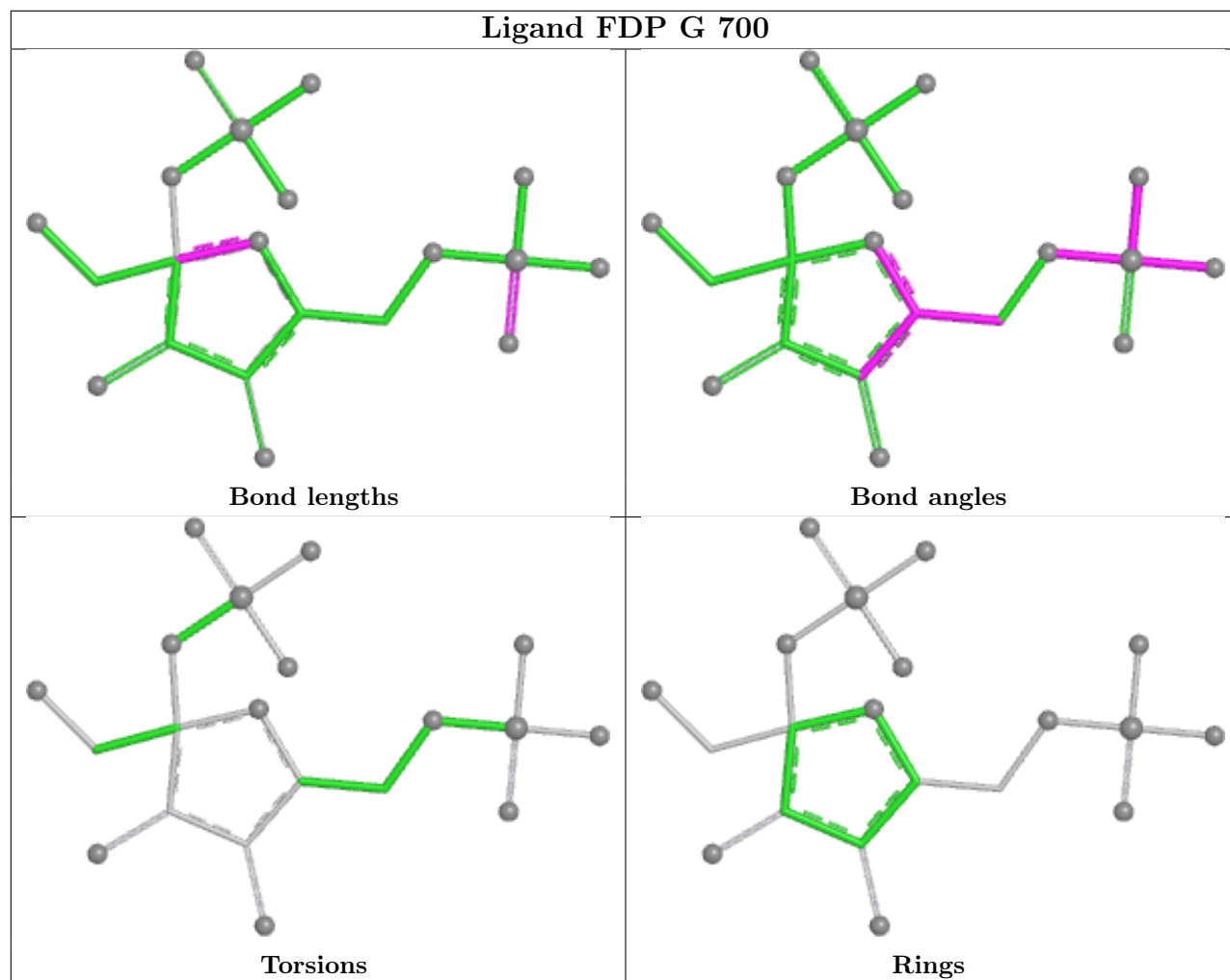




Ligand FDP I 700







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, 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%)	0.65	36 (7%) 21 23	19, 42, 59, 61	2 (0%)
1	B	498/499 (99%)	-0.22	2 (0%) 88 89	15, 25, 34, 42	0
1	C	498/499 (99%)	0.16	5 (1%) 79 80	16, 39, 50, 59	2 (0%)
1	D	498/499 (99%)	-0.21	1 (0%) 91 91	14, 27, 43, 45	1 (0%)
1	E	498/499 (99%)	0.45	26 (5%) 33 34	19, 42, 52, 56	1 (0%)
1	F	498/499 (99%)	0.66	25 (5%) 34 35	36, 52, 66, 70	0
1	G	498/499 (99%)	1.16	76 (15%) 5 6	44, 52, 60, 63	0
1	H	498/499 (99%)	0.50	14 (2%) 55 57	21, 46, 52, 55	2 (0%)
1	I	498/499 (99%)	-0.13	9 (1%) 67 69	7, 22, 47, 53	2 (0%)
1	J	498/499 (99%)	-0.22	4 (0%) 82 83	10, 22, 30, 41	3 (0%)
1	K	498/499 (99%)	-0.31	3 (0%) 85 86	10, 22, 31, 40	2 (0%)
1	L	498/499 (99%)	0.32	30 (6%) 27 29	19, 29, 60, 62	0
1	M	498/499 (99%)	0.46	21 (4%) 40 42	35, 47, 56, 59	0
1	N	498/499 (99%)	0.85	39 (7%) 19 21	23, 60, 69, 71	1 (0%)
1	O	498/499 (99%)	1.07	66 (13%) 7 8	35, 55, 84, 86	0
1	P	498/499 (99%)	1.08	59 (11%) 9 10	48, 60, 83, 86	0
All	All	7968/7984 (99%)	0.39	416 (5%) 33 34	7, 43, 65, 86	16 (0%)

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	7	LEU	5.4
1	L	172	SER	5.0
1	O	444	ALA	4.3
1	L	145	ASP	4.2
1	M	266	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	P	184	VAL	4.1
1	O	113	PRO	4.1
1	L	99	ALA	4.0
1	P	147	ILE	3.8
1	M	119	GLY	3.8
1	M	195	VAL	3.8
1	E	176	GLY	3.8
1	G	380	VAL	3.8
1	G	9	LEU	3.7
1	G	8	THR	3.7
1	G	100	VAL	3.6
1	N	444	ALA	3.6
1	E	147	ILE	3.6
1	O	83	ASP	3.6
1	G	109	VAL	3.6
1	A	163	CYS	3.5
1	P	134	VAL	3.5
1	G	87	PRO	3.5
1	M	182	CYS	3.5
1	G	3	LEU	3.5
1	F	11	ILE	3.5
1	P	100	VAL	3.4
1	L	143	ILE	3.4
1	F	3	LEU	3.4
1	K	183	ASP	3.4
1	F	12	PHE	3.4
1	A	20	ALA	3.4
1	M	191	ALA	3.4
1	P	431	LEU	3.4
1	L	146	GLY	3.4
1	P	78	ILE	3.3
1	G	99	ALA	3.3
1	P	252	ILE	3.3
1	O	100	VAL	3.3
1	E	100	VAL	3.3
1	L	195	VAL	3.3
1	M	105	ALA	3.2
1	O	475	TYR	3.2
1	G	186	LEU	3.2
1	P	161	LEU	3.2
1	G	12	PHE	3.2
1	F	109	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	4	ALA	3.2
1	O	481	ALA	3.2
1	L	196	ASP	3.2
1	H	168	SER	3.2
1	G	114	ALA	3.2
1	I	134	VAL	3.2
1	P	135	VAL	3.2
1	M	118	LYS	3.1
1	I	13	ASP	3.1
1	G	187	PRO	3.1
1	G	230	GLY	3.1
1	I	135	VAL	3.1
1	G	124	PHE	3.1
1	N	96	GLY	3.1
1	L	147	ILE	3.1
1	E	94	PHE	3.1
1	C	185	ASP	3.1
1	O	147	ILE	3.0
1	M	170	THR	3.0
1	O	120	THR	3.0
1	F	112	ASP	3.0
1	P	428	CYS	3.0
1	A	3	LEU	3.0
1	A	7	LEU	3.0
1	A	158	GLU	3.0
1	L	177	VAL	3.0
1	O	95	VAL	3.0
1	A	9	LEU	3.0
1	P	470	VAL	3.0
1	E	366	ILE	3.0
1	O	39	GLY	3.0
1	N	114	ALA	2.9
1	H	497	VAL	2.9
1	E	143	ILE	2.9
1	E	171	ILE	2.9
1	E	166	THR	2.9
1	G	108	TYR	2.9
1	F	1	SER	2.9
1	E	12	PHE	2.9
1	G	197	LEU	2.9
1	O	160	THR	2.9
1	P	9	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	201	VAL	2.9
1	G	82	LEU	2.9
1	O	216	ALA	2.9
1	O	496	LEU	2.9
1	P	410	ALA	2.9
1	A	165	VAL	2.9
1	H	34	VAL	2.9
1	O	234	MET	2.9
1	L	148	LEU	2.8
1	M	165	VAL	2.8
1	E	145	ASP	2.8
1	A	261	ALA	2.8
1	F	213	ILE	2.8
1	O	170	THR	2.8
1	O	483	HIS	2.7
1	O	492	THR	2.7
1	P	11	ILE	2.7
1	P	451	GLU	2.7
1	P	186	LEU	2.7
1	F	6	ASN	2.7
1	G	89	ILE	2.7
1	H	181	GLY	2.7
1	A	107	CYS	2.7
1	G	271	ALA	2.7
1	G	406	ALA	2.7
1	G	134	VAL	2.7
1	G	252	ILE	2.7
1	A	4	ALA	2.7
1	I	12	PHE	2.7
1	F	15	VAL	2.7
1	O	134	VAL	2.7
1	L	120	THR	2.7
1	A	97	GLY	2.7
1	G	176	GLY	2.7
1	G	1	SER	2.7
1	L	175	ARG	2.7
1	G	362	PHE	2.6
1	L	125	TYR	2.6
1	L	100	VAL	2.6
1	L	189	VAL	2.6
1	G	372	ILE	2.6
1	L	149	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	171	ILE	2.6
1	N	257	GLY	2.6
1	F	107	CYS	2.6
1	G	121	LYS	2.6
1	P	81	ALA	2.6
1	A	18	TYR	2.6
1	F	221	ASP	2.6
1	A	62	THR	2.6
1	G	31	THR	2.6
1	N	152	VAL	2.6
1	N	97	GLY	2.6
1	G	198	GLN	2.6
1	P	408	LEU	2.6
1	P	133	LYS	2.6
1	H	116	ALA	2.6
1	G	63	THR	2.6
1	L	119	GLY	2.6
1	O	140	TYR	2.6
1	M	190	SER	2.6
1	G	371	HIS	2.6
1	L	198	GLN	2.6
1	P	496	LEU	2.6
1	G	458	ALA	2.6
1	J	4	ALA	2.6
1	L	191	ALA	2.6
1	N	259	MET	2.6
1	G	14	PRO	2.6
1	N	111	THR	2.6
1	O	142	TYR	2.6
1	I	181	GLY	2.5
1	G	52	PHE	2.5
1	A	1	SER	2.5
1	A	76	VAL	2.5
1	I	177	VAL	2.5
1	I	189	VAL	2.5
1	N	245	VAL	2.5
1	N	125	TYR	2.5
1	F	183	ASP	2.5
1	K	185	ASP	2.5
1	K	464	ALA	2.5
1	O	116	ALA	2.5
1	P	105	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	444	ALA	2.5
1	P	187	PRO	2.5
1	N	140	TYR	2.5
1	H	20	ALA	2.5
1	A	8	THR	2.5
1	N	160	THR	2.5
1	L	194	ARG	2.5
1	M	156	GLU	2.5
1	O	233	ILE	2.5
1	O	275	VAL	2.5
1	E	148	LEU	2.5
1	G	98	ASP	2.5
1	A	14	PRO	2.5
1	F	263	GLY	2.5
1	G	147	ILE	2.4
1	N	177	VAL	2.4
1	E	142	TYR	2.4
1	F	7	LEU	2.4
1	E	144	ASP	2.4
1	N	483	HIS	2.4
1	O	70	ALA	2.4
1	P	107	CYS	2.4
1	N	109	VAL	2.4
1	P	89	ILE	2.4
1	J	7	LEU	2.4
1	E	108	TYR	2.4
1	G	377	ASP	2.4
1	P	232	ASP	2.4
1	E	99	ALA	2.4
1	P	481	ALA	2.4
1	P	160	THR	2.4
1	O	1	SER	2.4
1	A	34	VAL	2.4
1	A	100	VAL	2.4
1	A	201	VAL	2.4
1	H	147	ILE	2.4
1	P	233	ILE	2.4
1	E	162	GLU	2.4
1	F	184	VAL	2.4
1	G	95	VAL	2.4
1	G	219	VAL	2.4
1	M	186	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	451	GLU	2.4
1	N	271	ALA	2.3
1	A	11	ILE	2.3
1	C	184	VAL	2.3
1	H	12	PHE	2.3
1	P	124	PHE	2.3
1	P	398	VAL	2.3
1	L	179	LEU	2.3
1	P	325	ASP	2.3
1	E	345	TYR	2.3
1	G	18	TYR	2.3
1	N	113	PRO	2.3
1	O	108	TYR	2.3
1	P	125	TYR	2.3
1	P	191	ALA	2.3
1	F	60	HIS	2.3
1	G	5	HIS	2.3
1	G	269	ILE	2.3
1	O	235	ILE	2.3
1	O	494	ILE	2.3
1	O	485	VAL	2.3
1	N	161	LEU	2.3
1	C	304	TYR	2.3
1	F	4	ALA	2.3
1	F	16	ALA	2.3
1	G	20	ALA	2.3
1	F	111	THR	2.3
1	H	160	THR	2.3
1	P	106	THR	2.3
1	O	154	SER	2.3
1	O	115	PHE	2.3
1	P	421	VAL	2.3
1	F	9	LEU	2.3
1	O	431	LEU	2.3
1	C	183	ASP	2.3
1	A	200	GLY	2.3
1	O	207	MET	2.3
1	N	108	TYR	2.3
1	O	488	TYR	2.3
1	A	21	ALA	2.3
1	F	191	ALA	2.3
1	M	116	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	99	ALA	2.3
1	A	172	SER	2.3
1	G	439	SER	2.3
1	O	435	GLN	2.3
1	E	269	ILE	2.3
1	H	11	ILE	2.3
1	G	94	PHE	2.2
1	G	195	VAL	2.3
1	G	431	LEU	2.2
1	L	124	PHE	2.2
1	P	425	LEU	2.2
1	G	237	CYS	2.2
1	L	185	ASP	2.2
1	N	104	GLY	2.2
1	A	108	TYR	2.2
1	G	191	ALA	2.2
1	H	454	GLU	2.2
1	G	141	ILE	2.2
1	E	165	VAL	2.2
1	G	485	VAL	2.2
1	L	186	LEU	2.2
1	M	135	VAL	2.2
1	N	7	LEU	2.2
1	N	219	VAL	2.2
1	P	7	LEU	2.2
1	O	401	ASN	2.2
1	P	145	ASP	2.2
1	M	187	PRO	2.2
1	E	146	GLY	2.2
1	F	230	GLY	2.2
1	A	60	HIS	2.2
1	A	114	ALA	2.2
1	O	21	ALA	2.2
1	O	85	LYS	2.2
1	P	236	ILE	2.2
1	C	3	LEU	2.2
1	O	408	LEU	2.2
1	O	425	LEU	2.2
1	L	134	VAL	2.2
1	N	165	VAL	2.2
1	O	440	VAL	2.2
1	A	178	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASP	2.2
1	F	266	GLY	2.2
1	G	116	ALA	2.2
1	M	304	TYR	2.2
1	P	140	TYR	2.2
1	N	248	ILE	2.2
1	A	15	VAL	2.2
1	A	152	VAL	2.2
1	D	12	PHE	2.2
1	G	117	ASP	2.2
1	N	195	VAL	2.2
1	N	201	VAL	2.2
1	O	195	VAL	2.2
1	O	222	VAL	2.2
1	N	115	PHE	2.2
1	G	204	GLY	2.2
1	G	448	GLY	2.2
1	G	355	SER	2.2
1	L	170	THR	2.2
1	N	172	SER	2.2
1	O	210	ALA	2.2
1	P	489	ALA	2.2
1	G	262	ARG	2.1
1	O	125	TYR	2.1
1	G	24	ILE	2.1
1	H	131	LEU	2.1
1	O	131	LEU	2.1
1	P	495	LEU	2.1
1	N	95	VAL	2.1
1	O	206	ASP	2.1
1	O	221	ASP	2.1
1	G	363	PHE	2.1
1	P	115	PHE	2.1
1	A	483[A]	HIS	2.1
1	A	92	GLY	2.1
1	G	376	ALA	2.1
1	O	114	ALA	2.1
1	E	360	TYR	2.1
1	O	89	ILE	2.1
1	O	126	ILE	2.1
1	O	236	ILE	2.1
1	P	337	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	145	ASP	2.1
1	O	340	ASN	2.1
1	E	5	HIS	2.1
1	G	177	VAL	2.1
1	G	184	VAL	2.1
1	G	205	VAL	2.1
1	O	165	VAL	2.1
1	J	12	PHE	2.1
1	O	94	PHE	2.1
1	E	104	GLY	2.1
1	G	97	GLY	2.1
1	P	381	CYS	2.1
1	H	26	THR	2.1
1	E	4	ALA	2.1
1	I	190	SER	2.1
1	L	168	SER	2.1
1	M	330	SER	2.1
1	N	170	THR	2.1
1	B	7	LEU	2.1
1	G	447	LEU	2.1
1	O	399	LEU	2.1
1	G	193	ASP	2.1
1	I	185	ASP	2.1
1	J	185	ASP	2.1
1	P	27	ILE	2.1
1	P	494	ILE	2.1
1	O	129	GLN	2.1
1	E	363	PHE	2.1
1	O	204	GLY	2.1
1	P	28	GLY	2.1
1	M	106	THR	2.1
1	A	116	ALA	2.1
1	O	458	ALA	2.1
1	P	311	ALA	2.1
1	G	54	HIS	2.1
1	G	249	ASP	2.1
1	G	366	ILE	2.1
1	N	98	ASP	2.1
1	N	129	GLN	2.1
1	P	112	ASP	2.1
1	E	184	VAL	2.1
1	M	184	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	95	VAL	2.1
1	A	12	PHE	2.1
1	F	115	PHE	2.1
1	N	124	PHE	2.1
1	O	403	GLY	2.1
1	O	460	GLY	2.1
1	P	12	PHE	2.1
1	A	168	SER	2.0
1	F	8	THR	2.0
1	M	53	SER	2.0
1	N	211	SER	2.0
1	P	120	THR	2.0
1	P	423	THR	2.0
1	G	378	GLU	2.0
1	L	107	CYS	2.0
1	N	188	ALA	2.0
1	P	114	ALA	2.0
1	N	145	ASP	2.0
1	O	7	LEU	2.0
1	N	236	ILE	2.0
1	M	100	VAL	2.0
1	G	162	GLU	2.0
1	G	70	ALA	2.0
1	G	105	ALA	2.0
1	L	188	ALA	2.0
1	P	295	ALA	2.0
1	A	17	ASN	2.0
1	L	183	ASP	2.0
1	O	232	ASP	2.0
1	O	141	ILE	2.0
1	O	228	PRO	2.0
1	P	80	ILE	2.0
1	N	465	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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
3	K	G	501	1/1	0.31	0.15	137,137,137,137	0
3	K	N	499	1/1	0.57	0.15	107,107,107,107	0
4	OXL	P	510	6/6	0.65	0.15	85,85,85,86	0
7	GOL	I	501	6/6	0.74	0.15	85,85,85,85	0
3	K	A	504	1/1	0.75	0.22	106,106,106,106	0
7	GOL	J	499	6/6	0.75	0.18	69,71,71,72	0
3	K	P	499	1/1	0.76	0.11	119,119,119,119	0
2	MG	N	500	1/1	0.76	0.19	88,88,88,88	0
3	K	M	499	1/1	0.78	0.10	106,106,106,106	0
4	OXL	N	510	6/6	0.80	0.12	77,79,80,80	0
3	K	O	500	1/1	0.81	0.08	122,122,122,122	0
7	GOL	O	499	6/6	0.81	0.16	74,75,75,75	0
5	FDP	O	700	20/20	0.82	0.11	118,119,121,121	0
4	OXL	F	510	6/6	0.82	0.14	83,83,83,83	0
6	ATP	P	1001	31/31	0.83	0.12	132,134,134,134	0
4	OXL	G	510	6/6	0.83	0.13	71,74,75,75	0
7	GOL	G	499	6/6	0.84	0.12	97,97,97,97	0
6	ATP	G	1001	31/31	0.85	0.14	77,97,101,101	0
5	FDP	P	700	20/20	0.86	0.10	110,115,119,119	0
6	ATP	N	1001	31/31	0.86	0.13	83,94,95,95	0
7	GOL	I	499	6/6	0.86	0.09	91,91,91,92	0
2	MG	A	500	1/1	0.87	0.12	77,77,77,77	0
4	OXL	A	510	6/6	0.87	0.18	63,65,66,66	0
7	GOL	E	499	6/6	0.88	0.13	78,79,80,80	0
2	MG	G	500	1/1	0.88	0.14	81,81,81,81	0
6	ATP	A	1001	31/31	0.89	0.12	70,85,87,87	0
4	OXL	H	510	6/6	0.89	0.16	54,54,55,55	0
3	K	G	504	1/1	0.90	0.12	82,82,82,82	0
2	MG	P	500	1/1	0.90	0.11	94,94,94,94	0
5	FDP	G	700	20/20	0.90	0.10	69,74,75,75	0
3	K	N	504	1/1	0.91	0.09	84,84,84,84	0
4	OXL	C	510	6/6	0.91	0.12	39,40,41,41	0
3	K	P	504	1/1	0.91	0.11	98,98,98,98	0
2	MG	I	500	1/1	0.91	0.11	36,36,36,36	0
3	K	H	499	1/1	0.92	0.09	76,76,76,76	0
3	K	E	501	1/1	0.92	0.13	75,75,75,75	0
4	OXL	M	510	6/6	0.92	0.15	64,66,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FDP	N	700	20/20	0.92	0.09	76,78,81,82	0
3	K	F	504	1/1	0.93	0.13	69,69,69,69	0
6	ATP	M	1001	31/31	0.93	0.12	66,73,76,76	0
3	K	F	499	1/1	0.93	0.10	85,85,85,85	0
3	K	C	504	1/1	0.93	0.12	56,56,56,56	0
2	MG	H	502	1/1	0.93	0.09	61,61,61,61	0
4	OXL	L	510	6/6	0.94	0.14	37,38,38,39	0
6	ATP	C	1001	31/31	0.94	0.10	43,52,54,54	0
6	ATP	F	1001	31/31	0.94	0.10	64,73,76,76	0
2	MG	M	500	1/1	0.94	0.13	69,69,69,69	0
6	ATP	H	1001	31/31	0.94	0.10	62,69,72,72	0
2	MG	N	502	1/1	0.94	0.07	76,76,76,76	0
3	K	H	504	1/1	0.94	0.21	59,59,59,59	0
2	MG	D	500	1/1	0.95	0.09	37,37,37,37	0
3	K	O	501	1/1	0.95	0.50	30,30,30,30	0
6	ATP	L	1001	31/31	0.95	0.10	44,55,59,59	0
2	MG	F	500	1/1	0.95	0.09	67,67,67,67	0
6	ATP	E	1001	31/31	0.95	0.09	52,58,63,63	0
2	MG	A	502	1/1	0.95	0.09	58,58,58,58	0
5	FDP	H	700	20/20	0.96	0.07	54,57,59,60	0
5	FDP	K	700	20/20	0.96	0.08	36,38,42,43	0
5	FDP	M	700	20/20	0.96	0.07	55,59,62,64	0
3	K	C	499	1/1	0.96	0.11	68,68,68,68	0
2	MG	F	502	1/1	0.96	0.07	60,60,60,60	0
3	K	K	499	1/1	0.96	0.16	52,52,52,52	0
4	OXL	E	510	6/6	0.96	0.09	48,49,49,50	0
3	K	L	504	1/1	0.96	0.13	52,52,52,52	0
5	FDP	A	700	20/20	0.96	0.08	53,58,61,64	0
5	FDP	F	700	20/20	0.96	0.09	48,53,55,56	0
2	MG	G	502	1/1	0.96	0.08	66,66,66,66	0
6	ATP	D	1001	31/31	0.97	0.08	35,42,44,44	0
5	FDP	D	700	20/20	0.97	0.07	32,40,43,45	0
5	FDP	E	700	20/20	0.97	0.07	38,41,46,47	0
2	MG	P	502	1/1	0.97	0.09	64,64,64,64	0
2	MG	C	500	1/1	0.97	0.04	45,45,45,45	0
6	ATP	I	1001	31/31	0.97	0.07	36,37,39,40	0
6	ATP	K	1001	31/31	0.97	0.08	28,31,37,38	0
4	OXL	K	510	6/6	0.97	0.14	25,27,28,28	0
4	OXL	B	510	6/6	0.97	0.14	30,32,33,33	0
5	FDP	L	700	20/20	0.97	0.07	37,41,43,43	0
3	K	B	499	1/1	0.97	0.07	60,60,60,60	0
4	OXL	D	510	6/6	0.97	0.12	37,38,39,39	0

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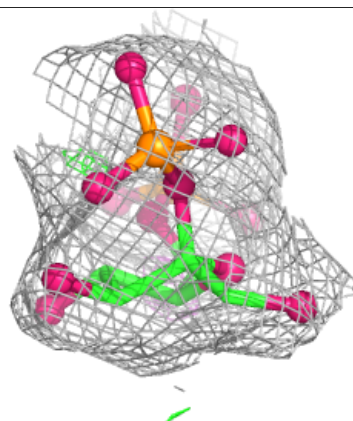
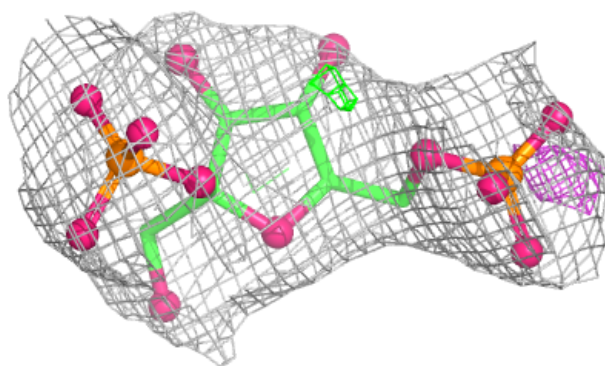
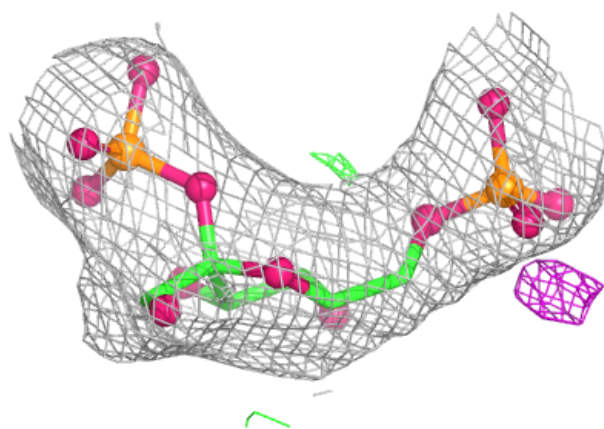
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	E	500	1/1	0.97	0.08	55,55,55,55	0
2	MG	H	500	1/1	0.97	0.05	63,63,63,63	0
5	FDP	B	700	20/20	0.97	0.07	37,40,45,46	0
6	ATP	B	1001	31/31	0.97	0.07	31,35,39,40	0
5	FDP	C	700	20/20	0.97	0.07	36,45,48,50	0
6	ATP	J	1001	31/31	0.98	0.07	26,34,36,36	0
4	OXL	J	510	6/6	0.98	0.10	30,31,32,33	0
3	K	I	504	1/1	0.98	0.18	36,36,36,36	0
3	K	I	503	1/1	0.98	0.23	47,47,47,47	0
2	MG	K	500	1/1	0.98	0.08	29,29,29,29	0
2	MG	B	502	1/1	0.98	0.07	28,28,28,28	0
5	FDP	I	700	20/20	0.98	0.06	29,32,34,35	0
5	FDP	J	700	20/20	0.98	0.07	25,32,34,35	0
3	K	L	499	1/1	0.98	0.10	47,47,47,47	0
3	K	M	504	1/1	0.98	0.15	61,61,61,61	0
2	MG	M	502	1/1	0.98	0.06	60,60,60,60	0
4	OXL	I	510	6/6	0.98	0.09	32,33,34,35	0
3	K	E	504	1/1	0.99	0.13	48,48,48,48	0
2	MG	I	502	1/1	0.99	0.05	30,30,30,30	0
2	MG	J	500	1/1	0.99	0.05	27,27,27,27	0
2	MG	J	502	1/1	0.99	0.09	26,26,26,26	0
2	MG	C	502	1/1	0.99	0.06	38,38,38,38	0
2	MG	L	500	1/1	0.99	0.05	46,46,46,46	0
3	K	A	499	1/1	0.99	0.11	60,60,60,60	0
3	K	B	504	1/1	0.99	0.12	38,38,38,38	0
2	MG	L	502	1/1	0.99	0.06	37,37,37,37	0
2	MG	E	502	1/1	0.99	0.05	48,48,48,48	0
3	K	J	504	1/1	0.99	0.10	35,35,35,35	0
3	K	J	501	1/1	0.99	0.14	50,50,50,50	0
2	MG	D	502	1/1	0.99	0.06	34,34,34,34	0
3	K	D	504	1/1	0.99	0.10	33,33,33,33	0
3	K	D	499	1/1	0.99	0.11	53,53,53,53	0
2	MG	B	500	1/1	1.00	0.06	35,35,35,35	0
2	MG	K	502	1/1	1.00	0.09	28,28,28,28	0
3	K	K	504	1/1	1.00	0.11	29,29,29,29	0

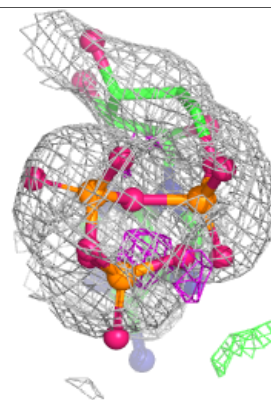
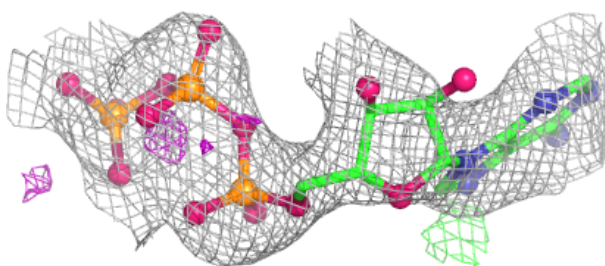
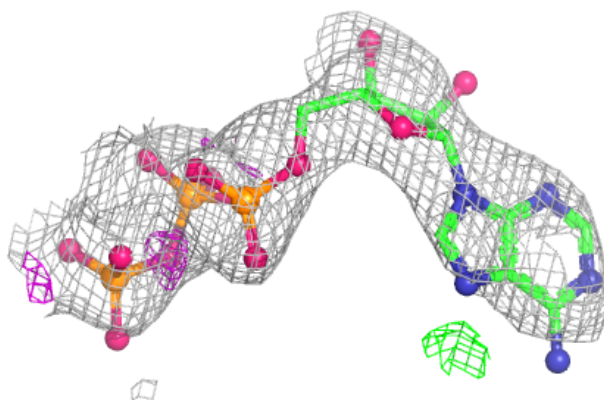
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDP 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)

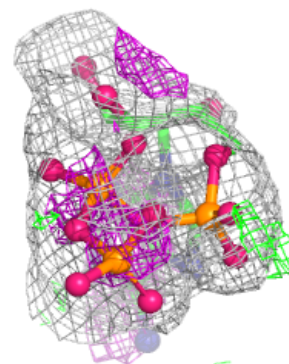
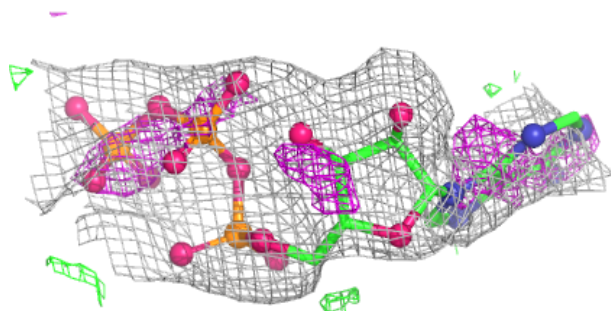
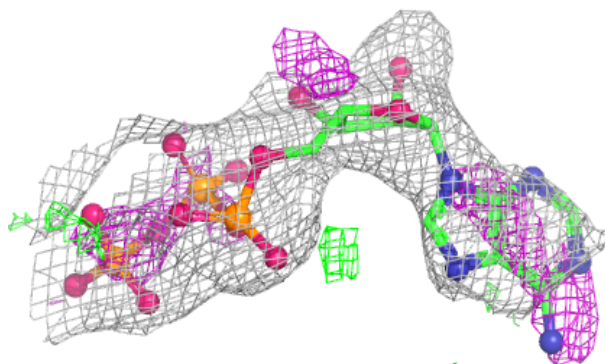
**Electron density around ATP P 1001:**

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

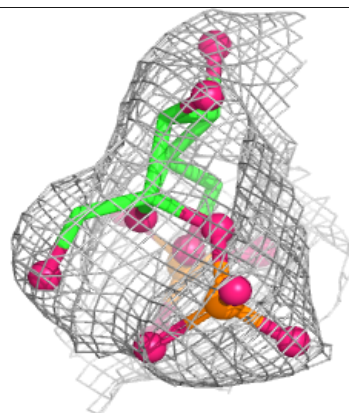
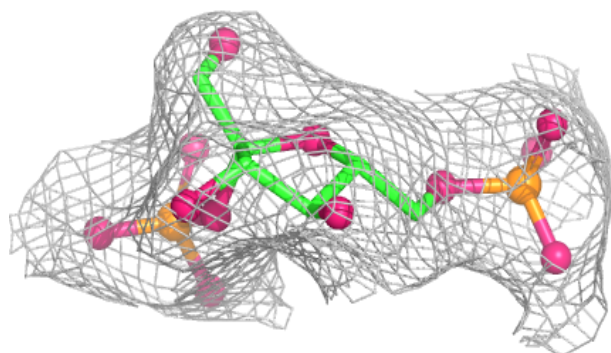
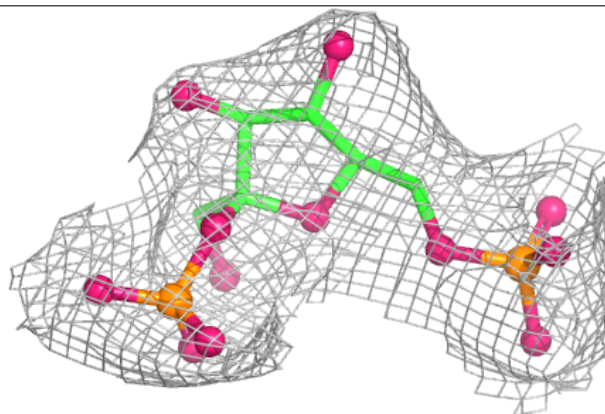


Electron density around ATP G 1001:

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

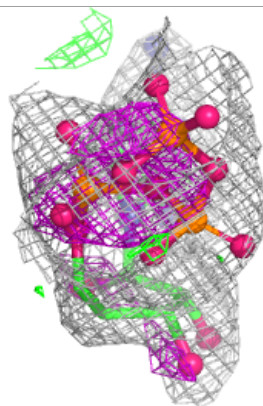
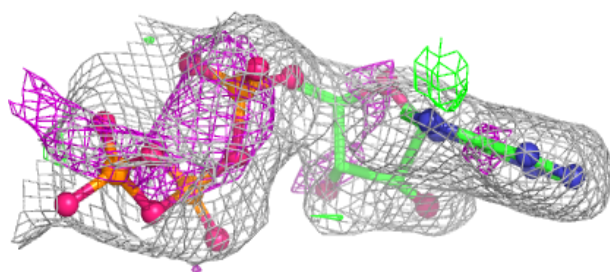
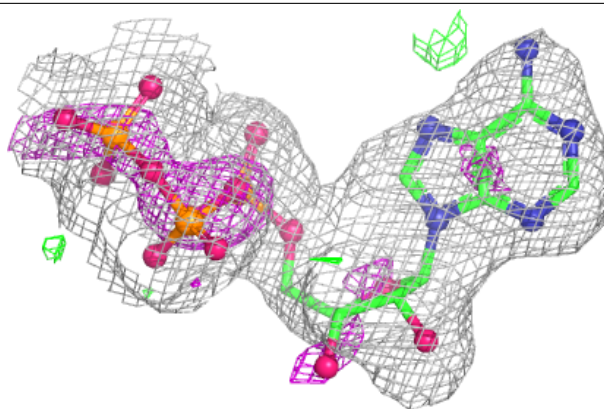
**Electron density around FDP P 700:**

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

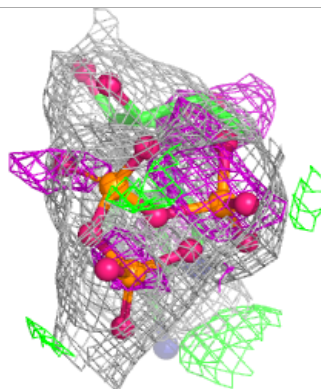
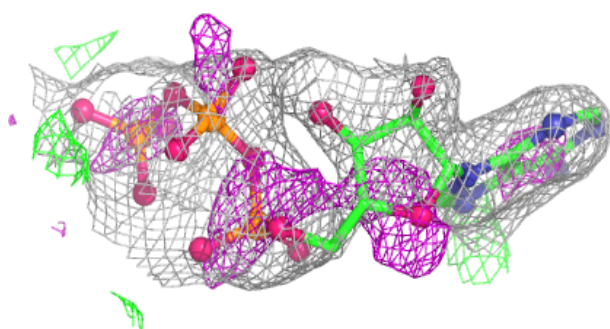
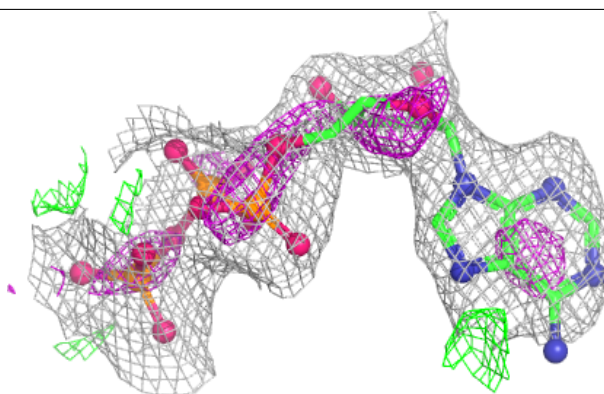


Electron density around ATP N 1001:

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

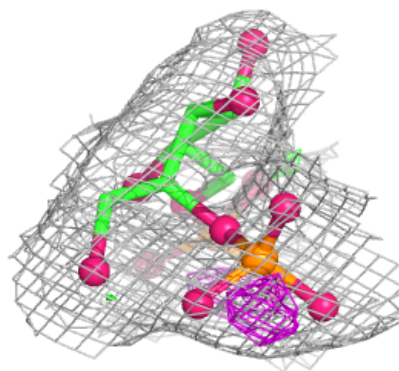
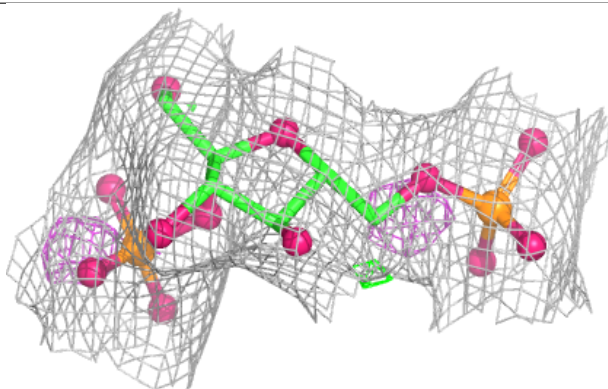
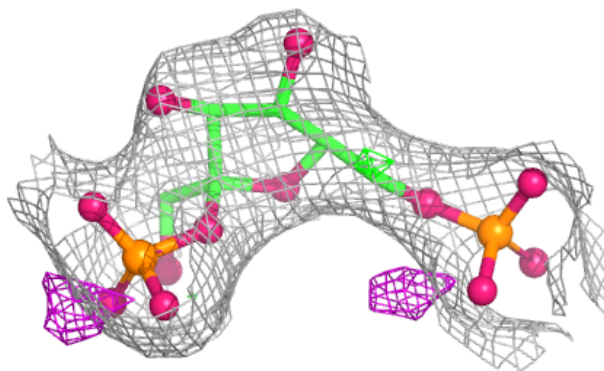
**Electron density around ATP A 1001:**

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

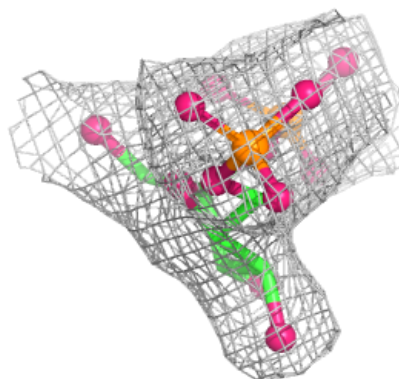
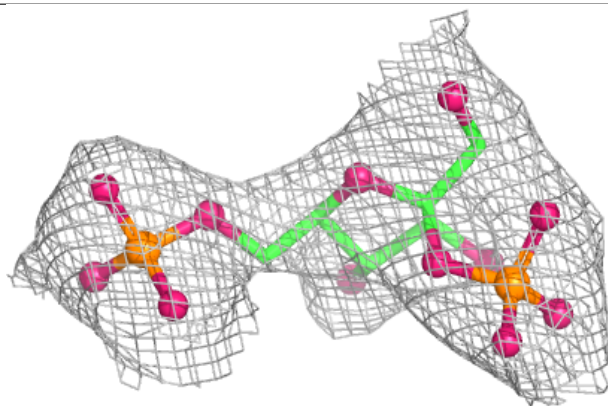
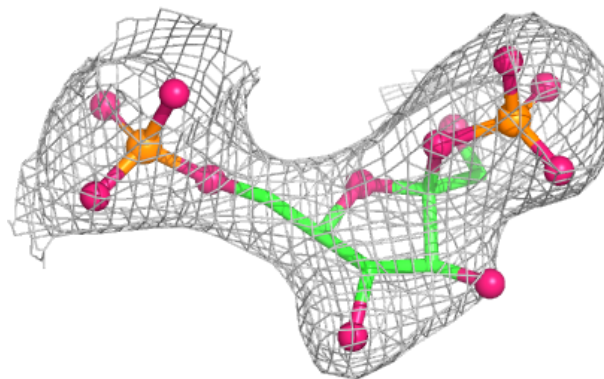


Electron density around FDP G 700:

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

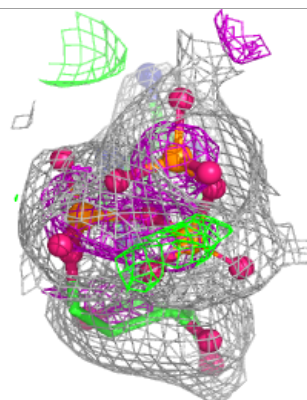
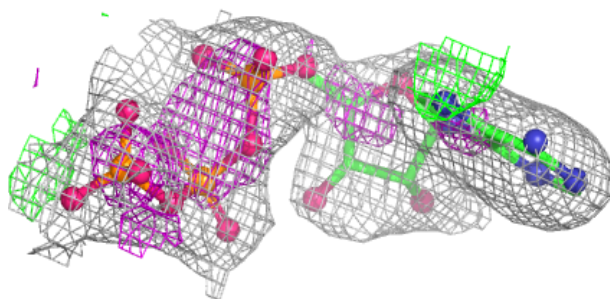
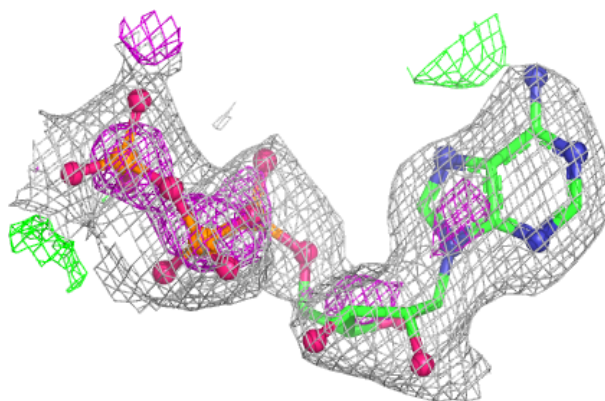
**Electron density around FDP N 700:**

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

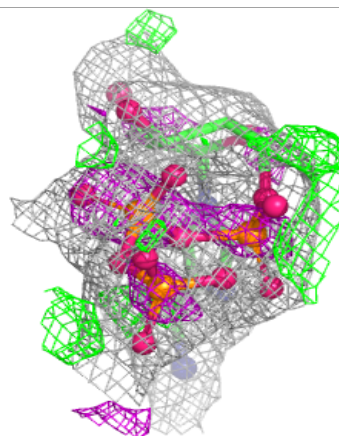
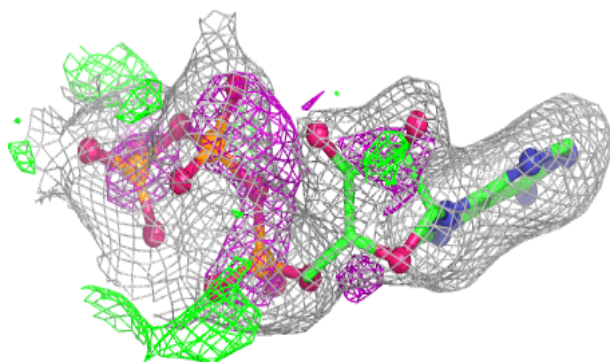
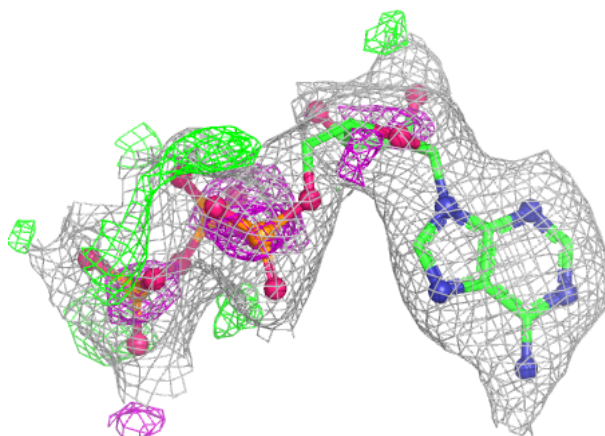


Electron density around ATP M 1001:

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

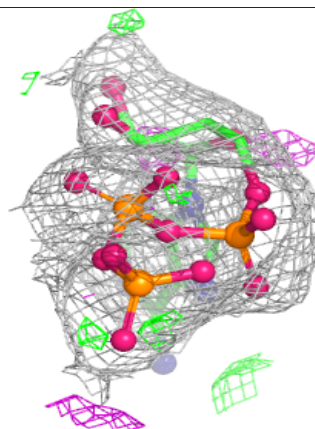
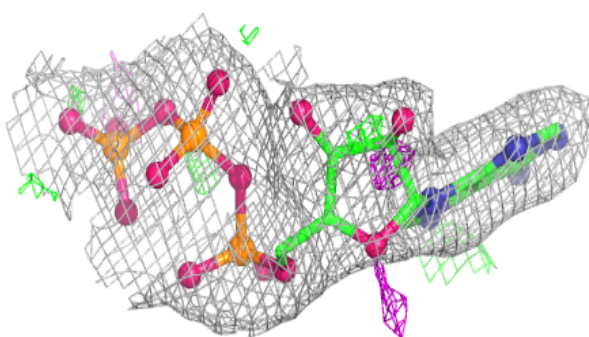
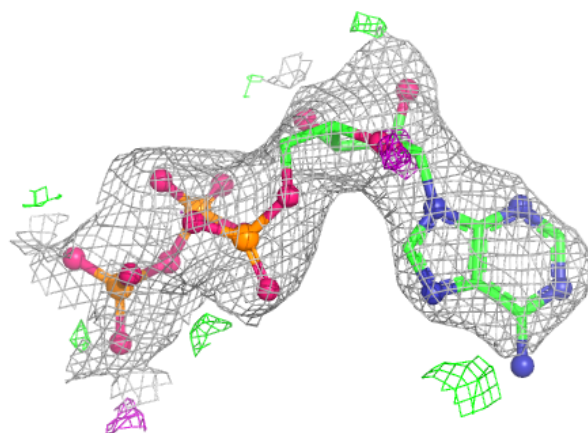
**Electron density around ATP C 1001:**

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

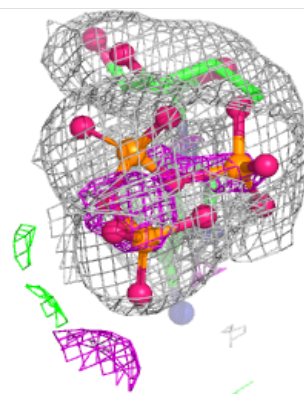
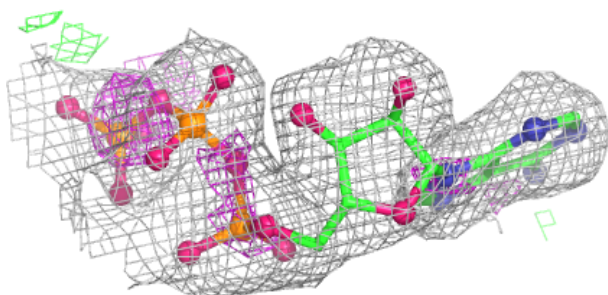
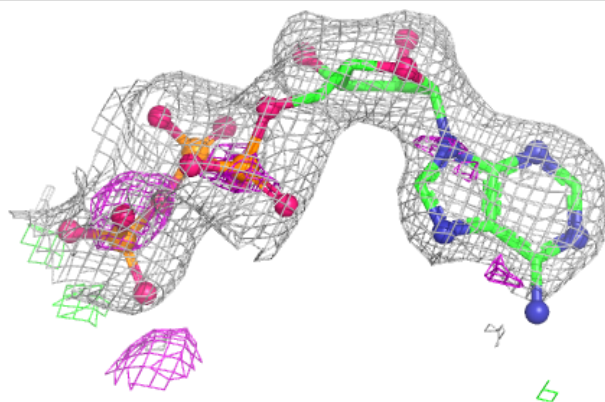


Electron density around ATP F 1001:

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

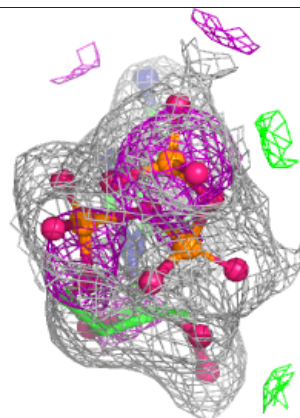
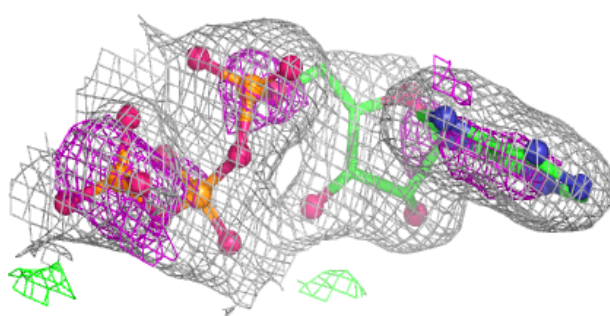
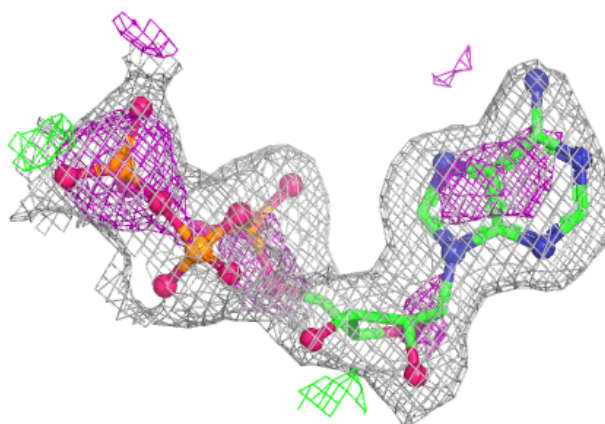
**Electron density around ATP H 1001:**

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

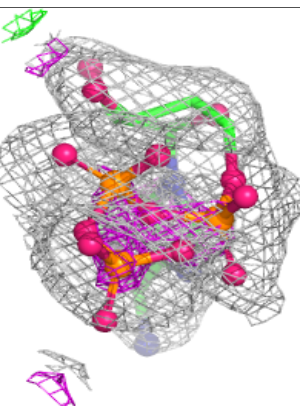
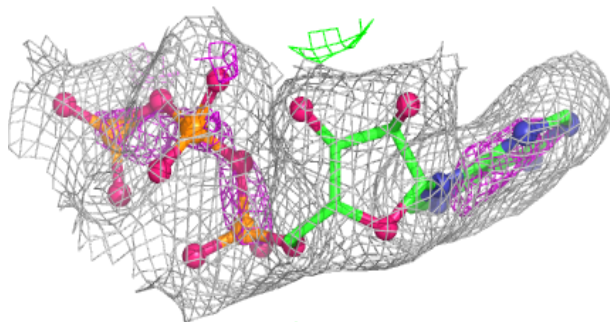
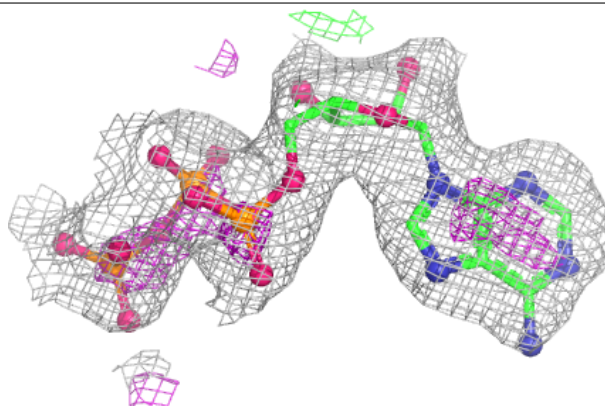


Electron density around ATP L 1001:

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

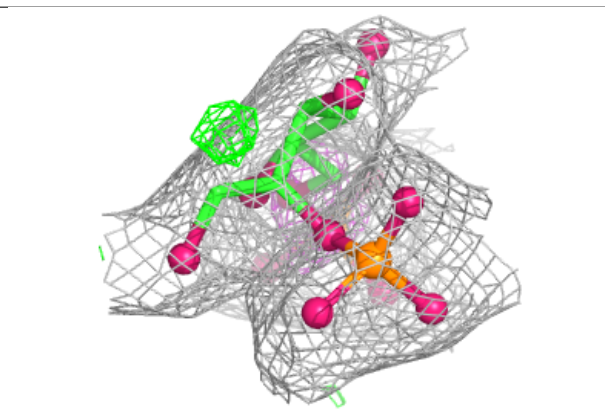
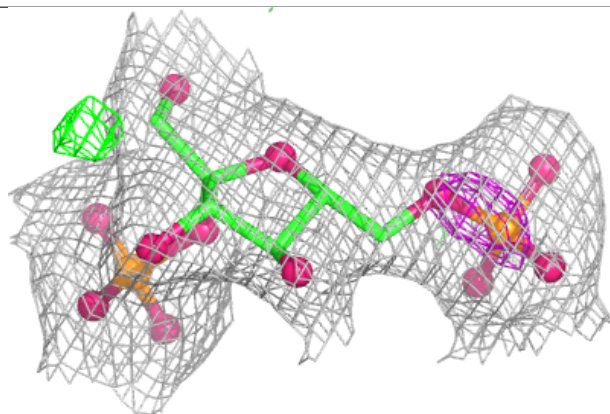
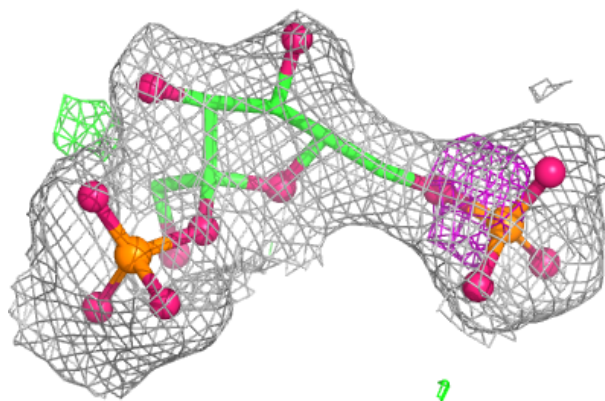
**Electron density around ATP E 1001:**

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

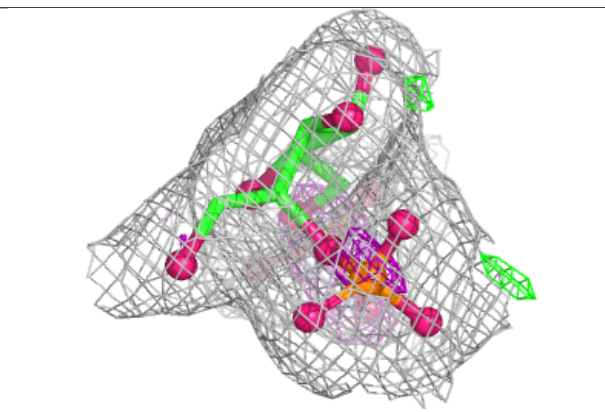
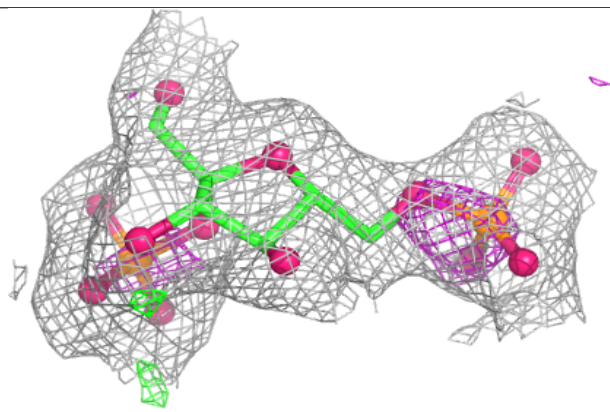
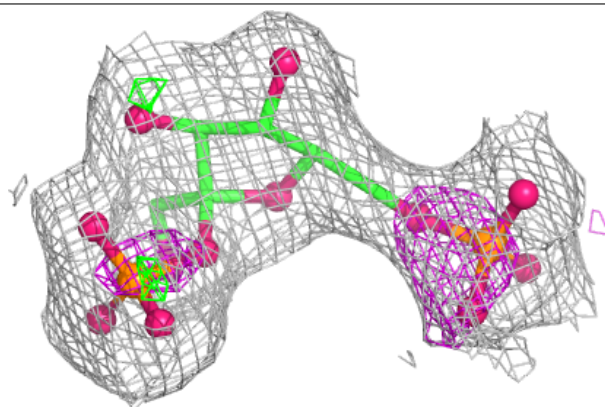


Electron density around FDP H 700:

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

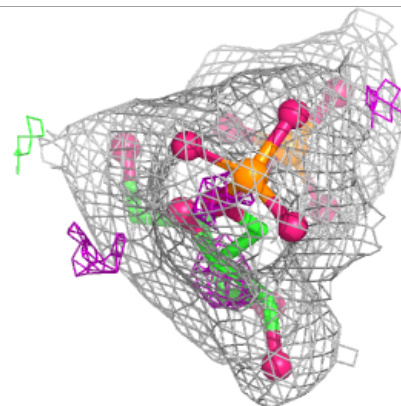
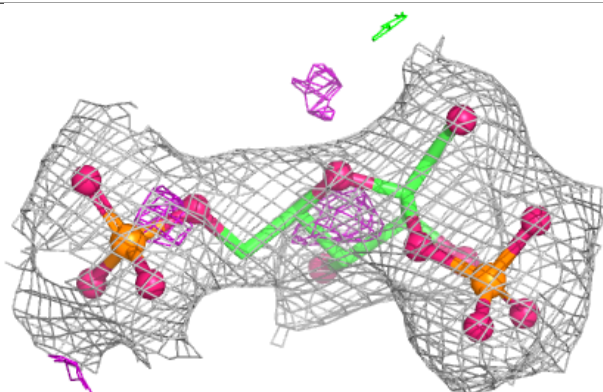
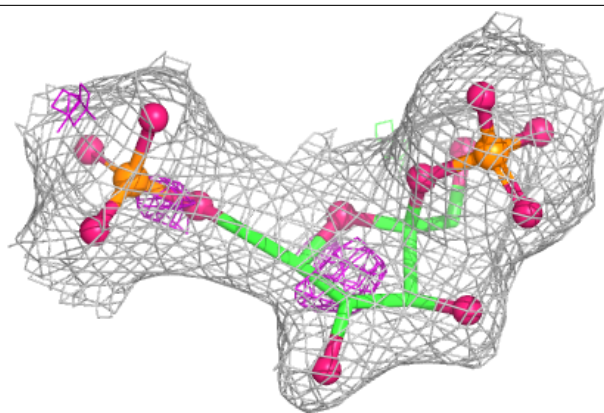
**Electron density around FDP K 700:**

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

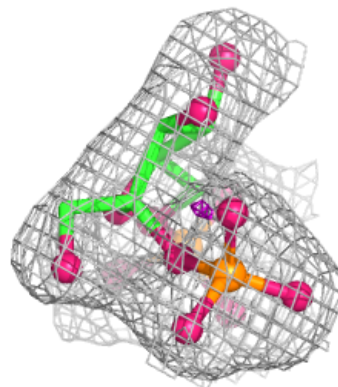
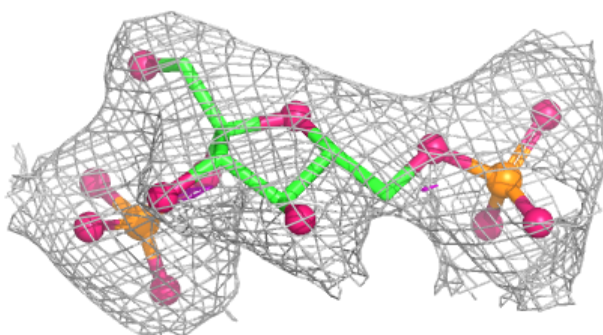
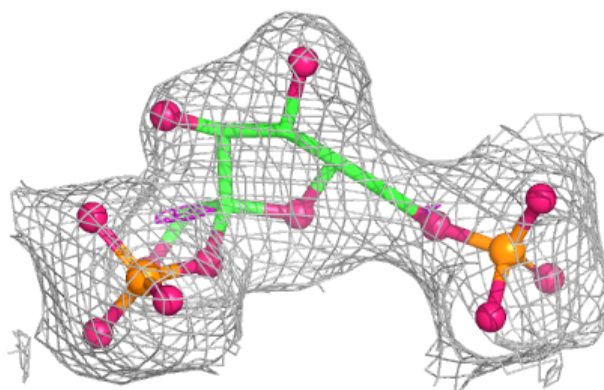


Electron density around FDP M 700:

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

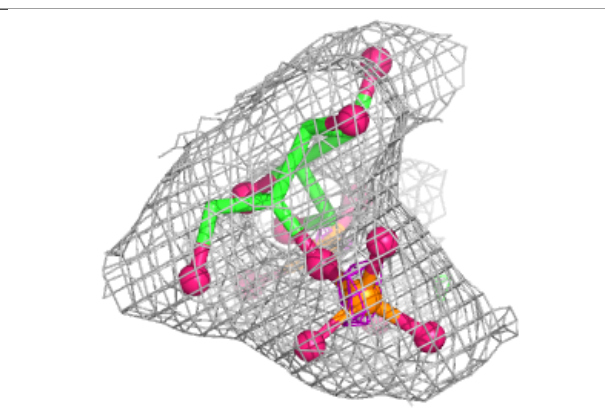
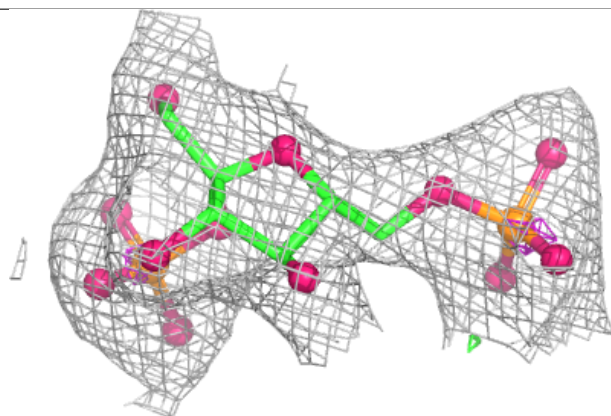
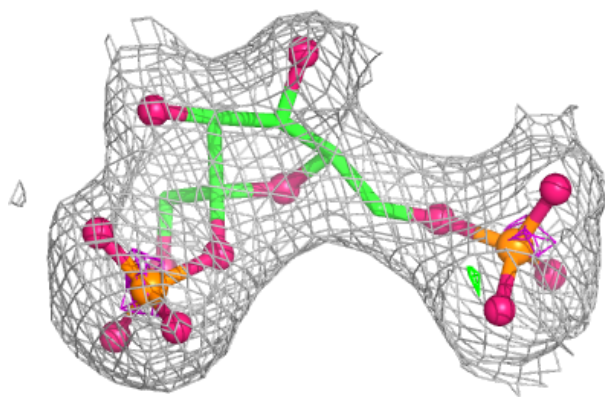
**Electron density around FDP A 700:**

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

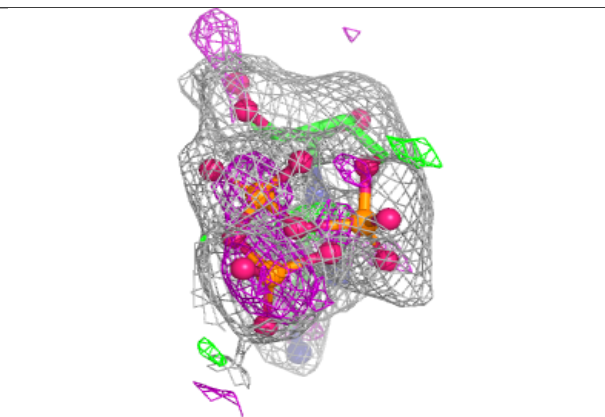
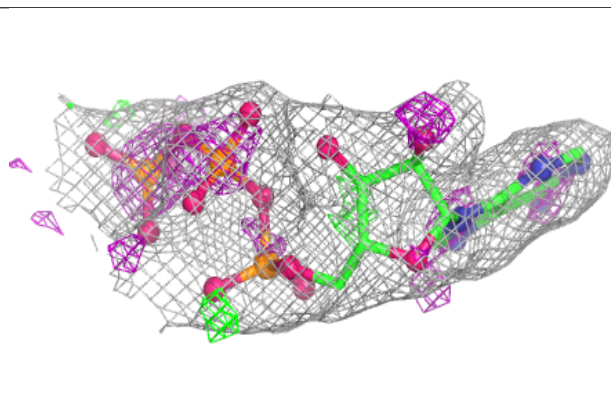
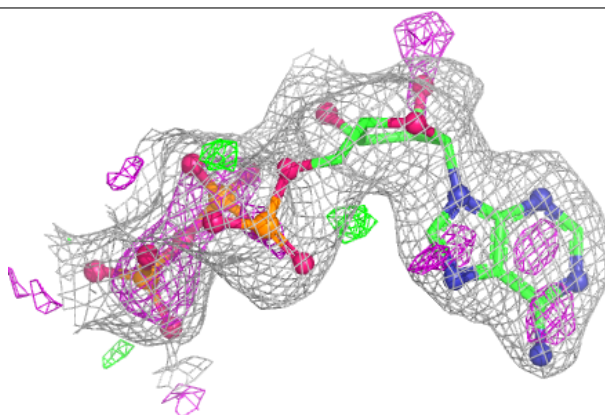


Electron density around FDP F 700:

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

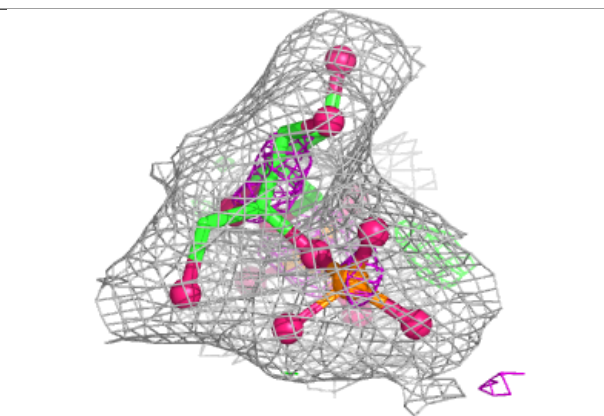
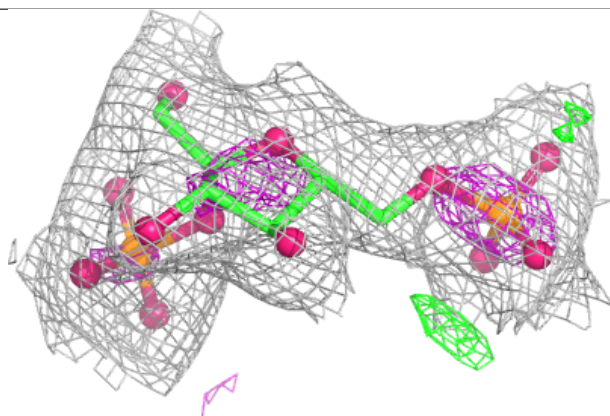
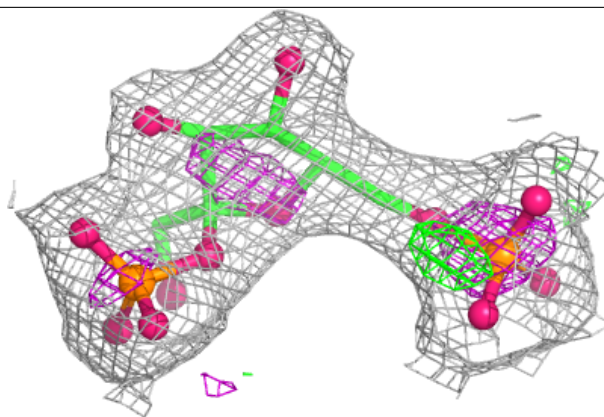
**Electron density around ATP D 1001:**

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

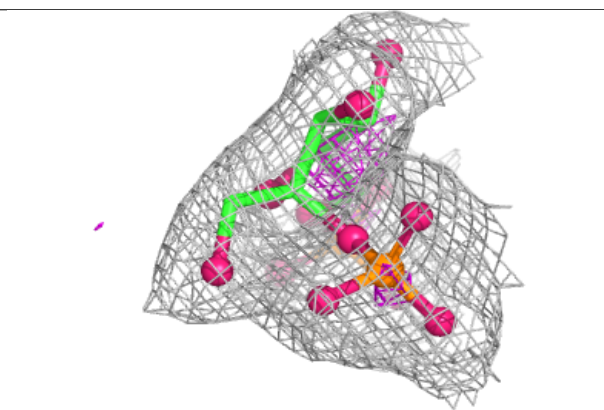
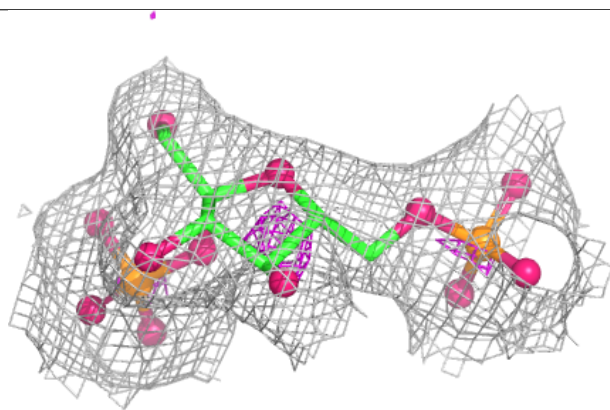
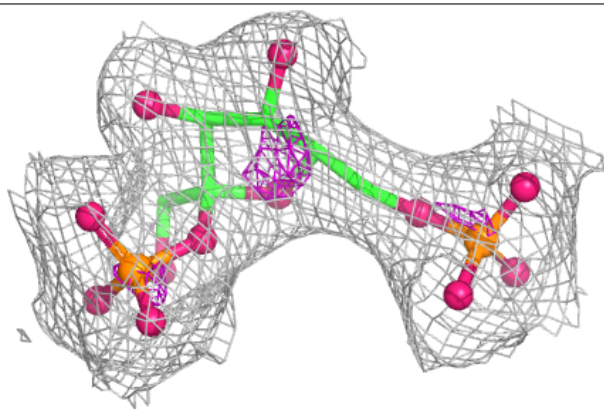


Electron density around FDP D 700:

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

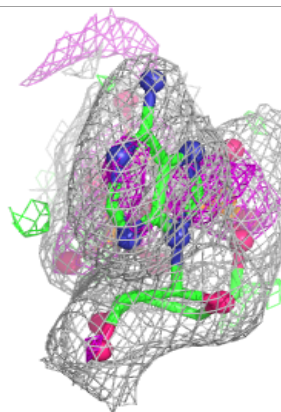
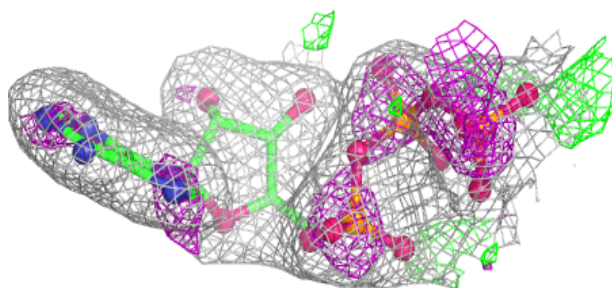
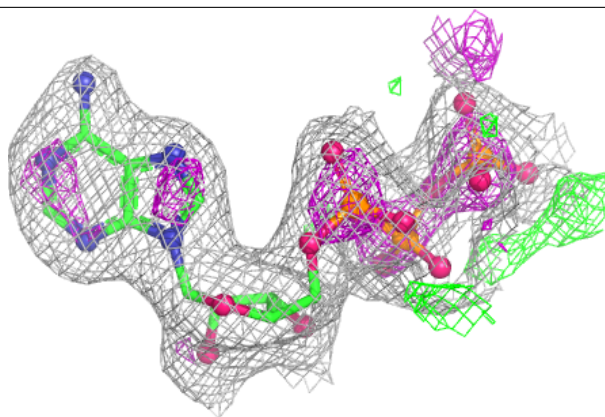
**Electron density around FDP E 700:**

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

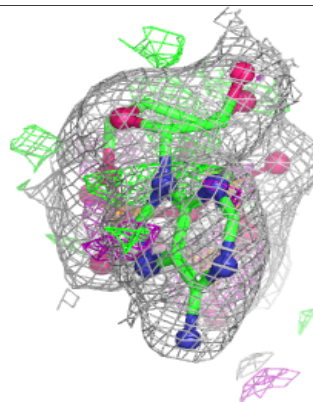
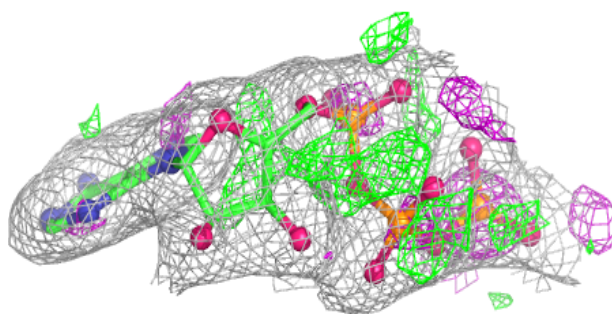
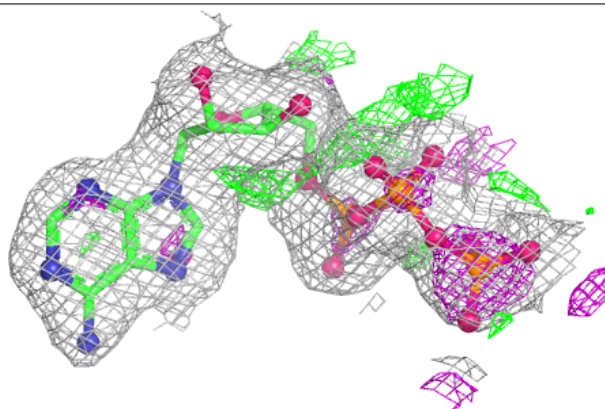


Electron density around ATP I 1001:

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

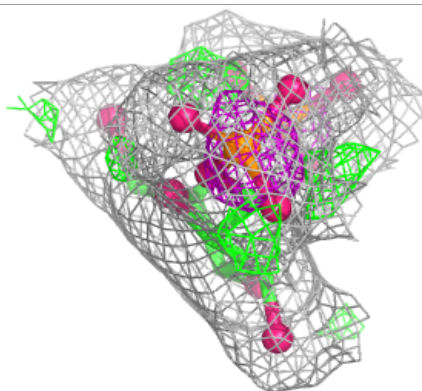
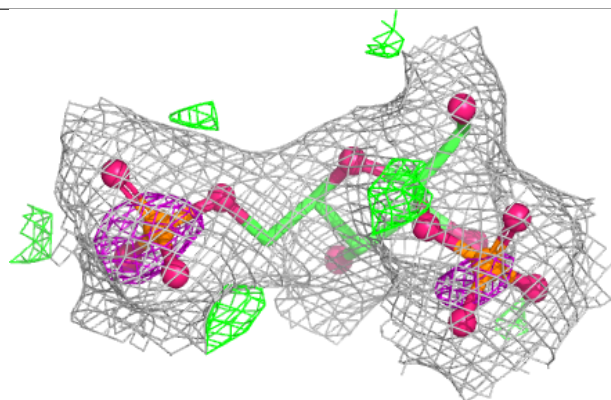
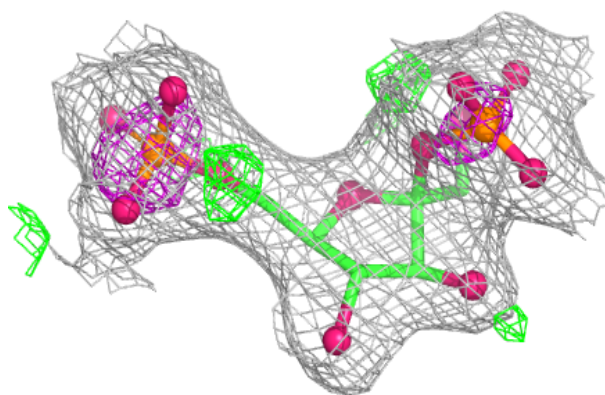
**Electron density around ATP K 1001:**

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

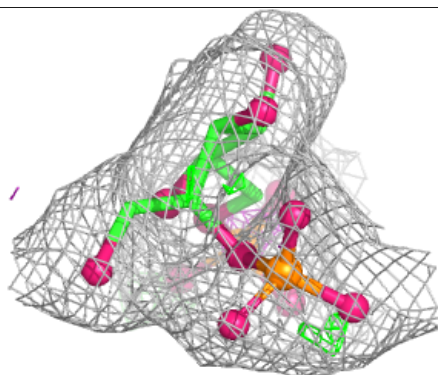
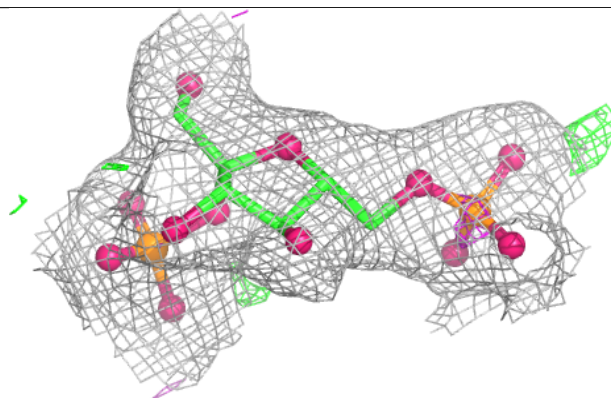
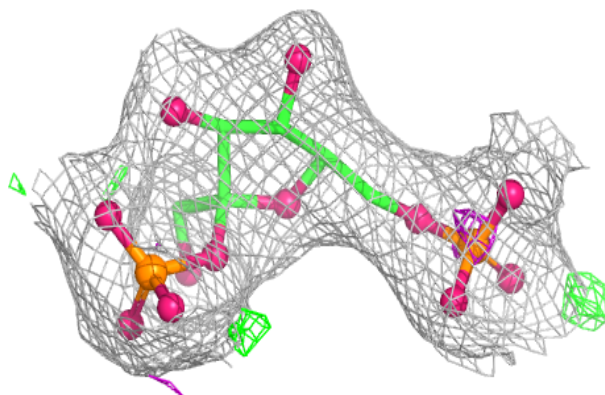


Electron density around FDP L 700:

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

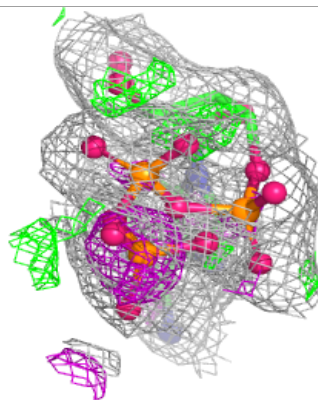
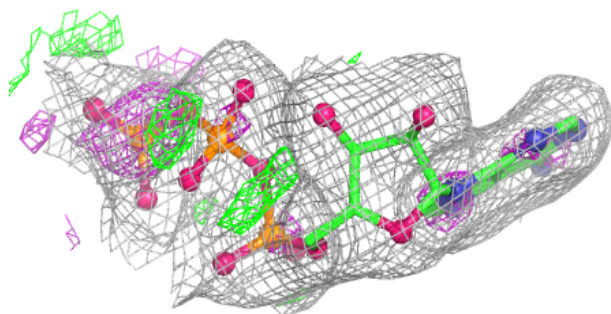
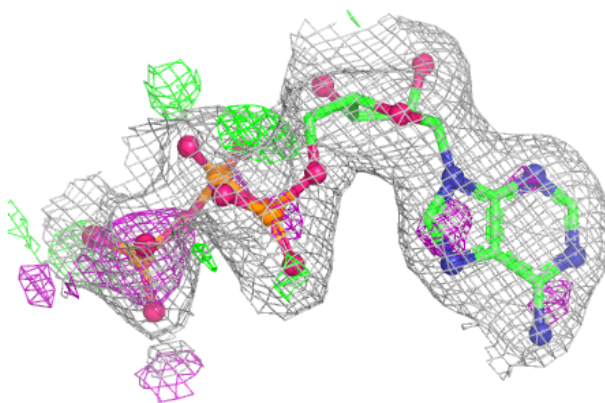
**Electron density around FDP B 700:**

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

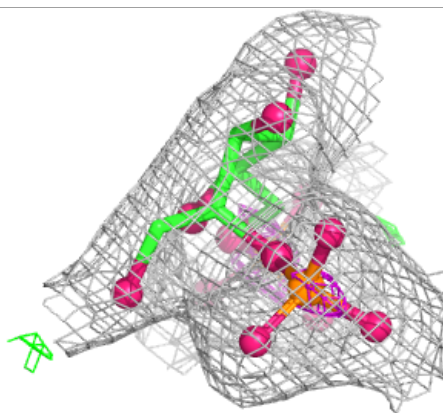
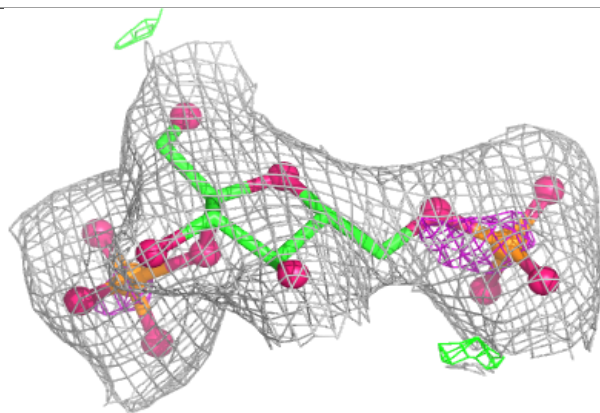
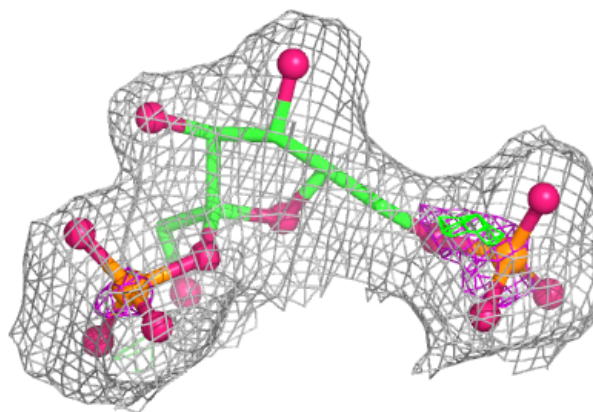


Electron density around ATP B 1001:

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

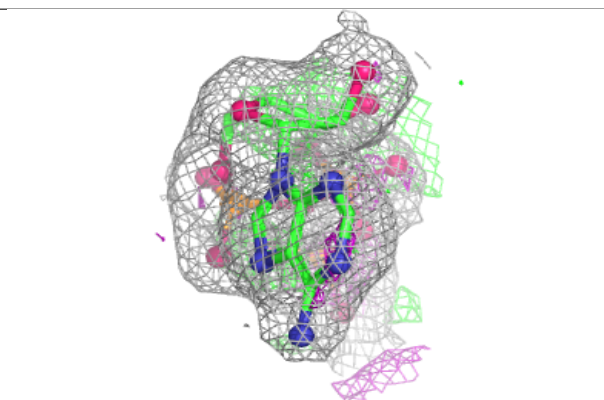
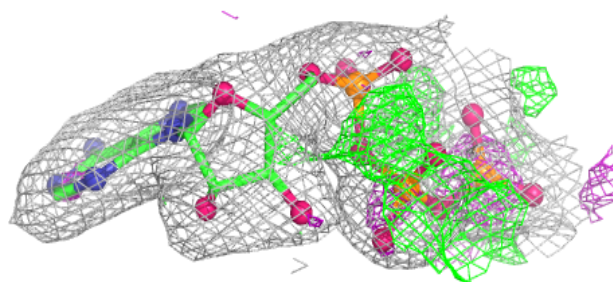
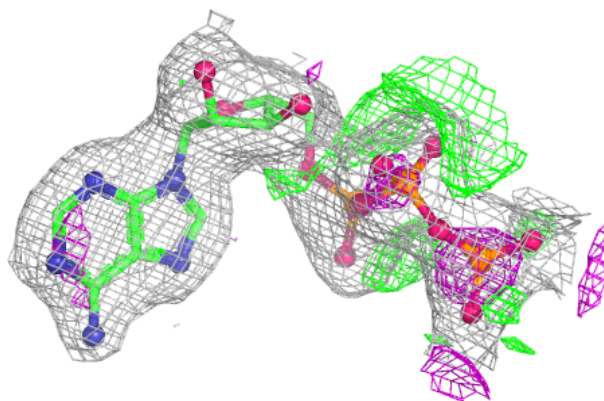
**Electron density around FDP C 700:**

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

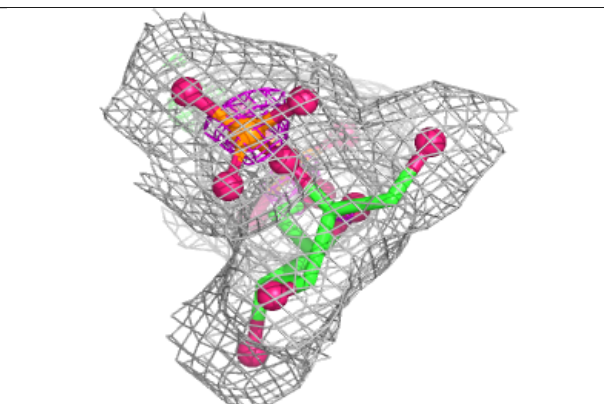
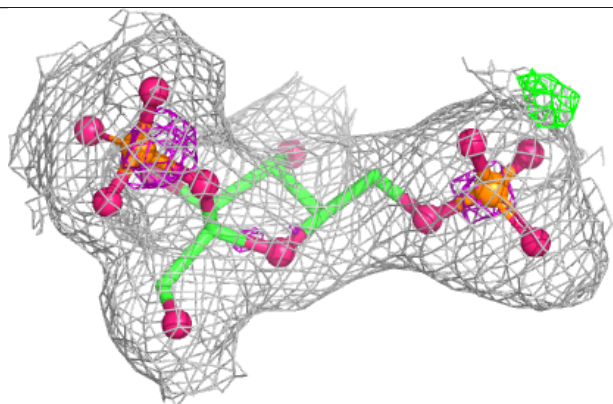
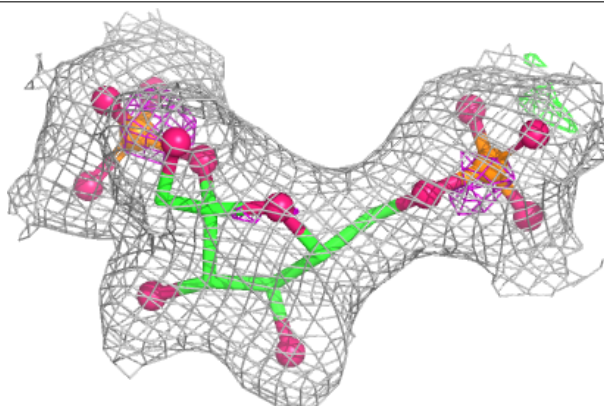


Electron density around ATP J 1001:

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

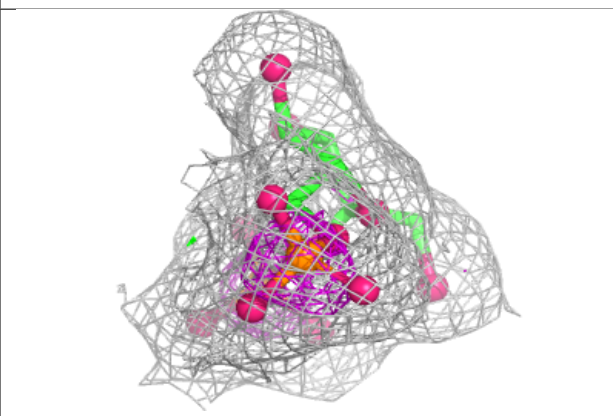
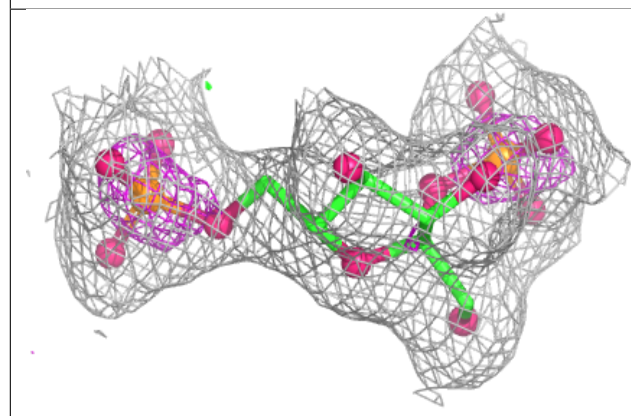
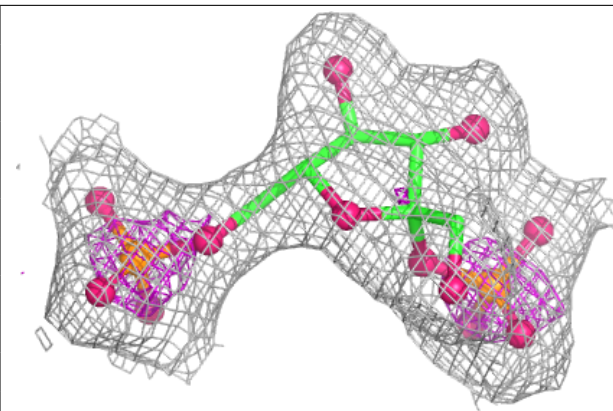
**Electron density around FDP I 700:**

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



Electron density around FDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.