



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 12:52 PM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

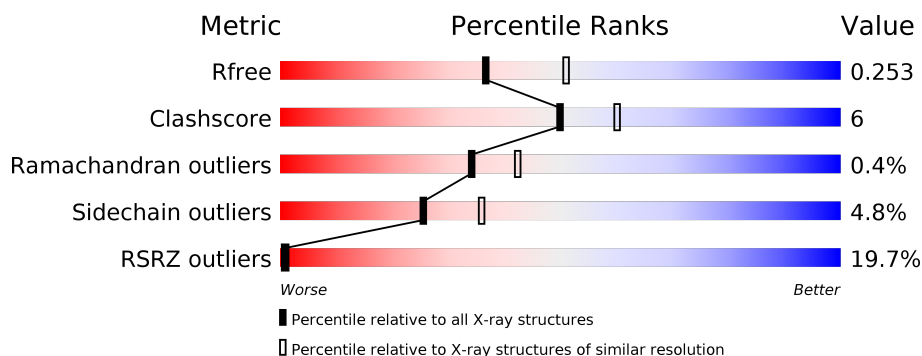
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	499	<div> <div>24%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	499	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
1	C	499	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	499	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	E	499	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	F	499	<div> <div>15%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

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

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 65997 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase.

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



There are 64 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

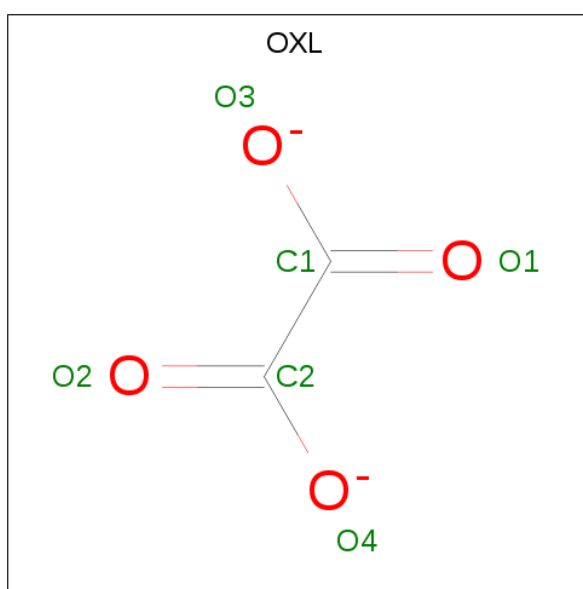
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total 2	K 2	0	0
3	G	2	Total 2	K 2	0	0
3	J	2	Total 2	K 2	0	0
3	D	2	Total 2	K 2	0	0
3	K	2	Total 2	K 2	0	0
3	E	2	Total 2	K 2	0	0
3	H	2	Total 2	K 2	0	0
3	B	2	Total 2	K 2	0	0
3	I	2	Total 2	K 2	0	0
3	C	2	Total 2	K 2	0	0
3	A	2	Total 2	K 2	0	0
3	N	2	Total 2	K 2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

*Continued on next page...*

Continued from previous page...

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

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



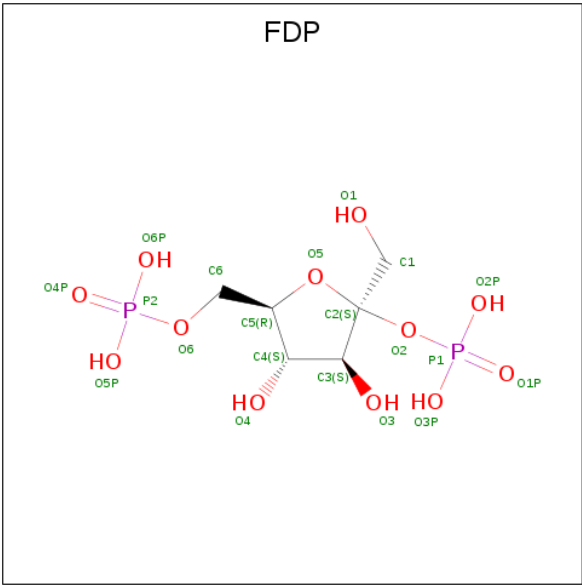
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 2	O 4	0	0
4	B	1	Total 6	C 2	O 4	0	0
4	C	1	Total 6	C 2	O 4	0	0
4	D	1	Total 6	C 2	O 4	0	0
4	E	1	Total 6	C 2	O 4	0	0
4	F	1	Total 6	C 2	O 4	0	0
4	G	1	Total 6	C 2	O 4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 2,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FDP) (formula:  $C_6H_{14}O_{12}P_2$ ).



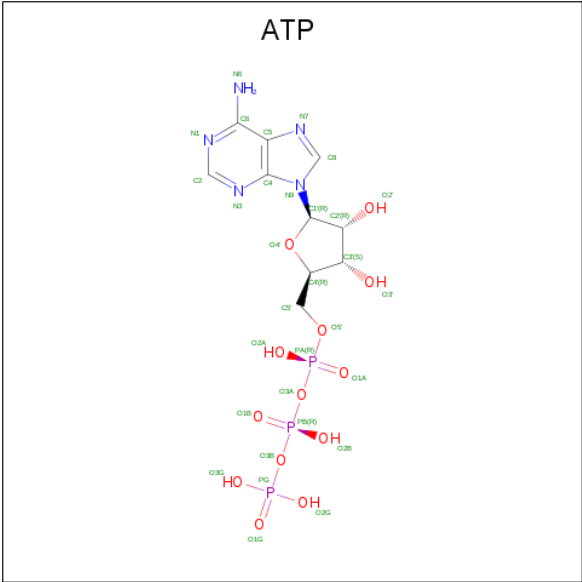
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			20	6	12	2		
5	B	1	Total	C	O	P	0	0
			20	6	12	2		
5	C	1	Total	C	O	P	0	0
			20	6	12	2		

Continued on next page...

*Continued from previous page...*

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

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



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

Continued on next page...

*Continued from previous page...*

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

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



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

- Molecule 8 is water.

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

*Continued on next page...*



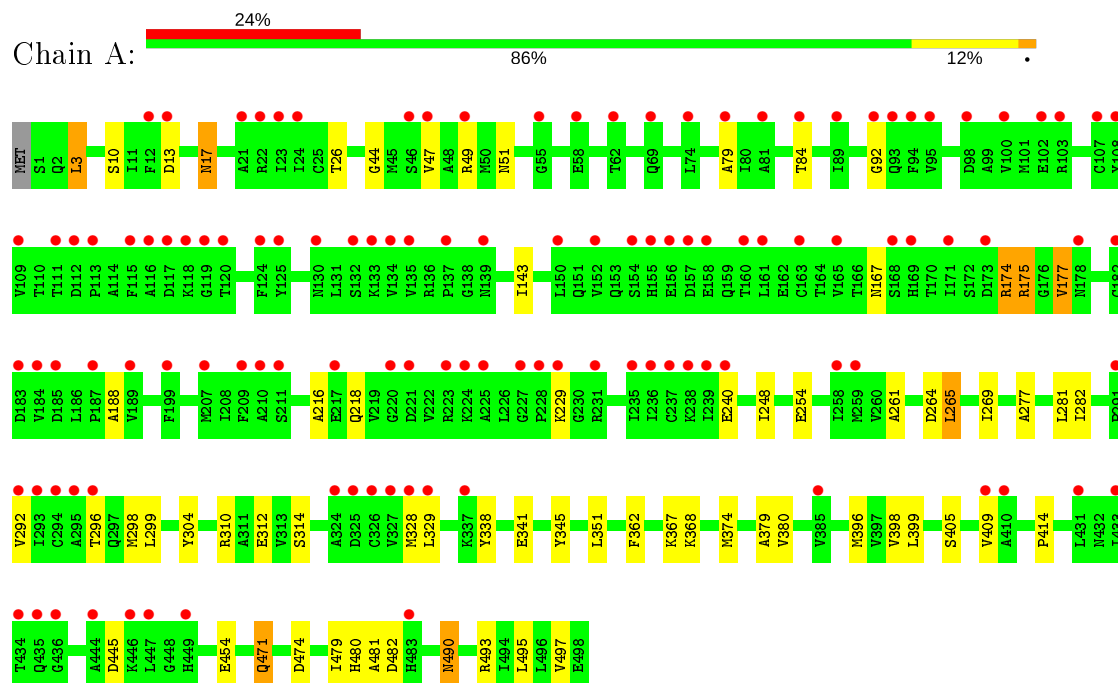
*Continued from previous page...*

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

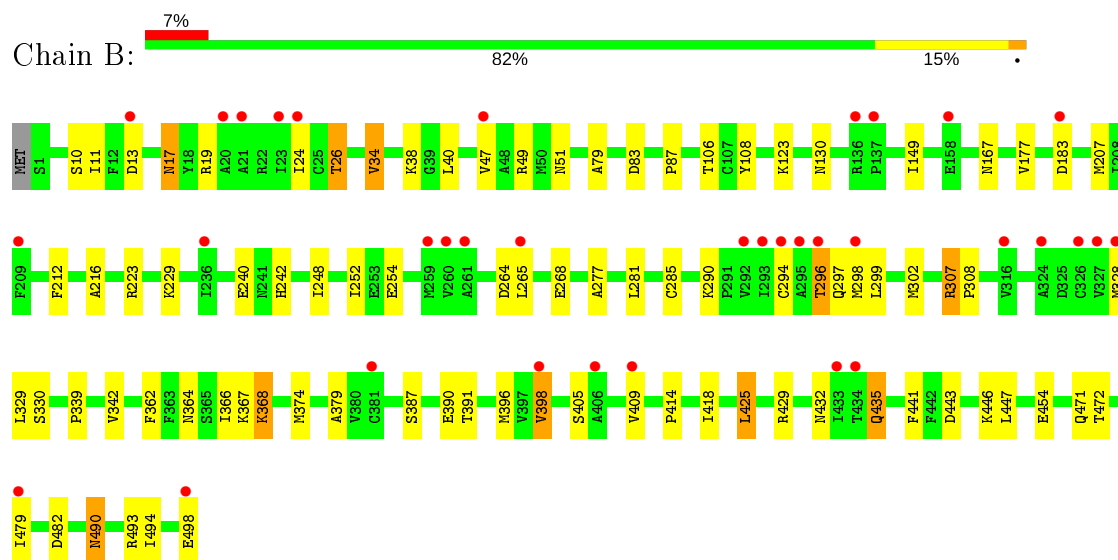
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

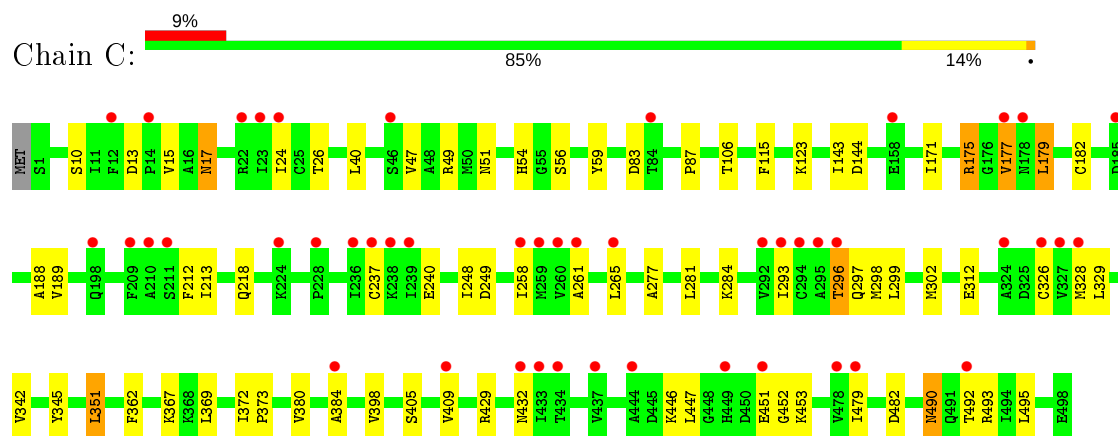
#### • Molecule 1: Pyruvate kinase



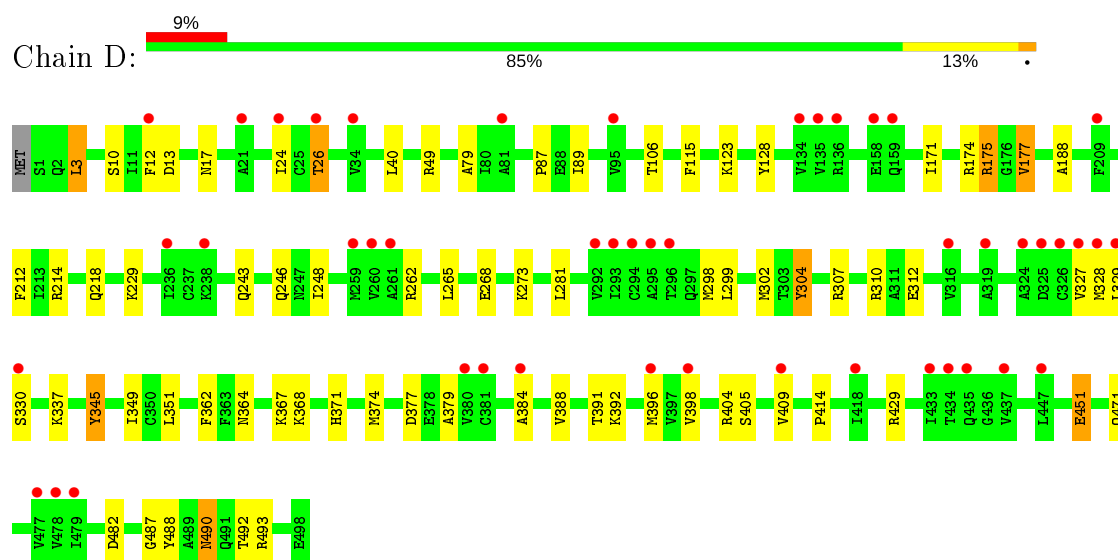
#### • Molecule 1: Pyruvate kinase



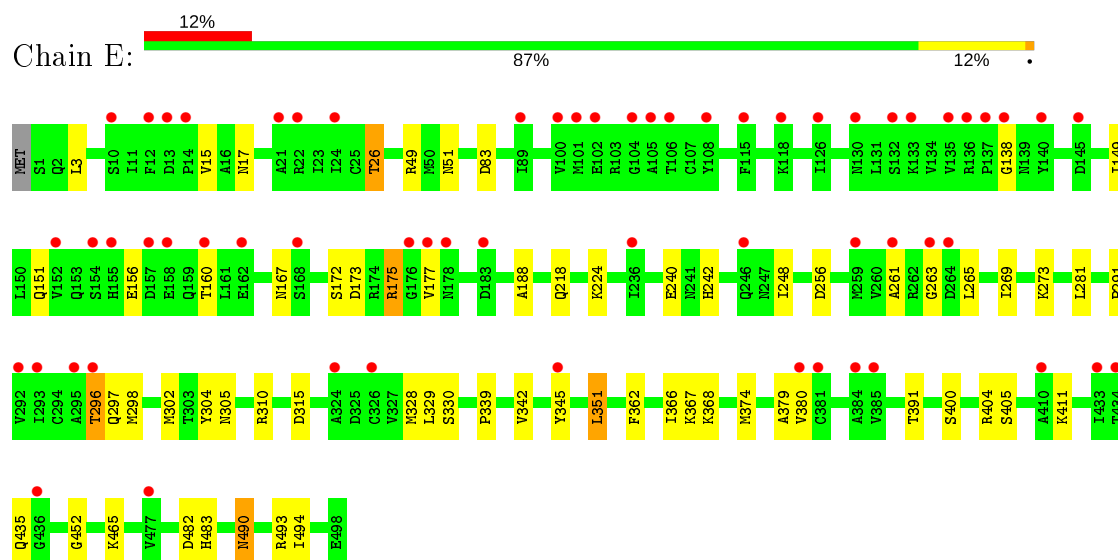
- Molecule 1: Pyruvate kinase



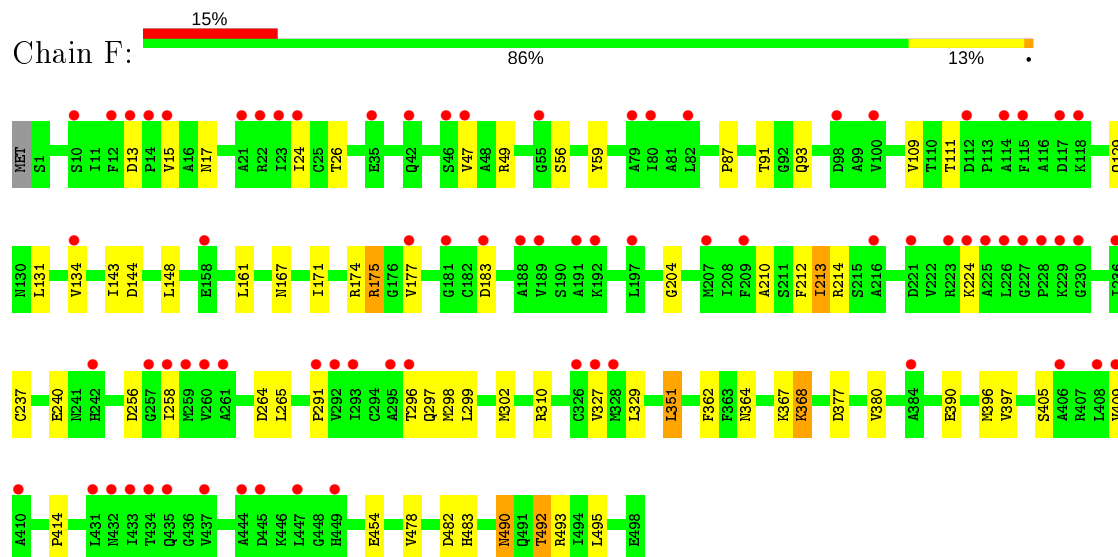
- Molecule 1: Pyruvate kinase



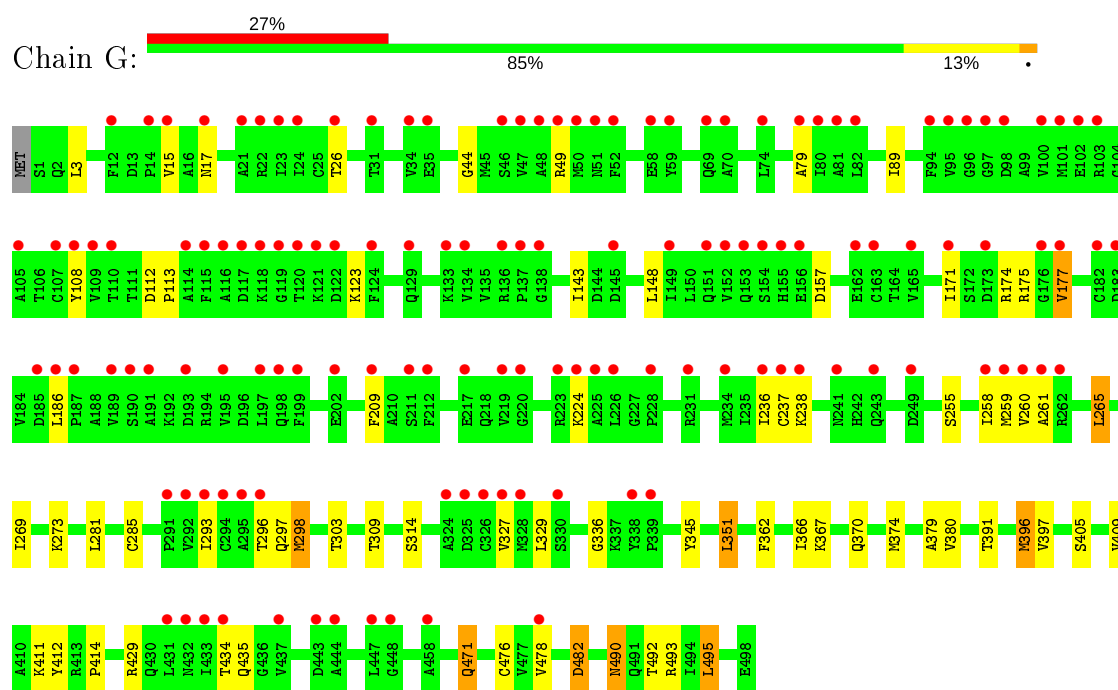
- Molecule 1: Pyruvate kinase



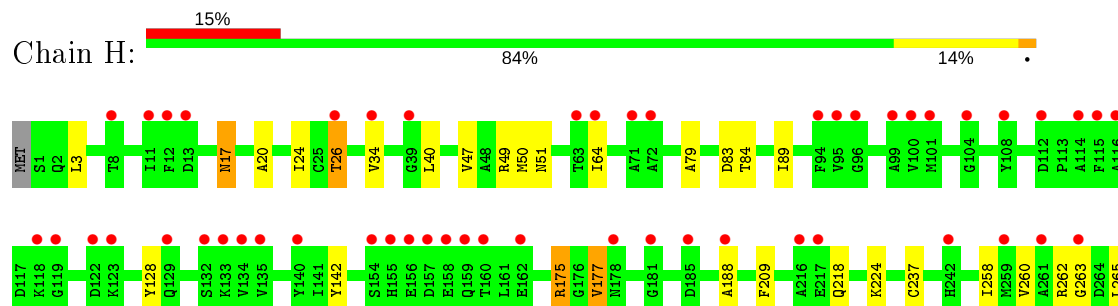
- Molecule 1: Pyruvate kinase

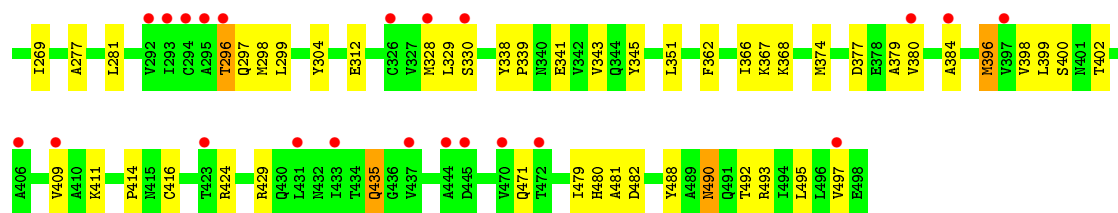


- Molecule 1: Pyruvate kinase

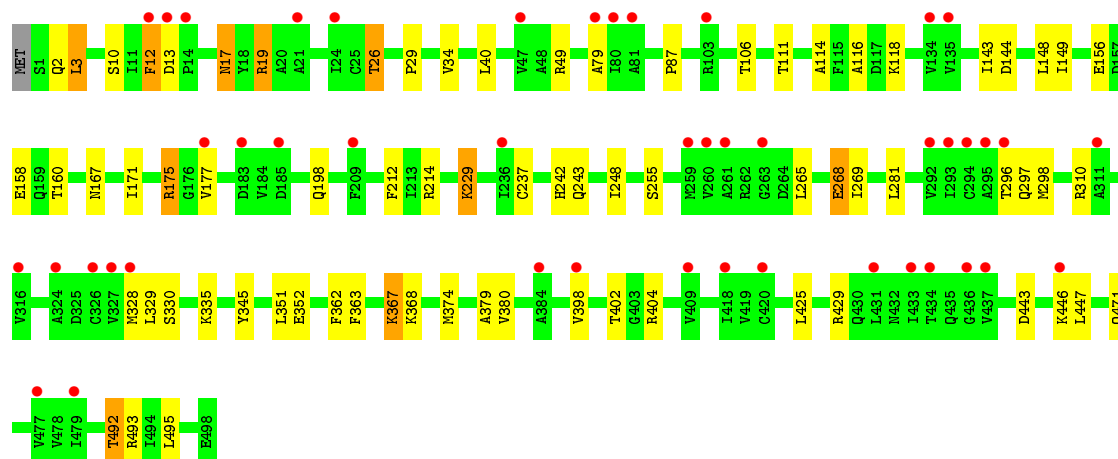
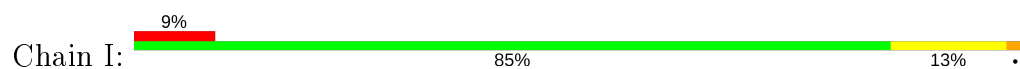


- Molecule 1: Pyruvate kinase

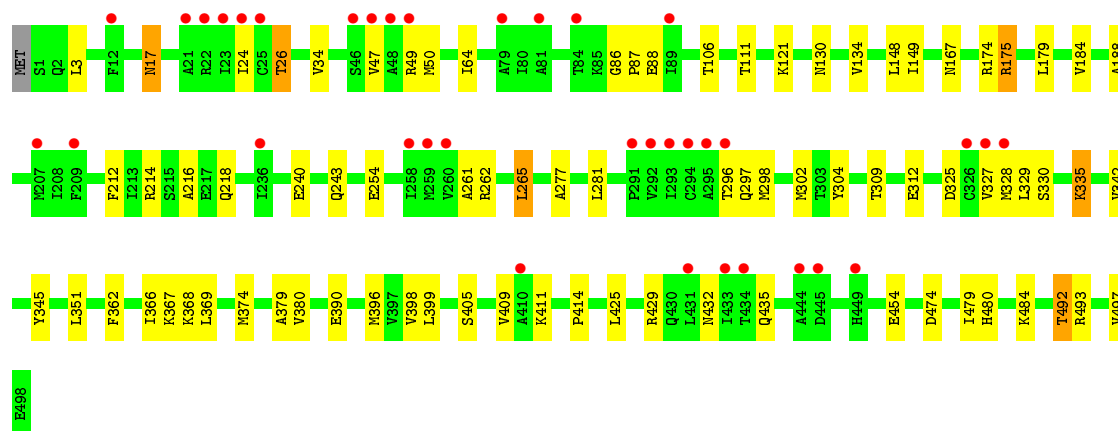
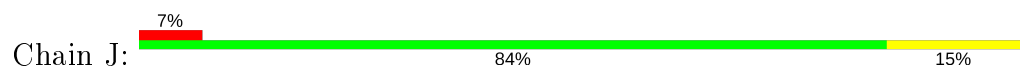




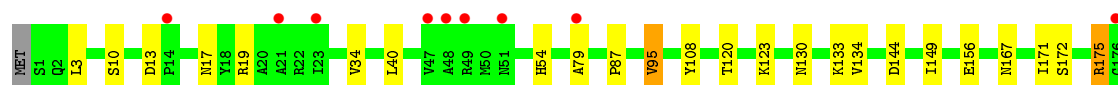
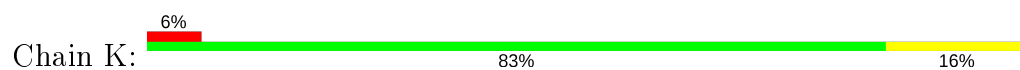
• Molecule 1: Pyruvate kinase

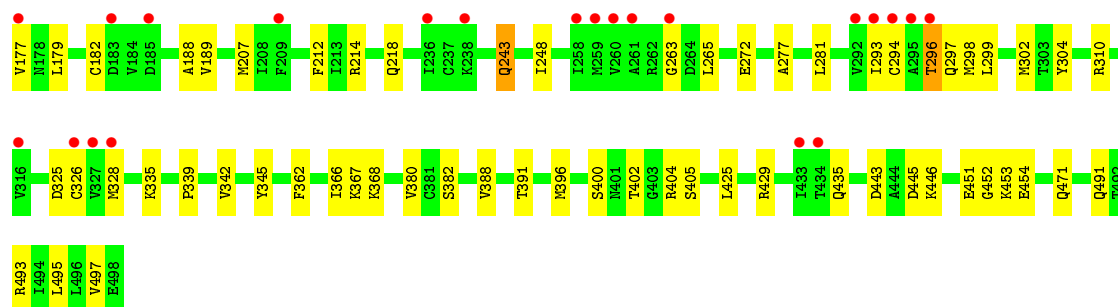


• Molecule 1: Pyruvate kinase

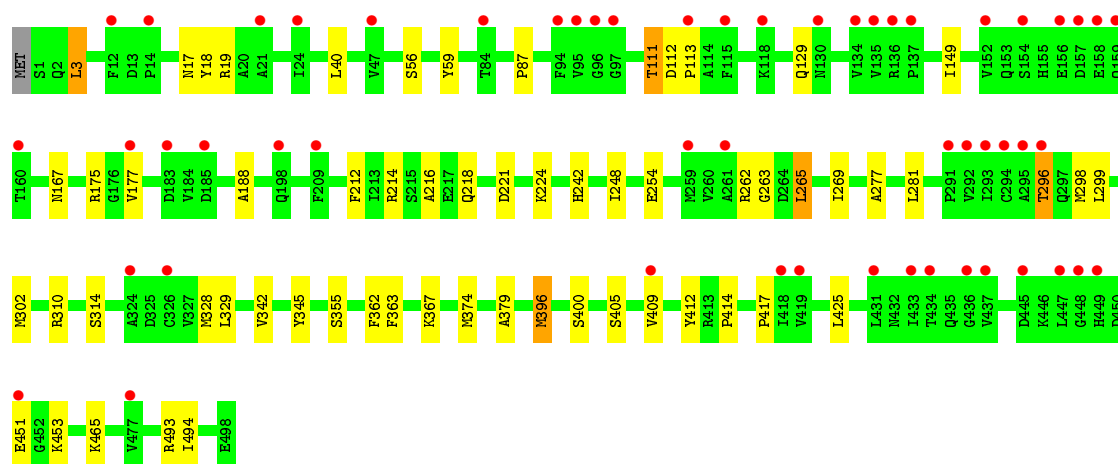
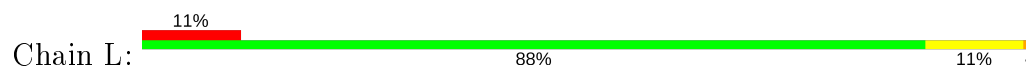


• Molecule 1: Pyruvate kinase

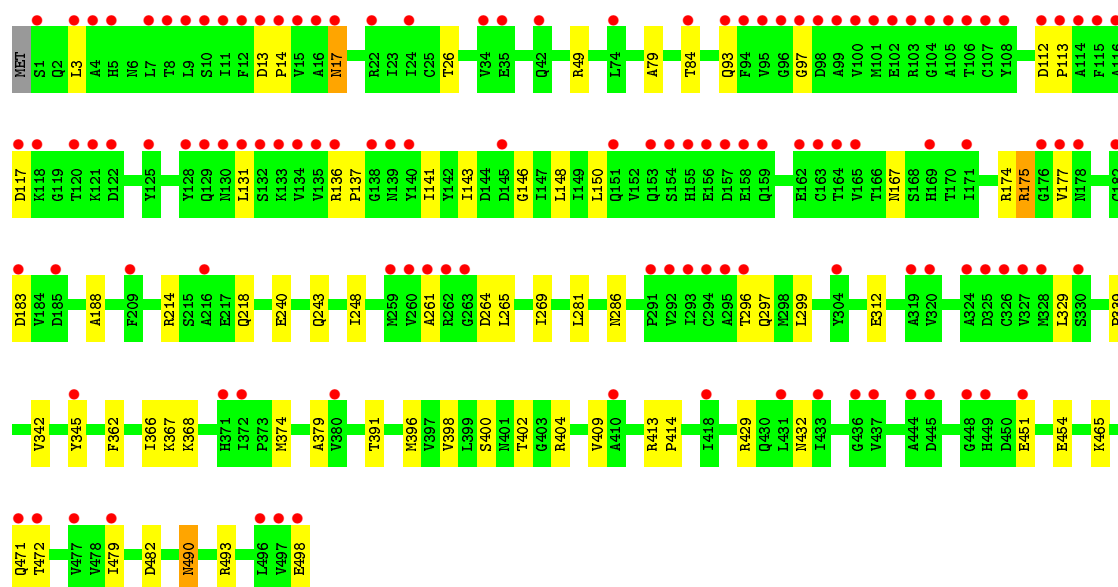
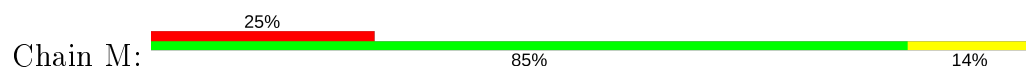




• Molecule 1: Pyruvate kinase



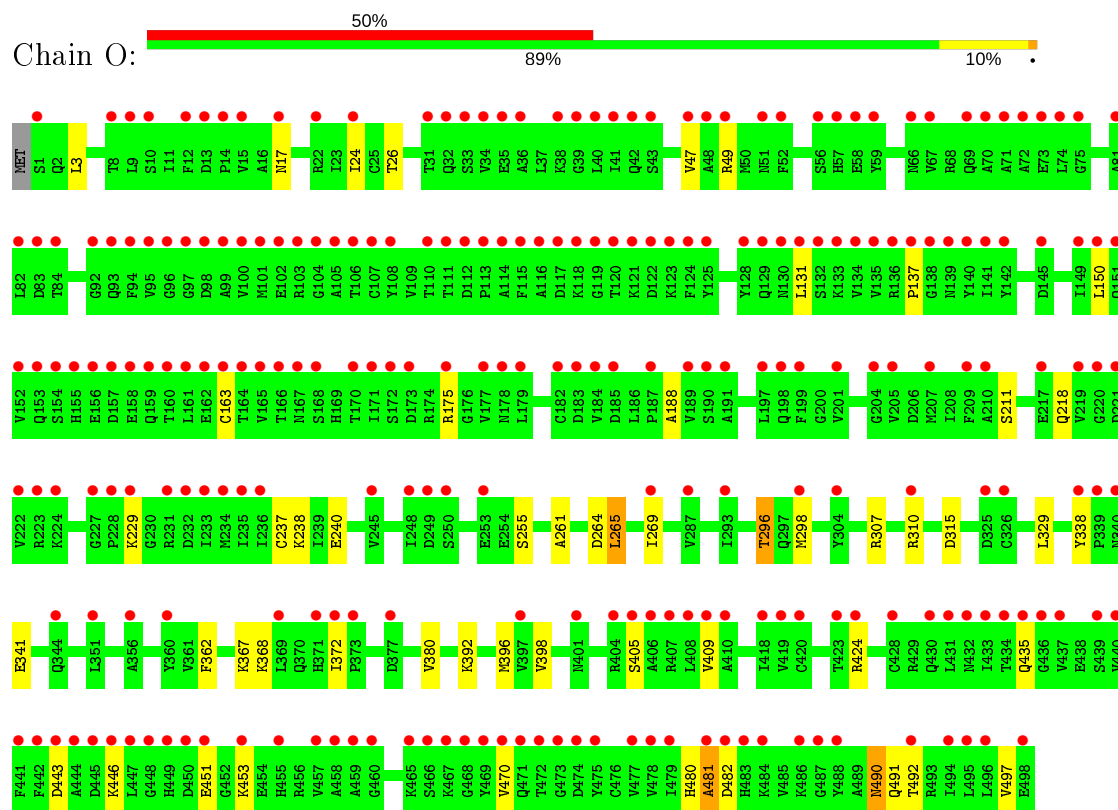
• Molecule 1: Pyruvate kinase



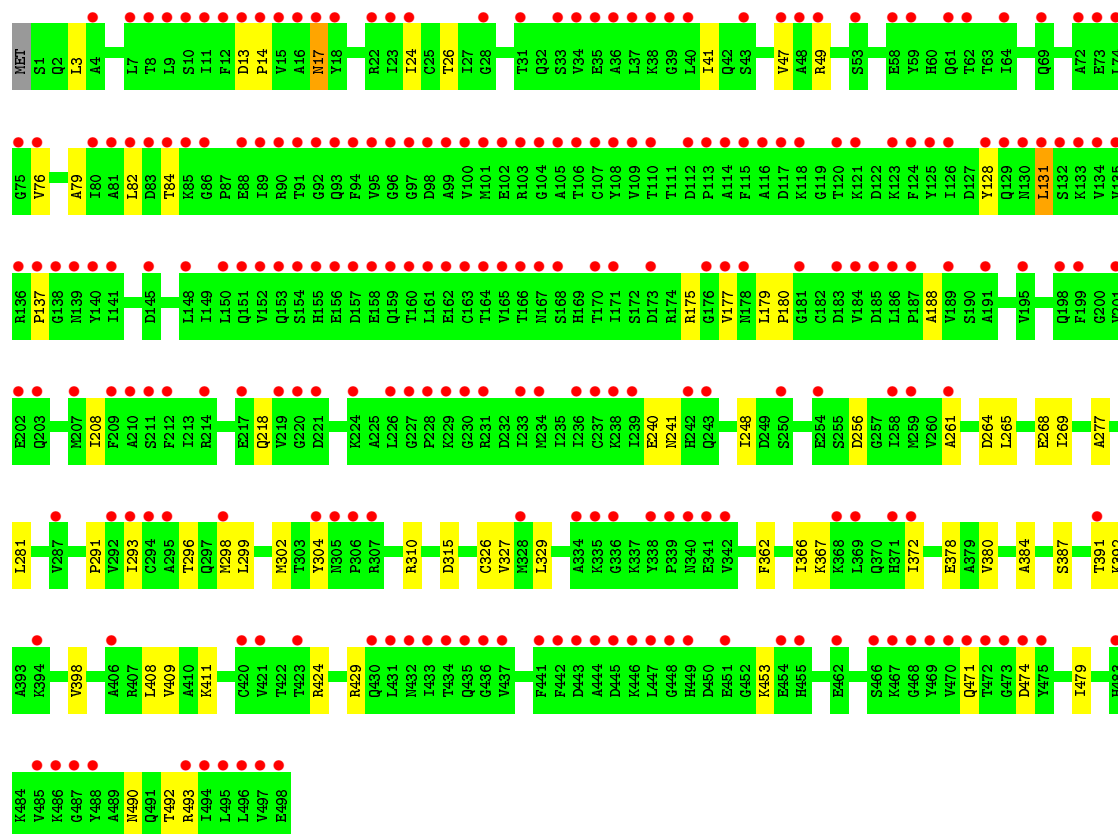
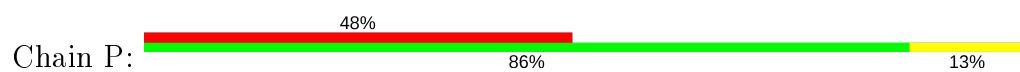
• Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase





## 4 Data and refinement statistics

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

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

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, K, OXL, FDP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/3876	0.50	0/5247
1	B	0.39	0/3856	0.55	0/5220
1	C	0.36	0/3872	0.53	0/5242
1	D	0.40	0/3867	0.55	0/5235
1	E	0.36	0/3865	0.51	0/5232
1	F	0.36	0/3856	0.51	0/5220
1	G	0.33	0/3856	0.49	0/5220
1	H	0.37	0/3874	0.51	0/5244
1	I	0.44	0/3874	0.59	1/5245 (0.0%)
1	J	0.44	0/3882	0.58	0/5256
1	K	0.45	0/3873	0.59	0/5243
1	L	0.41	0/3856	0.56	0/5220
1	M	0.35	0/3856	0.49	0/5220
1	N	0.35	0/3865	0.48	0/5232
1	O	0.34	0/3856	0.47	0/5220
1	P	0.33	0/3856	0.46	0/5220
All	All	0.38	0/61840	0.53	1/83716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (710) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:388:VAL:HG21	1:K:396:MET:HE1	1.34	1.09
1:C:26:THR:HG22	1:C:49:ARG:HD3	1.40	1.04
1:J:298:MET:HE3	1:J:327:VAL:HB	1.39	1.01
1:K:388:VAL:HG21	1:K:396:MET:CE	1.90	0.99
1:J:398[A]:VAL:HG11	1:J:409:VAL:HG21	1.50	0.92
1:B:396:MET:HE1	1:B:414:PRO:HG3	1.53	0.90
1:J:298:MET:HE1	1:J:328:MET:H	1.35	0.90
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:A:396:MET:HE1	1:A:414:PRO:HG3	1.54	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: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
5:N:700:FDP:H11	5:N:700:FDP:O3P	1.75	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: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:J:380:VAL:HG13	1:J:492:THR:HG22	1.61	0.81
1:J:26:THR:HG23	1:J:329:LEU:O	1.80	0.80
1:A:17:ASN:HD22	1:A:17:ASN:H	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: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: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:E:374:MET:HE2	1:F:390:GLU:HB3	1.69	0.75
1:B:396:MET:HE3	1:B:418:ILE:HG12	1.70	0.74

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:297:GLN:NE2	1:D:310:ARG:H	1.86	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: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:M:398:VAL:HG11	1:M:409:VAL:HG21	1.72	0.72
1:K:298:MET:CE	1:K:328:MET:H	2.03	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:L:302:MET:HE1	1:L:342:VAL:HA	1.73	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: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:374:MET:HE2	1:I:379:ALA:HA	1.73	0.69
1:A:396:MET:HE1	1:A:414:PRO:CG	2.21	0.69
1:I:297:GLN:HE21	1:K:310:ARG:H	1.41	0.69
1:B:398:VAL:HG11	1:B:409:VAL:HG21	1.75	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:D:298:MET:HE3	1:D:327:VAL:HB	1.74	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: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:L:302:MET:HE3	1:L:342:VAL:HG23	1.76	0.68
1:K:188:ALA:HB1	1:K:218:GLN:HG3	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:D:451:GLU:CD	1:D:451:GLU:H	1.98	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:N	1:A:17:ASN:HD22	1.93	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HG23	1:D:330:SER:HA	1.77	0.66
1:J:298:MET:CE	1:J:327:VAL:HB	2.23	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:B:298:MET:HE1	1:B:328:MET:H	1.59	0.65
1:N:398:VAL:HG11	1:N:409:VAL:HG21	1.79	0.65
1:E:26:THR:HG23	1:E:329:LEU:O	1.97	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:O:480:HIS:CA	1:O:481:ALA:HB3	2.26	0.64
1:E:298:MET:HE1	1:E:328:MET:H	1.61	0.64
1:J:374:MET:HE2	1:J:379:ALA:HA	1.79	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: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: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:D:388:VAL:HG21	1:D:396:MET:CE	2.27	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: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: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:B:277:ALA:O	1:B:281:LEU:HG	1.99	0.62
1:J:298:MET:HE1	1:J:328:MET:N	2.11	0.62
1:C:26:THR:HG21	1:C:49:ARG:HH11	1.65	0.61

*Continued on next page...*



*Continued from previous page...*

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:M:143:ILE:HB	1:M:148:LEU:HB3	1.81	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:D:299:LEU:HD13	1:D:302:MET:HE3	1.81	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:H:396:MET:HE1	1:H:414:PRO:CB	2.31	0.61
1:B:248:ILE:HG12	1:B:281:LEU:HD22	1.81	0.60
1:J:396:MET:HE1	1:J:414:PRO:CB	2.31	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:G:366:ILE:HD13	1:G:411:LYS:O	2.01	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:D:298:MET:HE1	1:D:328:MET:H	1.67	0.59
1:O:26:THR:HG22	1:O:49:ARG:HD3	1.84	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: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:A:474:ASP:O	1:A:497:VAL:HG22	2.03	0.58
1:A:3:LEU:HD13	1:C:369:LEU:HD12	1.85	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:K:325:ASP:HA	1:K:435:GLN:HB2	1.86	0.58
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:302:MET:HE3	1:C:342:VAL:HA	1.87	0.57
1:J:398[A]:VAL:CG1	1:J:409:VAL:HG21	2.31	0.57
1:K:388:VAL:HG21	1:K:396:MET:HE2	1.83	0.57
1:N:188:ALA:HB1	1:N:218:GLN:HG3	1.87	0.57
1:A:374:MET:HE3	1:A:379:ALA:HA	1.87	0.57
1:H:396:MET:HE2	1:H:416:CYS:SG	2.45	0.56
1:J:26:THR:HG21	1:J:49:ARG:HH11	1.69	0.56
1:K:248:ILE:HG12	1:K:281:LEU:HD22	1.87	0.56
1:F:87:PRO:HD2	1:F:212:PHE:HB2	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:L:405:SER:O	1:L:409:VAL:HG23	2.06	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:C:175:ARG:HH22	6:C:1001:ATP:HO3'	1.49	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:10:SER:OG	1:I:12:PHE:HD2	1.89	0.55
1:I:3:LEU:HD11	1:K:366:ILE:HG13	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
1:E:366:ILE:HD13	1:E:411:LYS:O	2.05	0.55
1:I:363:PHE:CZ	1:I:367:LYS:HE3	2.42	0.55
1:I:79:ALA:HB2	1:I:429:ARG:O	2.07	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:F:364:ASN:O	1:F:368:LYS:HD3	2.07	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:F:396:MET:HE1	1:F:414:PRO:CB	2.37	0.55
1:I:298:MET:CE	1:I:328:MET:H	2.19	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:M:490:ASN:HD22	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: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:C:87:PRO:HD2	1:C:212:PHE:HB2	1.87	0.54
1:H:374:MET:CE	1:H:379:ALA:HA	2.37	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: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:K:294:CYS:O	1:K:298:MET:HE1	2.08	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
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:D:298:MET:CE	1:D:327:VAL:HB	2.35	0.53
1:N:380:VAL:HG13	1:N:492:THR:HG23	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:N:482:ASP:H	1:N:490:ASN:HD21	1.56	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:374:MET:CE	1:A:379:ALA:HA	2.39	0.52
1:A:47:VAL:HG22	1:A:79:ALA:HB3	1.92	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:298:MET:HE1	1:I:328:MET:H	1.75	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: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
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:K:298:MET:HE1	1:K:328:MET:H	1.75	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:A:396:MET:CE	1:A:414:PRO:HG3	2.34	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: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:HD22	1:C:17:ASN:N	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:K:299:LEU:HD13	1:K:302:MET:CE	2.41	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: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:F:396:MET:HE3	1:F:414:PRO:HG3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:298:MET:CE	1:L:328:MET:H	2.24	0.51
5:N:700:FDP:C1	5:N:700:FDP:O3P	2.55	0.51
1:O:188:ALA:HB1	1:O:218:GLN:HG3	1.92	0.51
1:B:294:CYS:O	1:B:298:MET:HE1	2.10	0.50
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
1:P:277:ALA:O	1:P:281:LEU:HG	2.10	0.50
1:K:79:ALA:HB1	1:K:207:MET:HE3	1.92	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:B:299:LEU:HD13	1:B:302:MET:HE3	1.94	0.50
1:I:268:GLU:HG3	8:I:568:HOH:O	2.12	0.50
1:I:3:LEU:CD1	1:K:366:ILE:HG13	2.41	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:B:396:MET:CE	1:B:418:ILE:HG12	2.38	0.50
1:C:26:THR:HG23	1:C:329:LEU:O	2.11	0.50
1:D:388:VAL:HG21	1:D:396:MET:HE1	1.93	0.50
1:H:481:ALA:HA	1:H:490:ASN:HD22	1.76	0.50
1:N:396:MET:CE	1:N:414:PRO:HG3	2.42	0.50
1:O:380:VAL:HG21	1:O:490:ASN:HA	1.94	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:HD23	1:M:131:LEU:H	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:THR:HG22	1:M:49:ARG:HD3	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:G:396:MET:HE1	1:G:414:PRO:CB	2.42	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:J:87:PRO:HD2	1:J:212:PHE:HB2	1.95	0.49
1:J:262:ARG:NH2	1:J:298:MET:HG2	2.27	0.49
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:J:374:MET:HE1	1:J:379:ALA:HA	1.93	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: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: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:L:374:MET:HE3	1:L:379:ALA:HA	1.95	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:B:396:MET:HE2	1:B:414:PRO:HG3	1.92	0.48
1:C:54:HIS:HE1	6:C:1001:ATP:O2B	1.97	0.48
1:I:149:ILE:H	1:I:167:ASN:HD21	1.60	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:N:366:ILE:HD13	1:N:411:LYS:O	2.13	0.48
1:A:396:MET:HE1	1:A:414:PRO:CB	2.42	0.48
1:J:26:THR:CG2	1:J:329:LEU:O	2.58	0.48
1:D:374:MET:HE2	1:D:379:ALA:HA	1.96	0.47
1:D:388:VAL:HG21	1:D:396:MET:HE2	1.96	0.47
1:C:171:ILE:HB	1:C:175:ARG:HG2	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:THR:HG21	1:E:49:ARG:NH1	2.27	0.47
1:K:172:SER:O	1:K:175:ARG:CD	2.62	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:N:396:MET:HE1	1:N:414:PRO:CB	2.44	0.47
1:E:269:ILE:HG23	1:E:273:LYS:HB2	1.97	0.47
1:E:490:ASN:HD22	1:E:490:ASN:H	1.62	0.47
1:A:240:GLU:HB2	1:A:264:ASP:HB2	1.95	0.47
1:H:24:ILE:HB	1:H:328:MET:HG3	1.95	0.47
1:J:17:ASN:C	1:J:17:ASN:HD22	2.18	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: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: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:H	1:C:17:ASN:HD22	1.63	0.47
1:G:186:LEU:HB3	8:G:611:HOH:O	2.15	0.47
1:H:79:ALA:HB2	1:H:429:ARG:O	2.15	0.47
1:F:396:MET:HB2	1:F:396:MET:HE2	1.49	0.46
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:C:299:LEU:HB3	1:C:302:MET:HE2	1.98	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
1:A:216:ALA:HB1	1:A:254:GLU:HG3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:396:MET:HE1	1:M:414:PRO:HG3	1.96	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:G:260:VAL:HG22	1:G:281:LEU:HD12	1.96	0.46
1:E:297:GLN:HE21	1:G:309:THR:HB	1.81	0.46
1:M:374:MET:HE1	1:M:379:ALA:HA	1.98	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: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:396:MET:HE1	1:D:414:PRO:CB	2.46	0.46
1:E:172:SER:O	1:E:175:ARG:HD3	2.16	0.46
1:K:299:LEU:HD13	1:K:302:MET:HE3	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: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:L:242:HIS:HD2	8:L:662:HOH:O	1.99	0.45
1:M:17:ASN:N	1:M:17:ASN:HD22	2.13	0.45
1:D:396:MET:HE2	1:D:396:MET:HB2	1.78	0.45
1:I:26:THR:HG23	1:I:330:SER:HA	1.98	0.45
1:J:396:MET:HB2	1:J:396:MET:HE2	1.55	0.45
1:K:452:GLY:C	1:K:453:LYS:HG2	2.37	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:293:ILE:HG12	1:P:326:CYS:HB2	1.98	0.45
1:P:79:ALA:HB2	1:P:429:ARG:O	2.17	0.45
1:G:26:THR:HG23	1:G:329:LEU:O	2.16	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:396:MET:HE1	1:J:414:PRO:HB3	1.97	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:B:374:MET:HE3	1:B:379:ALA:HA	1.97	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: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: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:F:299:LEU:HD13	1:F:302: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:J:24:ILE:HG12	1:J:47:VAL:HB	1.98	0.44
1:M:374:MET:HE2	1:N:390:GLU:CD	2.37	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:L:396:MET:HE1	1:L:414:PRO:CB	2.48	0.44
1:M:429:ARG:O	1:M:432:ASN:HB2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:GLN:CD	1:F:129:GLN:H	2.20	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:P:299:LEU:HB3	1:P:302:MET:HE3	1.99	0.44
1:B:296:THR:HG22	1:B:297:GLN:HG3	1.98	0.44
1:L:277:ALA:O	1:L:281:LEU:HG	2.17	0.44
1:L:18:TYR:CD2	1:L:417:PRO:HG3	2.52	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: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: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:C:298:MET:HE3	1:C:328:MET:H	1.82	0.43
1:D:396:MET:HE1	1:D:414:PRO:HB3	2.00	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:339:PRO:O	1:M:342:VAL:HG12	2.18	0.43
1:B:79:ALA:HB1	1:B:207:MET:HE3	1.99	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
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:A:17:ASN:N	1:A:17:ASN:ND2	2.64	0.43
1:F:296:THR:HG22	1:F:297:GLN:HG3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:396:MET:HE2	1:L:396:MET:HB2	1.46	0.43
1:M:248:ILE:HG12	1:M:281:LEU:HD22	2.00	0.43
1:B:339:PRO:O	1:B:342:VAL:HG12	2.18	0.43
1:B:24:ILE:HG12	1:B:47:VAL:HB	2.00	0.43
1:I:214:ARG:HB2	1:I:243:GLN:HG3	2.00	0.43
1:K:293:ILE:HG12	1:K:326:CYS:HB2	2.00	0.43
1:P:47:VAL:HG13	1:P:79:ALA:HB3	2.00	0.43
1:F:396:MET:CE	1:F:414:PRO:HG3	2.48	0.43
1:K:175:ARG:N	1:K:175:ARG:HD2	2.34	0.43
1:C:446:LYS:HG3	1:C:447:LEU:HG	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:A:374:MET:HE1	1:B:390:GLU:CD	2.39	0.43
1:B:79:ALA:HB2	1:B:429:ARG:O	2.18	0.43
1:B:51:ASN:HA	1:B:83:ASP:HB3	2.01	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: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: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:P:380:VAL:HG13	1:P:492:THR:HG23	2.02	0.42
1:B:223:ARG:NH1	8:B:982:HOH:O	2.52	0.42
1:B:216:ALA:HB1	1:B:254:GLU:HG3	2.01	0.42
1:C:299:LEU:HD23	1:C:312:GLU:HB3	2.01	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:N:396:MET:HE1	1:N:414:PRO:HG3	2.01	0.42
1:B:285:CYS:HB3	1:B:290:LYS:O	2.19	0.42
1:B:49:ARG:NH2	8:B:1882:HOH:O	2.27	0.42
1:G:259:MET:HG3	1:G:293:ILE:HB	2.00	0.42
1:A:10:SER:HB3	1:A:13:ASP:OD1	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HD13	1:B:441:PHE:CG	2.54	0.42
1:G:396:MET:HE1	1:G:414:PRO:HB3	2.01	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: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:F:91:THR:O	1:F:174:ARG:HA	2.20	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:M:175:ARG:CA	1:M:175:ARG:HE	2.32	0.42
1:O:240:GLU:HB2	1:O:264:ASP:HB2	2.00	0.42
1:D:451:GLU:CD	1:D:451:GLU:N	2.71	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:M:400:SER:OG	1:M:402:THR:O	2.25	0.42
1:B:307:ARG:HB2	1:B:308:PRO:HD2	2.02	0.41
1:C:17:ASN:ND2	1:C:17:ASN:N	2.67	0.41
1:K:171:ILE:HB	1:K:175:ARG:HG2	2.02	0.41
1:K:144:ASP:HB2	1:K:175:ARG:HG3	2.03	0.41
1:A:481:ALA:HA	1:A:490:ASN:HD22	1.85	0.41
1:B:10:SER:HB3	1:B:13:ASP:CG	2.41	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:L:374:MET:CE	1:L:379:ALA:CA	2.94	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HD13	1:C:177:VAL:HB	2.02	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:298:MET:HE3	1:K:328:MET:H	1.80	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:J:302:MET:CE	1:J:342:VAL:HG23	2.50	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: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:F:396:MET:HE1	1:F:414:PRO:HB2	2.03	0.41
1:G:298:MET:HE1	1:G:327:VAL:HG12	2.01	0.41
1:H:24:ILE:HG12	1:H:47:VAL:HB	2.02	0.41
1:I:242:HIS:ND1	1:I:269:ILE:HG22	2.35	0.41
1:I:2:GLN:NE2	8:I:683:HOH:O	2.53	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:H:396:MET:HE1	1:H:414:PRO:HB2	2.01	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:D:24:ILE:HG21	1:D:328:MET:HE2	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:LEU:O	1:K:182:CYS:HB2	2.20	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:M:146:GLY:O	1:O:307:ARG:HD2	2.21	0.41
1:C:452:GLY:C	1:C:453:LYS:HG2	2.41	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:N:85:LYS:HE2	1:N:192:LYS:HD3	2.03	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:490:ASN:HD22	1:G:490:ASN:H	1.69	0.41
1:G:26:THR:CG2	1:G:49:ARG:HD3	2.42	0.41
1:L:56:SER:H	1:L:59:TYR:HB3	1.85	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:F:298:MET:CE	1:F:327:VAL:HB	2.51	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:HA	1:O:229:LYS:HE2	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: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:484:LYS:NZ	8:J:595:HOH:O	2.54	0.40
1:J:474:ASP:O	1:J:497:VAL:HG13	2.20	0.40
1:L:299:LEU:HD12	1:L:329:LEU:HD21	2.02	0.40
1:N:298:MET:CE	1:N:328:MET:H	2.34	0.40
1:O:237:CYS:SG	1:O:255:SER:HB3	2.61	0.40
1:B:34:VAL:O	1:B:38:LYS:HG3	2.21	0.40
1:C:213:ILE:HA	1:C:218:GLN:OE1	2.20	0.40
1:C:56:SER:H	1:C:59:TYR:HB3	1.86	0.40
6:D:1001:ATP:O1A	6:D:1001:ATP:O1G	2.40	0.40
1:D:115:PHE:CE2	1:D:123:LYS:HD3	2.56	0.40
1:F:24:ILE:HG12	1:F:47:VAL:HB	2.03	0.40
1:H:260:VAL:HG22	1:H:281:LEU:HD12	2.02	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:378:GLU:HA	1:P:408:LEU:HD21	2.02	0.40
1:P:26:THR:HG22	1:P:49:ARG:HD3	2.03	0.40
1:E:26:THR:CG2	1:E:49:ARG:HH11	2.34	0.40
1:H:402:THR:HG22	1:H:424:ARG:NH2	2.36	0.40
1:M:396:MET:HE1	1:M:414:PRO:CB	2.51	0.40
1:N:396:MET:HE3	1:N:414:PRO:HG3	2.03	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

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/499 (100%)	481 (97%)	14 (3%)	3 (1%)	25	31
1	B	496/499 (99%)	486 (98%)	8 (2%)	2 (0%)	34	42
1	C	498/499 (100%)	482 (97%)	15 (3%)	1 (0%)	47	58
1	D	497/499 (100%)	483 (97%)	14 (3%)	0	100	100
1	E	497/499 (100%)	477 (96%)	19 (4%)	1 (0%)	47	58
1	F	496/499 (99%)	480 (97%)	14 (3%)	2 (0%)	34	42
1	G	496/499 (99%)	465 (94%)	27 (5%)	4 (1%)	19	23
1	H	498/499 (100%)	477 (96%)	20 (4%)	1 (0%)	47	58
1	I	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	47	58
1	J	499/499 (100%)	483 (97%)	15 (3%)	1 (0%)	47	58

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	47	58
1	L	496/499 (99%)	477 (96%)	18 (4%)	1 (0%)	47	58
1	M	496/499 (99%)	472 (95%)	20 (4%)	4 (1%)	19	23
1	N	497/499 (100%)	476 (96%)	20 (4%)	1 (0%)	47	58
1	O	496/499 (99%)	466 (94%)	27 (5%)	3 (1%)	25	31
1	P	496/499 (99%)	469 (95%)	25 (5%)	2 (0%)	34	42
All	All	7952/7984 (100%)	7646 (96%)	278 (4%)	28 (0%)	34	42

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
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%)	397 (95%)	21 (5%)	24	34
1	B	416/417 (100%)	395 (95%)	21 (5%)	24	34
1	C	418/417 (100%)	401 (96%)	17 (4%)	30	43
1	D	417/417 (100%)	395 (95%)	22 (5%)	22	31
1	E	417/417 (100%)	398 (95%)	19 (5%)	27	38
1	F	416/417 (100%)	398 (96%)	18 (4%)	29	40
1	G	416/417 (100%)	396 (95%)	20 (5%)	25	36
1	H	418/417 (100%)	394 (94%)	24 (6%)	20	28
1	I	418/417 (100%)	391 (94%)	27 (6%)	17	23
1	J	419/417 (100%)	398 (95%)	21 (5%)	24	34
1	K	418/417 (100%)	392 (94%)	26 (6%)	18	25
1	L	416/417 (100%)	400 (96%)	16 (4%)	33	47
1	M	416/417 (100%)	397 (95%)	19 (5%)	27	38
1	N	417/417 (100%)	397 (95%)	20 (5%)	25	36
1	O	416/417 (100%)	401 (96%)	15 (4%)	35	49
1	P	416/417 (100%)	400 (96%)	16 (4%)	33	47
All	All	6672/6672 (100%)	6350 (95%)	322 (5%)	25	36

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	ASN
1	A	84	THR
1	A	167	ASN
1	A	175	ARG
1	A	177	VAL
1	A	229	LYS
1	A	265	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	304	TYR
1	A	314	SER
1	A	345	TYR
1	A	351	LEU
1	A	362	PHE
1	A	367	LYS
1	A	368	LYS
1	A	445	ASP
1	A	454	GLU
1	A	471	GLN
1	A	490	ASN
1	A	493	ARG
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	177	VAL
1	B	229	LYS
1	B	240	GLU
1	B	265	LEU
1	B	307	ARG
1	B	362	PHE
1	B	367	LYS
1	B	368	LYS
1	B	398	VAL
1	B	425	LEU
1	B	435	GLN
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	345	TYR
1	C	351	LEU
1	C	362	PHE
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	D	3	LEU
1	D	17	ASN
1	D	26	THR
1	D	40	LEU
1	D	106	THR
1	D	174	ARG
1	D	175	ARG
1	D	177	VAL
1	D	229	LYS
1	D	265	LEU
1	D	304	TYR
1	D	307	ARG
1	D	345	TYR
1	D	351	LEU
1	D	362	PHE
1	D	367	LYS
1	D	391	THR
1	D	398	VAL
1	D	451	GLU
1	D	471	GLN
1	D	490	ASN
1	D	493	ARG
1	E	3	LEU
1	E	17	ASN
1	E	26	THR
1	E	175	ARG
1	E	177	VAL
1	E	224	LYS
1	E	265	LEU
1	E	304	TYR
1	E	345	TYR
1	E	351	LEU
1	E	362	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	367	LYS
1	E	368	LYS
1	E	391	THR
1	E	404	ARG
1	E	435	GLN
1	E	465	LYS
1	E	490	ASN
1	E	493	ARG
1	F	13	ASP
1	F	17	ASN
1	F	111	THR
1	F	167	ASN
1	F	175	ARG
1	F	177	VAL
1	F	213	ILE
1	F	214	ARG
1	F	224	LYS
1	F	351	LEU
1	F	362	PHE
1	F	367	LYS
1	F	368	LYS
1	F	454	GLU
1	F	483	HIS
1	F	490	ASN
1	F	492	THR
1	F	493	ARG
1	G	3	LEU
1	G	17	ASN
1	G	157	ASP
1	G	177	VAL
1	G	224	LYS
1	G	265	LEU
1	G	298	MET
1	G	314	SER
1	G	345	TYR
1	G	351	LEU
1	G	362	PHE
1	G	367	LYS
1	G	391	THR
1	G	396	MET
1	G	434	THR
1	G	435	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	471	GLN
1	G	490	ASN
1	G	493	ARG
1	G	495	LEU
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	224	LYS
1	H	265	LEU
1	H	269	ILE
1	H	304	TYR
1	H	345	TYR
1	H	351	LEU
1	H	362	PHE
1	H	367	LYS
1	H	368	LYS
1	H	396	MET
1	H	400	SER
1	H	435	GLN
1	H	471	GLN
1	H	490	ASN
1	H	493	ARG
1	H	495	LEU
1	H	497	VAL
1	I	3	LEU
1	I	12	PHE
1	I	17	ASN
1	I	26	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	229	LYS
1	I	265	LEU
1	I	268	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	335	LYS
1	I	345	TYR
1	I	351	LEU
1	I	362	PHE
1	I	367	LYS
1	I	368	LYS
1	I	398[A]	VAL
1	I	398[B]	VAL
1	I	425	LEU
1	I	471	GLN
1	I	492	THR
1	I	493	ARG
1	I	495	LEU
1	J	3	LEU
1	J	17	ASN
1	J	26	THR
1	J	34	VAL
1	J	106	THR
1	J	121	LYS
1	J	134	VAL
1	J	175	ARG
1	J	179	LEU
1	J	265	LEU
1	J	304	TYR
1	J	335	LYS
1	J	345	TYR
1	J	351	LEU
1	J	362	PHE
1	J	367	LYS
1	J	368	LYS
1	J	425	LEU
1	J	454	GLU
1	J	492	THR
1	J	493	ARG
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	189	VAL
1	K	243	GLN
1	K	265	LEU
1	K	304	TYR
1	K	335	LYS
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	425	LEU
1	K	445	ASP
1	K	451	GLU
1	K	454	GLU
1	K	471	GLN
1	K	495	LEU
1	K	497	VAL
1	L	3	LEU
1	L	17	ASN
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	362	PHE
1	L	367	LYS
1	L	396	MET
1	L	425	LEU
1	L	465	LYS
1	L	493	ARG
1	M	3	LEU
1	M	17	ASN
1	M	84	THR
1	M	167	ASN
1	M	175	ARG
1	M	177	VAL
1	M	265	LEU
1	M	269	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	345	TYR
1	M	367	LYS
1	M	368	LYS
1	M	391	THR
1	M	404	ARG
1	M	451	GLU
1	M	454	GLU
1	M	465	LYS
1	M	471	GLN
1	M	490	ASN
1	M	493	ARG
1	N	3	LEU
1	N	17	ASN
1	N	175	ARG
1	N	177	VAL
1	N	231	ARG
1	N	265	LEU
1	N	307	ARG
1	N	345	TYR
1	N	359	GLU
1	N	362	PHE
1	N	367	LYS
1	N	368	LYS
1	N	391	THR
1	N	398	VAL
1	N	404	ARG
1	N	424	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	131	LEU
1	O	175	ARG
1	O	265	LEU
1	O	269	ILE
1	O	296	THR
1	O	362	PHE
1	O	367	LYS
1	O	368	LYS
1	O	396	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	131	LEU
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	362	PHE
1	P	367	LYS
1	P	424	ARG
1	P	471	GLN
1	P	474	ASP
1	P	493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	17	ASN
1	A	54	HIS
1	A	65	ASN
1	A	167	ASN
1	A	286	ASN
1	A	297	GLN
1	A	322	ASN
1	A	344	GLN
1	A	471	GLN
1	A	490	ASN
1	B	2	GLN
1	B	17	ASN
1	B	42	GLN
1	B	167	ASN
1	B	178	ASN
1	B	242	HIS
1	B	243	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	297	GLN
1	B	305	ASN
1	B	322	ASN
1	B	344	GLN
1	B	490	ASN
1	B	491	GLN
1	C	17	ASN
1	C	54	HIS
1	C	178	ASN
1	C	243	GLN
1	C	286	ASN
1	C	297	GLN
1	C	305	ASN
1	C	322	ASN
1	C	344	GLN
1	C	490	ASN
1	D	2	GLN
1	D	17	ASN
1	D	42	GLN
1	D	167	ASN
1	D	178	ASN
1	D	305	ASN
1	D	344	GLN
1	D	435	GLN
1	D	490	ASN
1	E	17	ASN
1	E	151	GLN
1	E	167	ASN
1	E	178	ASN
1	E	297	GLN
1	E	401	ASN
1	E	483	HIS
1	E	490	ASN
1	E	491	GLN
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	490	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	17	ASN
1	G	57	HIS
1	G	139	ASN
1	G	167	ASN
1	G	243	GLN
1	G	297	GLN
1	G	322	ASN
1	G	386	ASN
1	G	471	GLN
1	G	490	ASN
1	H	17	ASN
1	H	93	GLN
1	H	167	ASN
1	H	297	GLN
1	H	386	ASN
1	H	401	ASN
1	H	490	ASN
1	I	2	GLN
1	I	17	ASN
1	I	167	ASN
1	I	178	ASN
1	I	297	GLN
1	I	305	ASN
1	I	344	GLN
1	I	401	ASN
1	I	435	GLN
1	J	17	ASN
1	J	54	HIS
1	J	93	GLN
1	J	167	ASN
1	J	246	GLN
1	J	297	GLN
1	J	305	ASN
1	J	401	ASN
1	K	17	ASN
1	K	54	HIS
1	K	130	ASN
1	K	167	ASN
1	K	178	ASN
1	K	243	GLN
1	K	305	ASN
1	K	344	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	435	GLN
1	K	471	GLN
1	L	2	GLN
1	L	17	ASN
1	L	42	GLN
1	L	54	HIS
1	L	167	ASN
1	L	178	ASN
1	L	242	HIS
1	L	243	GLN
1	L	318	ASN
1	L	344	GLN
1	L	401	ASN
1	M	17	ASN
1	M	167	ASN
1	M	178	ASN
1	M	278	GLN
1	M	286	ASN
1	M	297	GLN
1	M	322	ASN
1	M	401	ASN
1	M	490	ASN
1	N	17	ASN
1	N	42	GLN
1	N	51	ASN
1	N	54	HIS
1	N	167	ASN
1	N	198	GLN
1	N	242	HIS
1	N	243	GLN
1	N	286	ASN
1	N	344	GLN
1	N	471	GLN
1	N	490	ASN
1	O	17	ASN
1	O	42	GLN
1	O	480	HIS
1	O	490	ASN
1	O	491	GLN
1	P	17	ASN
1	P	318	ASN
1	P	322	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 114 ligands modelled in this entry, 62 are monoatomic - leaving 52 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
7	GOL	E	499	-	5,5,5	0.39	0	5,5,5	0.30	0
5	FDP	N	700	-	19,20,20	1.13	2 (10%)	30,32,32	1.16	1 (3%)
7	GOL	O	499	-	5,5,5	0.38	0	5,5,5	0.23	0
6	ATP	P	1001	3,2	26,33,33	0.99	1 (3%)	31,52,52	1.46	5 (16%)
5	FDP	M	700	-	19,20,20	0.74	0	30,32,32	1.10	3 (10%)
4	OXL	N	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	L	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	H	1001	3,2	26,33,33	0.97	1 (3%)	31,52,52	1.31	4 (12%)
5	FDP	E	700	-	19,20,20	1.21	2 (10%)	30,32,32	1.08	2 (6%)
6	ATP	L	1001	3,2	26,33,33	1.06	3 (11%)	31,52,52	1.36	5 (16%)
5	FDP	A	700	-	19,20,20	0.87	0	30,32,32	1.30	3 (10%)
6	ATP	B	1001	3,2	26,33,33	0.92	1 (3%)	31,52,52	1.32	3 (9%)
4	OXL	I	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	F	1001	3,2	26,33,33	1.05	3 (11%)	31,52,52	1.30	3 (9%)
5	FDP	H	700	-	19,20,20	0.92	1 (5%)	30,32,32	1.38	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	G	499	-	5,5,5	0.38	0	5,5,5	0.25	0
4	OXL	A	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	E	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	J	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	O	700	-	19,20,20	1.02	0	30,32,32	1.01	1 (3%)
7	GOL	J	499	-	5,5,5	0.37	0	5,5,5	0.32	0
6	ATP	I	1001	3,2	26,33,33	1.07	3 (11%)	31,52,52	1.34	6 (19%)
6	ATP	J	1001	3,2	26,33,33	1.03	2 (7%)	31,52,52	1.27	2 (6%)
5	FDP	G	700	-	19,20,20	1.24	2 (10%)	30,32,32	1.33	3 (10%)
6	ATP	M	1001	3,2	26,33,33	1.01	2 (7%)	31,52,52	1.32	4 (12%)
4	OXL	F	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	C	700	-	19,20,20	0.91	0	30,32,32	1.51	5 (16%)
4	OXL	D	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	E	1001	3,2	26,33,33	1.03	3 (11%)	31,52,52	1.34	4 (12%)
6	ATP	D	1001	3,2	26,33,33	1.02	2 (7%)	31,52,52	1.47	6 (19%)
5	FDP	D	700	-	19,20,20	1.13	1 (5%)	30,32,32	1.36	3 (10%)
4	OXL	P	510	2	0,5,5	0.00	-	0,6,6	0.00	-
7	GOL	I	499	-	5,5,5	0.37	0	5,5,5	0.28	0
4	OXL	H	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	K	700	-	19,20,20	1.13	3 (15%)	30,32,32	1.47	7 (23%)
4	OXL	B	510	2	0,5,5	0.00	-	0,6,6	0.00	-
7	GOL	I	501	-	5,5,5	0.41	0	5,5,5	0.35	0
6	ATP	N	1001	3,2	26,33,33	1.02	2 (7%)	31,52,52	1.50	5 (16%)
6	ATP	A	1001	3,2	26,33,33	1.01	2 (7%)	31,52,52	1.34	5 (16%)
4	OXL	K	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	G	1001	2	26,33,33	0.99	2 (7%)	31,52,52	1.39	4 (12%)
5	FDP	J	700	-	19,20,20	1.08	2 (10%)	30,32,32	1.36	4 (13%)
5	FDP	F	700	-	19,20,20	1.17	2 (10%)	30,32,32	1.38	4 (13%)
5	FDP	B	700	-	19,20,20	1.50	3 (15%)	30,32,32	1.54	6 (20%)
4	OXL	G	510	2	0,5,5	0.00	-	0,6,6	0.00	-
6	ATP	C	1001	3,2	26,33,33	1.03	3 (11%)	31,52,52	1.34	4 (12%)
5	FDP	I	700	-	19,20,20	1.58	3 (15%)	30,32,32	1.44	3 (10%)
5	FDP	P	700	-	19,20,20	1.17	1 (5%)	30,32,32	0.80	1 (3%)
5	FDP	L	700	-	19,20,20	1.04	1 (5%)	30,32,32	1.39	4 (13%)
6	ATP	K	1001	3,2	26,33,33	0.97	1 (3%)	31,52,52	1.19	3 (9%)
4	OXL	M	510	2	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	C	510	2	0,5,5	0.00	-	0,6,6	0.00	-

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

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

*Continued on next page...*

*Continued from previous page...*

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

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	700	FDP	P2-O6	-4.52	1.45	1.60
5	I	700	FDP	P1-O2P	-3.84	1.40	1.54
5	I	700	FDP	O3-C3	-3.16	1.36	1.42
5	E	700	FDP	P2-O6	-2.98	1.50	1.60
5	D	700	FDP	O5-C5	2.90	1.50	1.43
5	G	700	FDP	O5-C2	2.82	1.48	1.42
5	I	700	FDP	P2-O6	-2.80	1.51	1.60
6	L	1001	ATP	C5-C4	2.79	1.48	1.40
6	C	1001	ATP	C5-C4	2.77	1.48	1.40
6	M	1001	ATP	C5-C4	2.76	1.48	1.40
6	A	1001	ATP	C5-C4	2.75	1.48	1.40
5	E	700	FDP	O5-C2	2.74	1.48	1.42
6	N	1001	ATP	C5-C4	2.73	1.48	1.40
6	D	1001	ATP	C5-C4	2.70	1.48	1.40
6	G	1001	ATP	C5-C4	2.67	1.48	1.40
6	F	1001	ATP	C5-C4	2.64	1.47	1.40
6	H	1001	ATP	C5-C4	2.64	1.47	1.40
6	E	1001	ATP	C5-C4	2.64	1.47	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1001	ATP	C5-C4	2.62	1.47	1.40
6	I	1001	ATP	C5-C4	2.59	1.47	1.40
5	F	700	FDP	P1-O2	2.52	1.64	1.59
6	B	1001	ATP	C5-C4	2.52	1.47	1.40
6	J	1001	ATP	C5-C4	2.52	1.47	1.40
5	J	700	FDP	O4-C4	-2.44	1.37	1.43
6	K	1001	ATP	C5-C4	2.42	1.47	1.40
6	I	1001	ATP	O4'-C1'	2.37	1.44	1.41
6	L	1001	ATP	O4'-C1'	2.33	1.44	1.41
5	L	700	FDP	P2-O6	-2.33	1.52	1.60
6	F	1001	ATP	O4'-C1'	2.31	1.44	1.41
5	P	700	FDP	P1-O3P	2.30	1.63	1.54
5	J	700	FDP	P2-O5P	-2.22	1.46	1.54
5	B	700	FDP	P1-O2	2.22	1.63	1.59
5	K	700	FDP	O5-C2	2.20	1.47	1.42
5	H	700	FDP	P1-O2	2.17	1.63	1.59
6	F	1001	ATP	C2-N3	2.15	1.35	1.32
5	K	700	FDP	P1-O2P	-2.14	1.46	1.54
6	C	1001	ATP	O4'-C1'	2.14	1.44	1.41
6	J	1001	ATP	O4'-C1'	2.13	1.44	1.41
5	F	700	FDP	O5-C2	-2.12	1.37	1.42
5	N	700	FDP	P2-O5P	2.11	1.63	1.54
6	E	1001	ATP	O4'-C1'	2.10	1.44	1.41
6	A	1001	ATP	C2-N3	2.10	1.35	1.32
5	G	700	FDP	P2-O6P	2.09	1.62	1.54
6	C	1001	ATP	C2-N3	2.07	1.35	1.32
5	B	700	FDP	P1-O3P	-2.07	1.46	1.54
6	E	1001	ATP	C2-N3	2.06	1.35	1.32
6	I	1001	ATP	C2-N3	2.06	1.35	1.32
6	L	1001	ATP	C2-N3	2.05	1.35	1.32
6	D	1001	ATP	C2-N3	2.05	1.35	1.32
6	M	1001	ATP	O4'-C1'	2.04	1.43	1.41
6	N	1001	ATP	C2-N3	2.04	1.35	1.32
5	K	700	FDP	P1-O2	2.04	1.63	1.59
5	N	700	FDP	P1-O2	2.03	1.63	1.59
6	G	1001	ATP	C2-N3	2.02	1.35	1.32

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	FDP	O2-C2-C3	3.96	120.92	108.18
5	I	700	FDP	O2-C2-C3	3.91	120.74	108.18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1001	ATP	N3-C2-N1	-3.91	122.57	128.68
5	B	700	FDP	O2-C2-C3	3.89	120.67	108.18
5	L	700	FDP	O2-C2-C3	3.81	120.44	108.18
5	C	700	FDP	O6-P2-O4P	3.76	117.01	106.47
5	I	700	FDP	O5-C2-C3	-3.71	97.83	105.49
6	E	1001	ATP	N3-C2-N1	-3.66	122.95	128.68
5	G	700	FDP	C6-C5-C4	-3.65	101.50	115.18
5	L	700	FDP	O2-P1-O1P	3.59	123.24	109.39
6	J	1001	ATP	N3-C2-N1	-3.58	123.09	128.68
5	H	700	FDP	C6-C5-C4	-3.55	101.88	115.18
6	G	1001	ATP	N3-C2-N1	-3.50	123.20	128.68
6	L	1001	ATP	N3-C2-N1	-3.48	123.23	128.68
6	P	1001	ATP	N3-C2-N1	-3.47	123.25	128.68
5	F	700	FDP	O2-C2-C3	3.46	119.30	108.18
6	K	1001	ATP	N3-C2-N1	-3.45	123.29	128.68
6	P	1001	ATP	C3'-C2'-C1'	3.42	106.13	100.98
5	B	700	FDP	C6-C5-C4	-3.41	102.39	115.18
6	N	1001	ATP	N3-C2-N1	-3.41	123.35	128.68
6	D	1001	ATP	PA-O3A-PB	-3.40	121.17	132.83
6	M	1001	ATP	N3-C2-N1	-3.37	123.41	128.68
6	I	1001	ATP	N3-C2-N1	-3.37	123.41	128.68
6	F	1001	ATP	N3-C2-N1	-3.36	123.42	128.68
6	H	1001	ATP	N3-C2-N1	-3.28	123.55	128.68
6	N	1001	ATP	PB-O3B-PG	-3.27	121.60	132.83
5	B	700	FDP	O5-C2-C3	-3.26	98.77	105.49
6	N	1001	ATP	C3'-C2'-C1'	3.24	105.86	100.98
6	A	1001	ATP	N3-C2-N1	-3.23	123.62	128.68
5	F	700	FDP	O6P-P2-O6	-3.23	98.14	106.73
5	J	700	FDP	O2-C2-C3	3.21	118.48	108.18
5	F	700	FDP	O5-C2-C3	-3.18	98.93	105.49
6	F	1001	ATP	PB-O3B-PG	-3.17	121.95	132.83
6	D	1001	ATP	N3-C2-N1	-3.17	123.73	128.68
6	C	1001	ATP	N3-C2-N1	-3.16	123.74	128.68
6	G	1001	ATP	PA-O3A-PB	-3.12	122.11	132.83
5	J	700	FDP	O6-P2-O4P	3.06	115.06	106.47
5	H	700	FDP	O3P-P1-O1P	3.02	122.49	110.68
5	K	700	FDP	C6-C5-C4	-2.99	103.96	115.18
6	P	1001	ATP	PB-O3B-PG	-2.97	122.63	132.83
5	K	700	FDP	O2-C2-C3	2.94	117.63	108.18
6	G	1001	ATP	PB-O3B-PG	-2.94	122.75	132.83
6	M	1001	ATP	PB-O3B-PG	-2.86	123.00	132.83
5	D	700	FDP	O2-P1-O1P	2.83	120.30	109.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	700	FDP	C6-C5-C4	-2.82	104.61	115.18
6	C	1001	ATP	PB-O3B-PG	-2.78	123.30	132.83
6	L	1001	ATP	PB-O3B-PG	-2.77	123.31	132.83
6	A	1001	ATP	PA-O3A-PB	-2.77	123.33	132.83
5	C	700	FDP	O5P-P2-O6	-2.75	99.42	106.73
6	H	1001	ATP	PA-O3A-PB	-2.74	123.42	132.83
6	C	1001	ATP	C4-C5-N7	-2.74	106.55	109.40
6	L	1001	ATP	PA-O3A-PB	-2.70	123.57	132.83
6	N	1001	ATP	C4-C5-N7	-2.69	106.59	109.40
6	J	1001	ATP	C4-C5-N7	-2.69	106.60	109.40
5	L	700	FDP	O5-C2-C3	-2.66	100.00	105.49
6	I	1001	ATP	C4-C5-N7	-2.65	106.64	109.40
5	M	700	FDP	O6-P2-O4P	2.65	113.90	106.47
5	J	700	FDP	C6-C5-C4	-2.63	105.34	115.18
5	D	700	FDP	O3P-P1-O2	-2.60	94.36	105.99
5	A	700	FDP	C6-C5-C4	-2.59	105.48	115.18
6	D	1001	ATP	C4-C5-N7	-2.58	106.71	109.40
5	N	700	FDP	O6-P2-O4P	2.58	113.70	106.47
6	F	1001	ATP	C4-C5-N7	-2.56	106.73	109.40
6	E	1001	ATP	PB-O3B-PG	-2.54	124.10	132.83
5	C	700	FDP	O6P-P2-O4P	2.54	120.61	110.68
6	A	1001	ATP	PB-O3B-PG	-2.53	124.16	132.83
6	M	1001	ATP	C4-C5-N7	-2.53	106.77	109.40
6	B	1001	ATP	C3'-C2'-C1'	2.52	104.77	100.98
6	E	1001	ATP	PA-O3A-PB	-2.51	124.23	132.83
6	P	1001	ATP	C4-C5-N7	-2.49	106.81	109.40
6	N	1001	ATP	PA-O3A-PB	-2.49	124.29	132.83
6	I	1001	ATP	PB-O3B-PG	-2.48	124.33	132.83
6	A	1001	ATP	C3'-C2'-C1'	2.47	104.69	100.98
6	E	1001	ATP	C4-C5-N7	-2.46	106.83	109.40
5	E	700	FDP	O5-C2-C3	-2.46	100.42	105.49
6	H	1001	ATP	C4-C5-N7	-2.44	106.86	109.40
6	M	1001	ATP	PA-O3A-PB	-2.43	124.50	132.83
6	A	1001	ATP	C4-C5-N7	-2.39	106.91	109.40
5	B	700	FDP	O6-P2-O4P	2.38	113.16	106.47
5	K	700	FDP	C2-C3-C4	-2.38	96.65	102.10
5	A	700	FDP	O6-P2-O4P	2.38	113.15	106.47
5	D	700	FDP	C6-C5-C4	-2.36	106.33	115.18
6	D	1001	ATP	PB-O3B-PG	-2.36	124.74	132.83
5	B	700	FDP	O3P-P1-O2	-2.34	95.49	105.99
6	K	1001	ATP	C4-C5-N7	-2.34	106.96	109.40
6	G	1001	ATP	C4-C5-N7	-2.32	106.98	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	700	FDP	C5-C4-C3	-2.32	94.46	101.91
5	K	700	FDP	O4-C4-C5	-2.29	104.42	111.05
6	H	1001	ATP	PB-O3B-PG	-2.28	125.01	132.83
5	K	700	FDP	O6P-P2-O4P	2.26	119.53	110.68
5	G	700	FDP	O6-P2-O4P	2.25	112.80	106.47
6	B	1001	ATP	C2-N1-C6	2.24	122.59	118.75
5	H	700	FDP	O2-C2-C3	2.24	115.37	108.18
6	I	1001	ATP	O3G-PG-O2G	2.23	116.17	107.64
6	L	1001	ATP	C4-C5-N7	-2.22	107.08	109.40
5	B	700	FDP	O2-P1-O1P	2.21	117.92	109.39
5	J	700	FDP	O5-C2-C3	-2.21	100.94	105.49
5	K	700	FDP	O5-C5-C6	2.20	114.29	109.45
5	F	700	FDP	O6-P2-O4P	2.19	112.62	106.47
5	E	700	FDP	O6-P2-O4P	2.19	112.60	106.47
6	I	1001	ATP	PA-O3A-PB	-2.18	125.34	132.83
5	G	700	FDP	O5-C5-C6	2.18	114.25	109.45
5	M	700	FDP	C6-C5-C4	-2.16	107.07	115.18
6	P	1001	ATP	PA-O3A-PB	-2.16	125.43	132.83
6	C	1001	ATP	O3G-PG-O2G	2.14	115.83	107.64
5	C	700	FDP	C6-C5-C4	-2.07	107.41	115.18
5	M	700	FDP	O2-C2-C1	2.05	115.72	109.57
6	I	1001	ATP	C3'-C2'-C1'	2.05	104.06	100.98
6	D	1001	ATP	O3G-PG-O2G	2.04	115.42	107.64
6	D	1001	ATP	C3'-C2'-C1'	2.03	104.04	100.98
5	C	700	FDP	O6P-P2-O6	-2.03	101.33	106.73
6	L	1001	ATP	C2-N1-C6	2.02	122.21	118.75
5	H	700	FDP	O6-P2-O4P	2.02	112.14	106.47
5	I	700	FDP	O6P-P2-O6	2.02	112.11	106.73
6	K	1001	ATP	PB-O3B-PG	-2.02	125.90	132.83
5	K	700	FDP	C1-C2-C3	-2.01	108.62	114.56
5	P	700	FDP	O6-P2-O4P	2.01	112.11	106.47

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	O	499	GOL	O1-C1-C2-C3
7	O	499	GOL	C1-C2-C3-O3
6	I	1001	ATP	PB-O3B-PG-O3G
6	E	1001	ATP	PB-O3B-PG-O3G
5	N	700	FDP	O1-C1-C2-C3
5	N	700	FDP	C6-O6-P2-O4P

*Continued on next page...*

*Continued from previous page...*

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
7	J	499	GOL	C1-C2-C3-O3
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
7	I	499	GOL	O1-C1-C2-C3
7	I	501	GOL	C1-C2-C3-O3
6	G	1001	ATP	C5'-O5'-PA-O1A
6	P	1001	ATP	O4'-C4'-C5'-O5'
6	H	1001	ATP	C5'-O5'-PA-O1A
6	H	1001	ATP	C5'-O5'-PA-O2A
6	L	1001	ATP	C5'-O5'-PA-O1A
6	L	1001	ATP	C5'-O5'-PA-O2A
6	M	1001	ATP	PB-O3B-PG-O3G
5	P	700	FDP	O1-C1-C2-C3
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	A	1001	ATP	C5'-O5'-PA-O1A
6	A	1001	ATP	C5'-O5'-PA-O2A
5	O	700	FDP	C4-C5-C6-O6
6	P	1001	ATP	C3'-C4'-C5'-O5'
6	L	1001	ATP	O4'-C4'-C5'-O5'
7	J	499	GOL	O2-C2-C3-O3
7	I	501	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
7	J	499	GOL	O1-C1-C2-C3
7	E	499	GOL	O1-C1-C2-C3
7	I	501	GOL	O1-C1-C2-C3
7	O	499	GOL	O1-C1-C2-O2
7	O	499	GOL	O2-C2-C3-O3
7	I	499	GOL	O1-C1-C2-O2
5	O	700	FDP	O5-C5-C6-O6
6	H	1001	ATP	O4'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
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
5	F	700	FDP	C6-O6-P2-O4P
5	F	700	FDP	O1-C1-C2-O2
5	M	700	FDP	O1-C1-C2-O5
6	A	1001	ATP	O4'-C4'-C5'-O5'
7	I	501	GOL	O1-C1-C2-O2
5	P	700	FDP	O5-C5-C6-O6
5	N	700	FDP	C6-O6-P2-O6P
5	E	700	FDP	O1-C1-C2-O5
6	H	1001	ATP	PB-O3B-PG-O1G
6	L	1001	ATP	PB-O3B-PG-O1G
6	J	1001	ATP	PB-O3B-PG-O3G
6	K	1001	ATP	PB-O3B-PG-O3G
6	B	1001	ATP	PB-O3B-PG-O3G
6	G	1001	ATP	C5'-O5'-PA-O3A
6	H	1001	ATP	C5'-O5'-PA-O3A
6	D	1001	ATP	C5'-O5'-PA-O3A
6	A	1001	ATP	C5'-O5'-PA-O3A
6	G	1001	ATP	PA-O3A-PB-O2B
6	C	1001	ATP	PB-O3A-PA-O1A
6	M	1001	ATP	PB-O3A-PA-O1A
6	D	1001	ATP	PA-O3A-PB-O1B
6	A	1001	ATP	PA-O3A-PB-O1B
6	G	1001	ATP	C5'-O5'-PA-O2A
6	N	1001	ATP	O4'-C4'-C5'-O5'
5	P	700	FDP	O1-C1-C2-O5
5	H	700	FDP	C6-O6-P2-O4P
5	F	700	FDP	C4-C5-C6-O6
5	F	700	FDP	O5-C5-C6-O6
6	I	1001	ATP	PB-O3A-PA-O1A
5	M	700	FDP	O1-C1-C2-O2
6	N	1001	ATP	C3'-C4'-C5'-O5'
5	L	700	FDP	C2-O2-P1-O3P
5	P	700	FDP	C2-O2-P1-O2P
6	J	1001	ATP	PB-O3A-PA-O1A
6	B	1001	ATP	PA-O3A-PB-O1B
6	G	1001	ATP	PA-O3A-PB-O1B
5	H	700	FDP	O1-C1-C2-C3
5	M	700	FDP	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

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

There are no ring outliers.

16 monomers are involved in 24 short contacts:

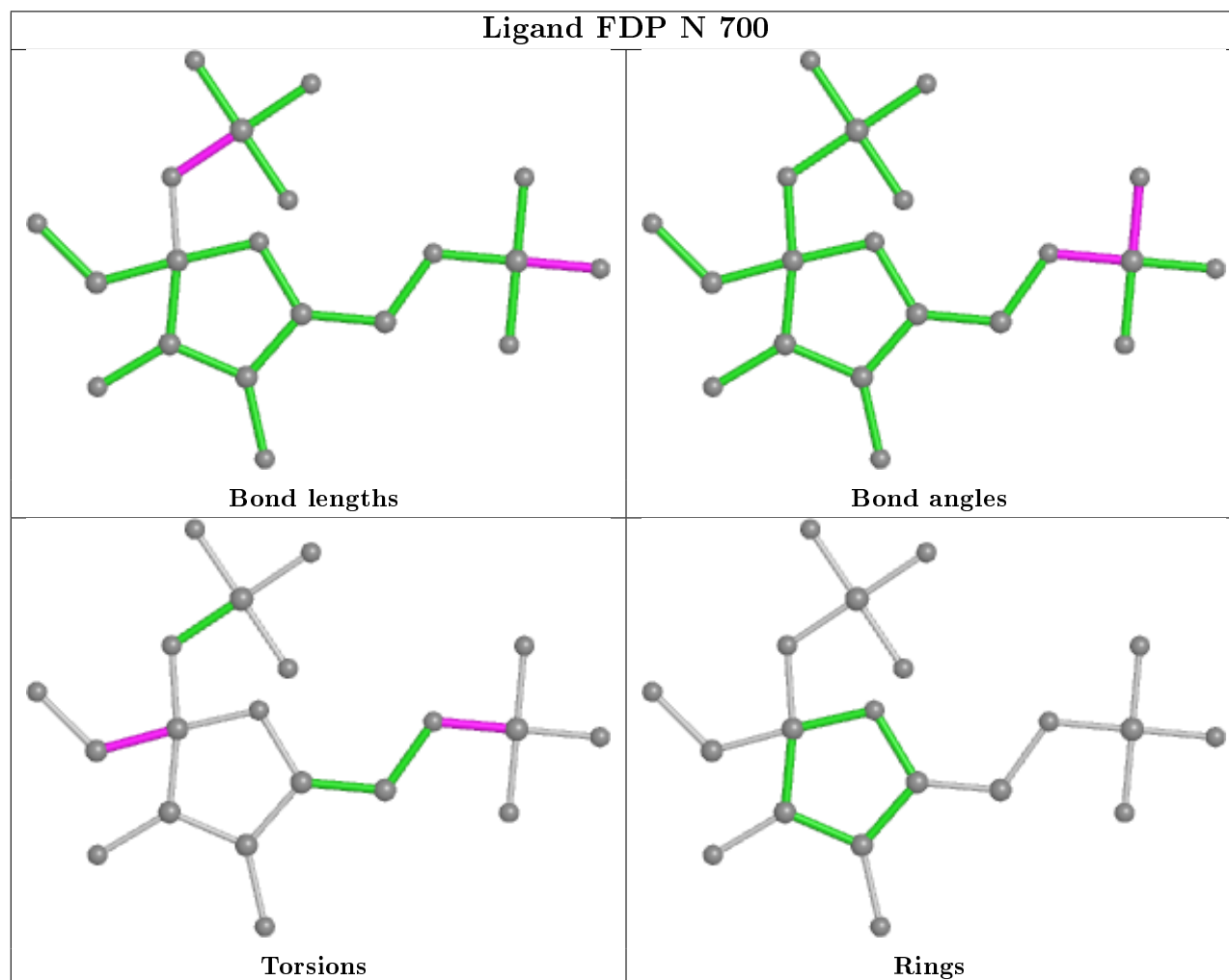
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	700	FDP	2	0
6	H	1001	ATP	1	0
6	F	1001	ATP	1	0
5	O	700	FDP	1	0
7	J	499	GOL	1	0
6	E	1001	ATP	1	0
6	D	1001	ATP	3	0
5	D	700	FDP	2	0
7	I	499	GOL	1	0
6	A	1001	ATP	2	0
6	G	1001	ATP	1	0
6	C	1001	ATP	3	0
5	I	700	FDP	1	0

*Continued on next page...*

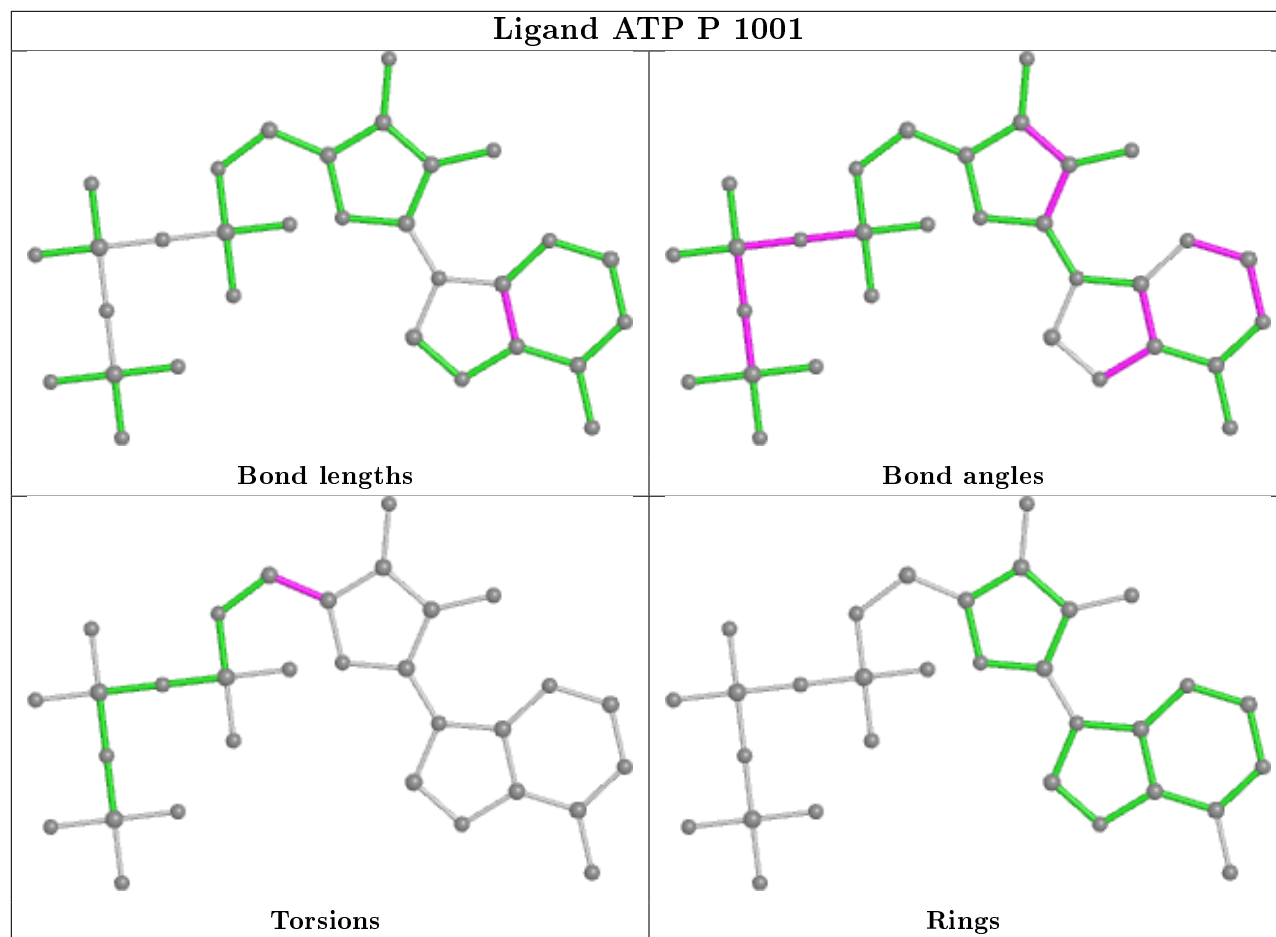
*Continued from previous page...*

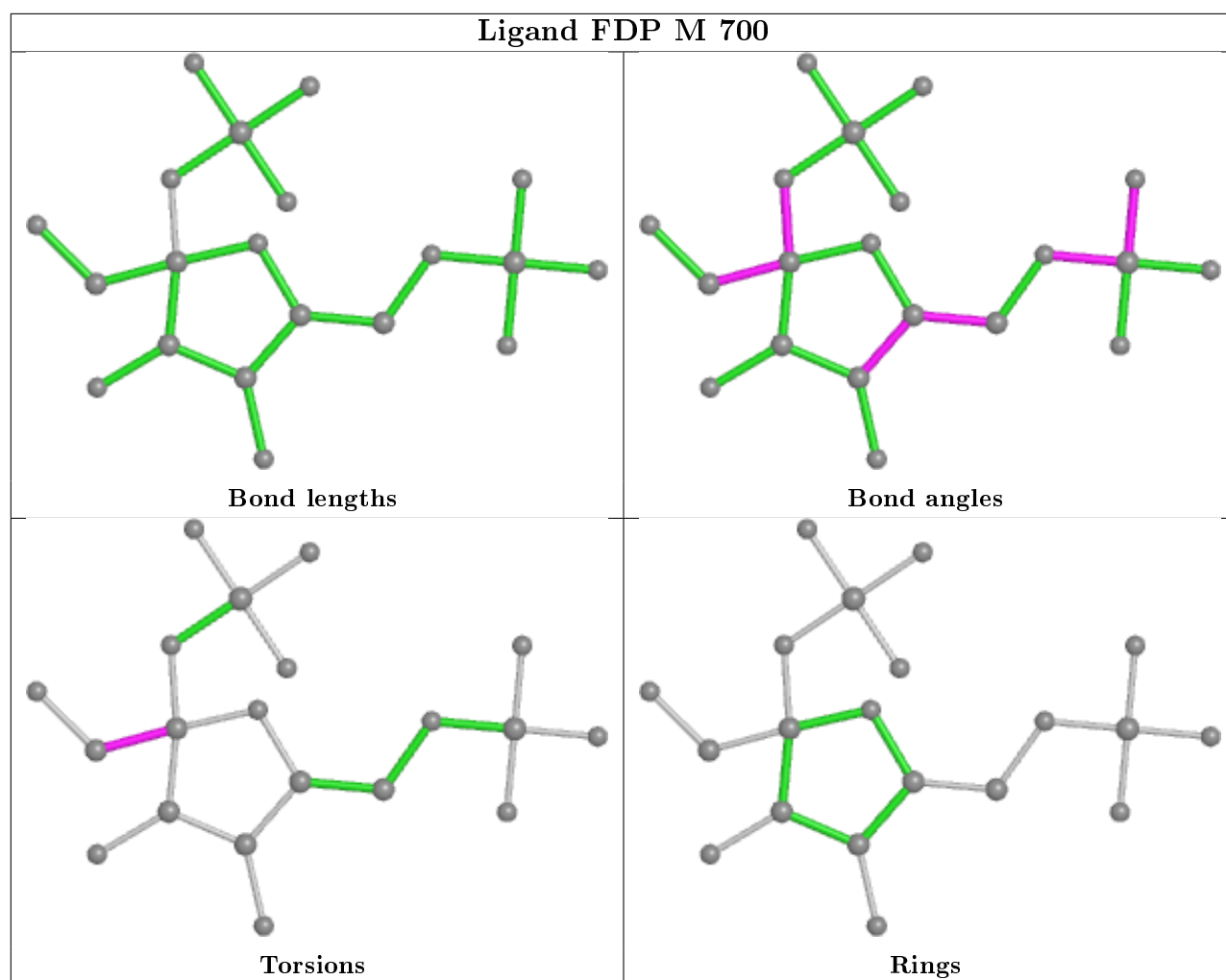
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	700	FDP	1	0
6	K	1001	ATP	2	0
4	M	510	OXL	1	0

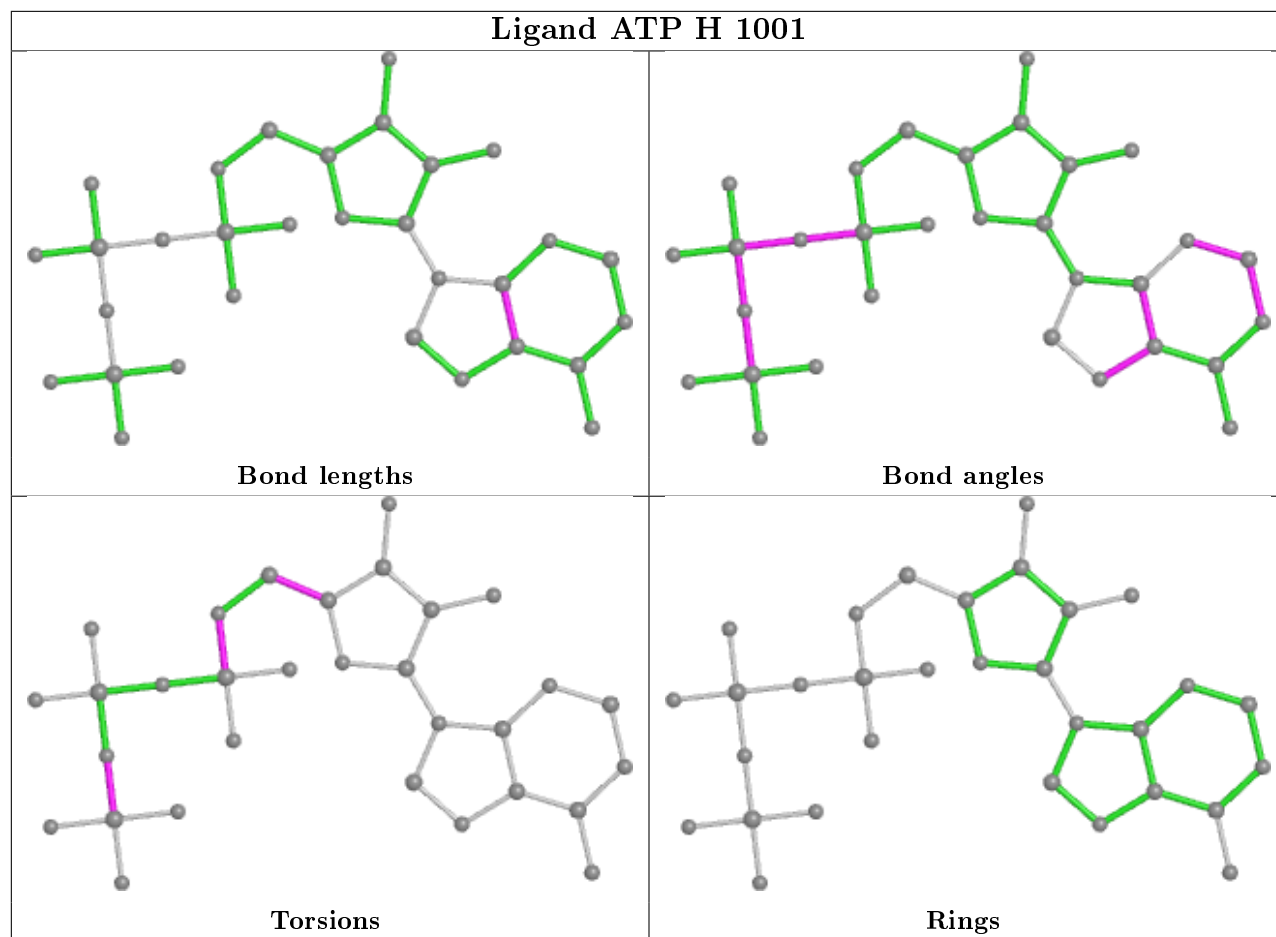
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



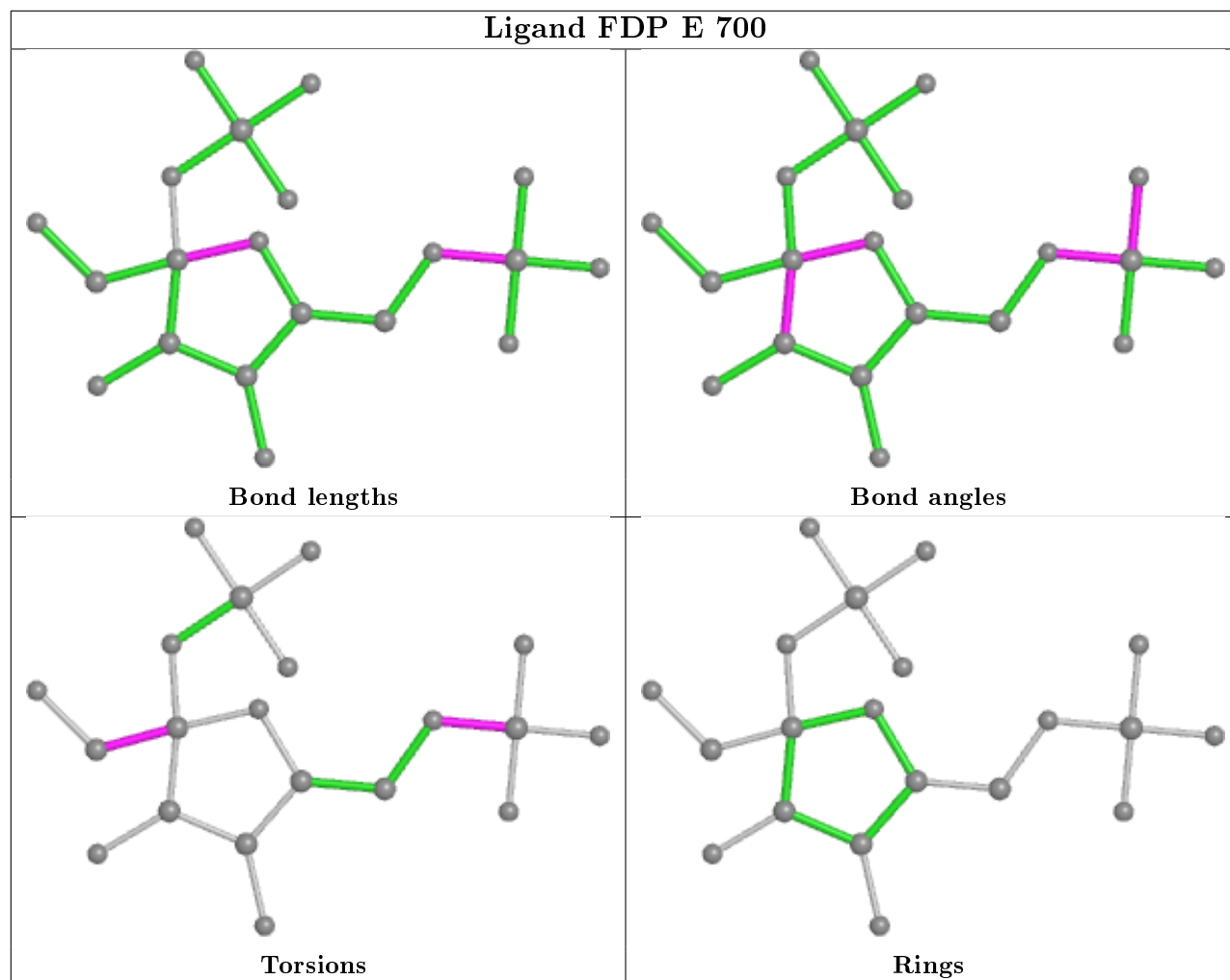


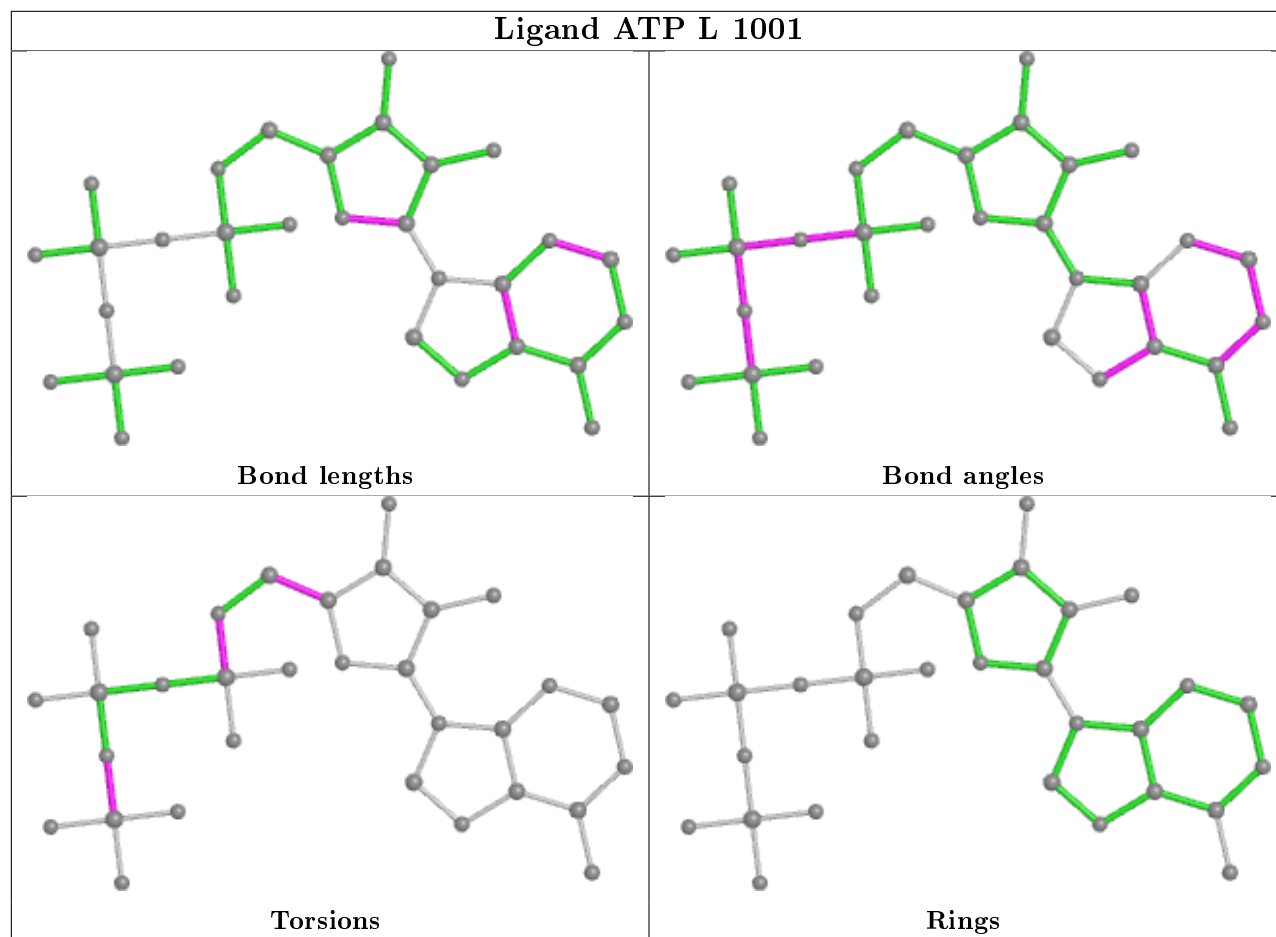


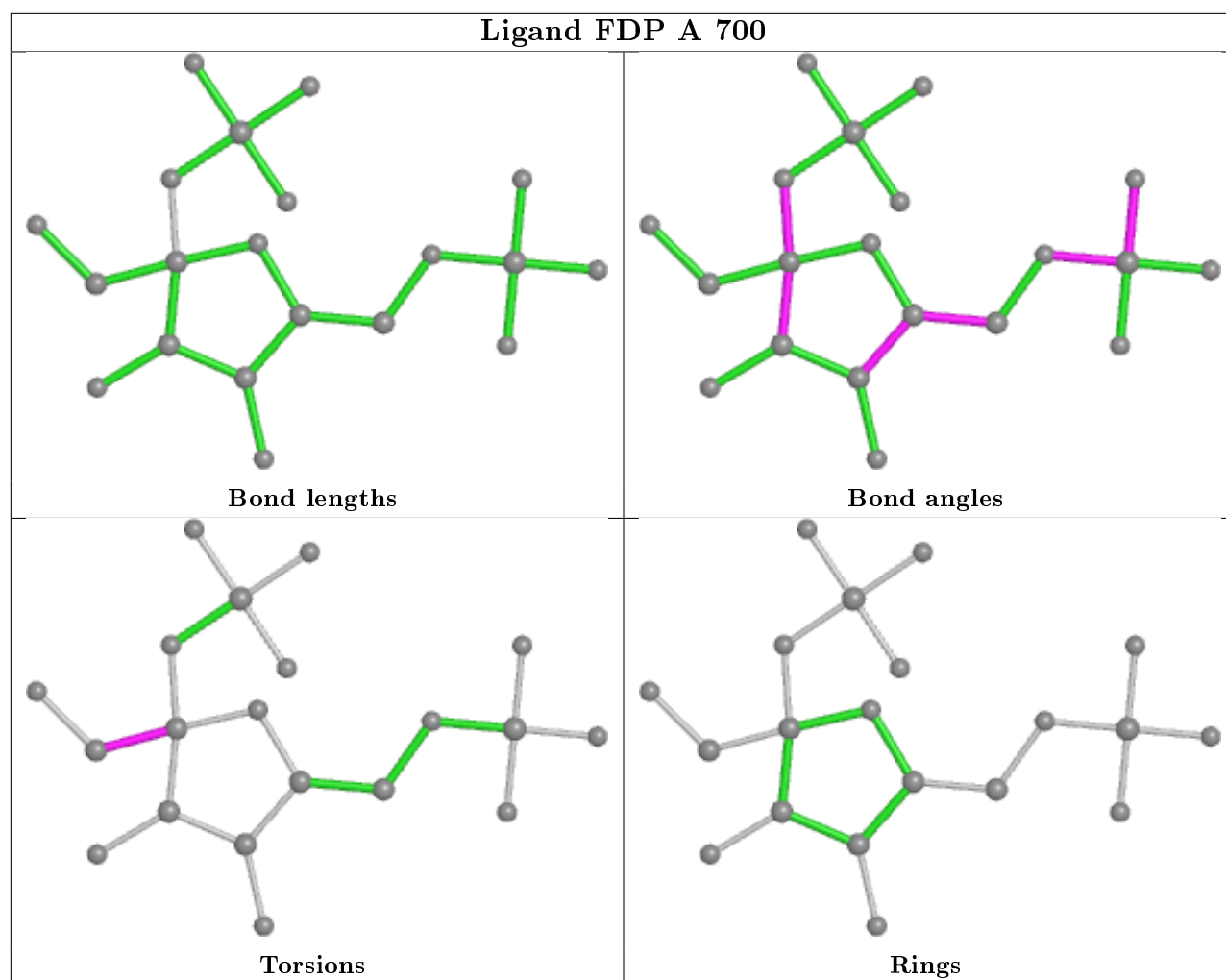


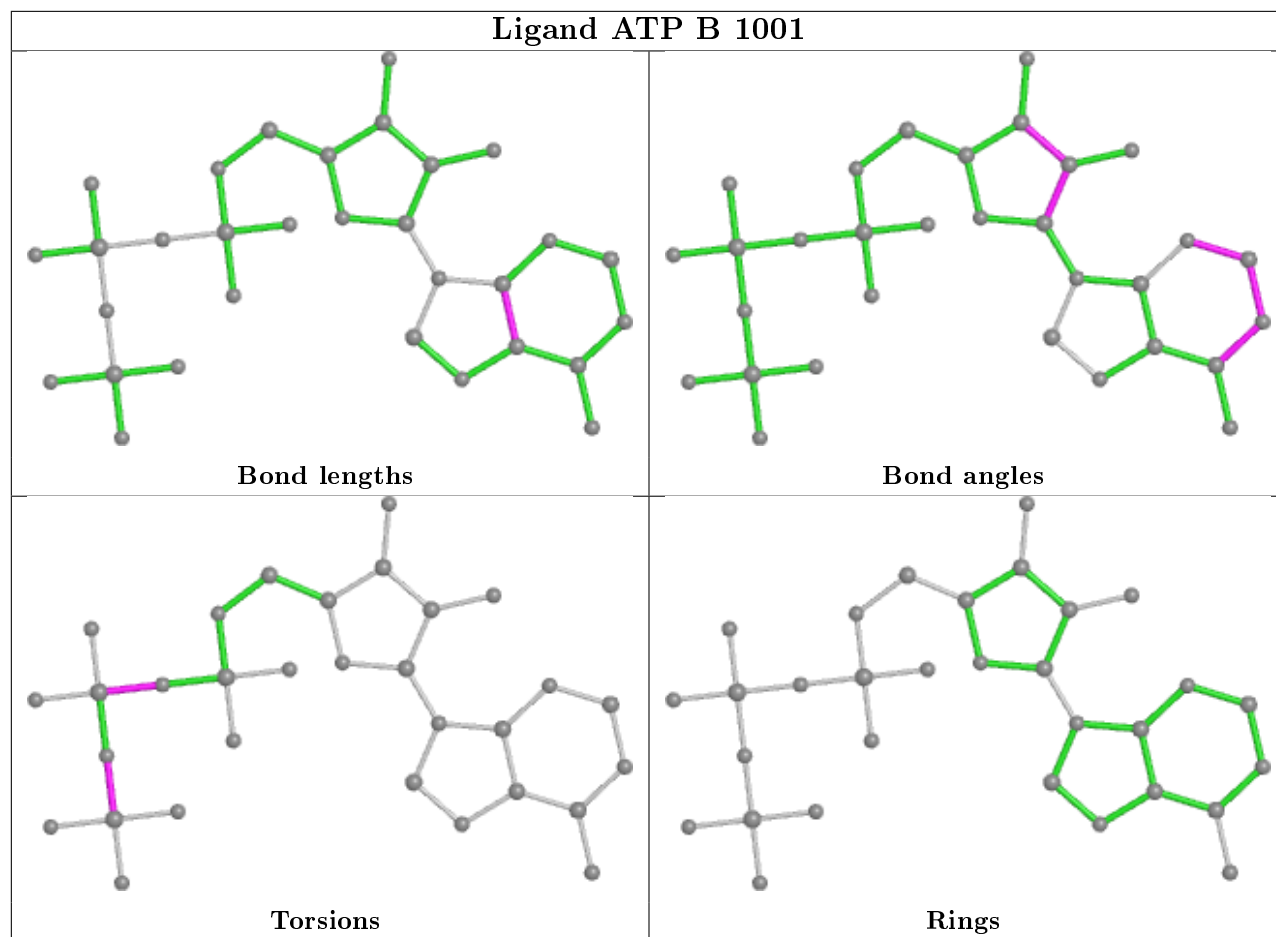


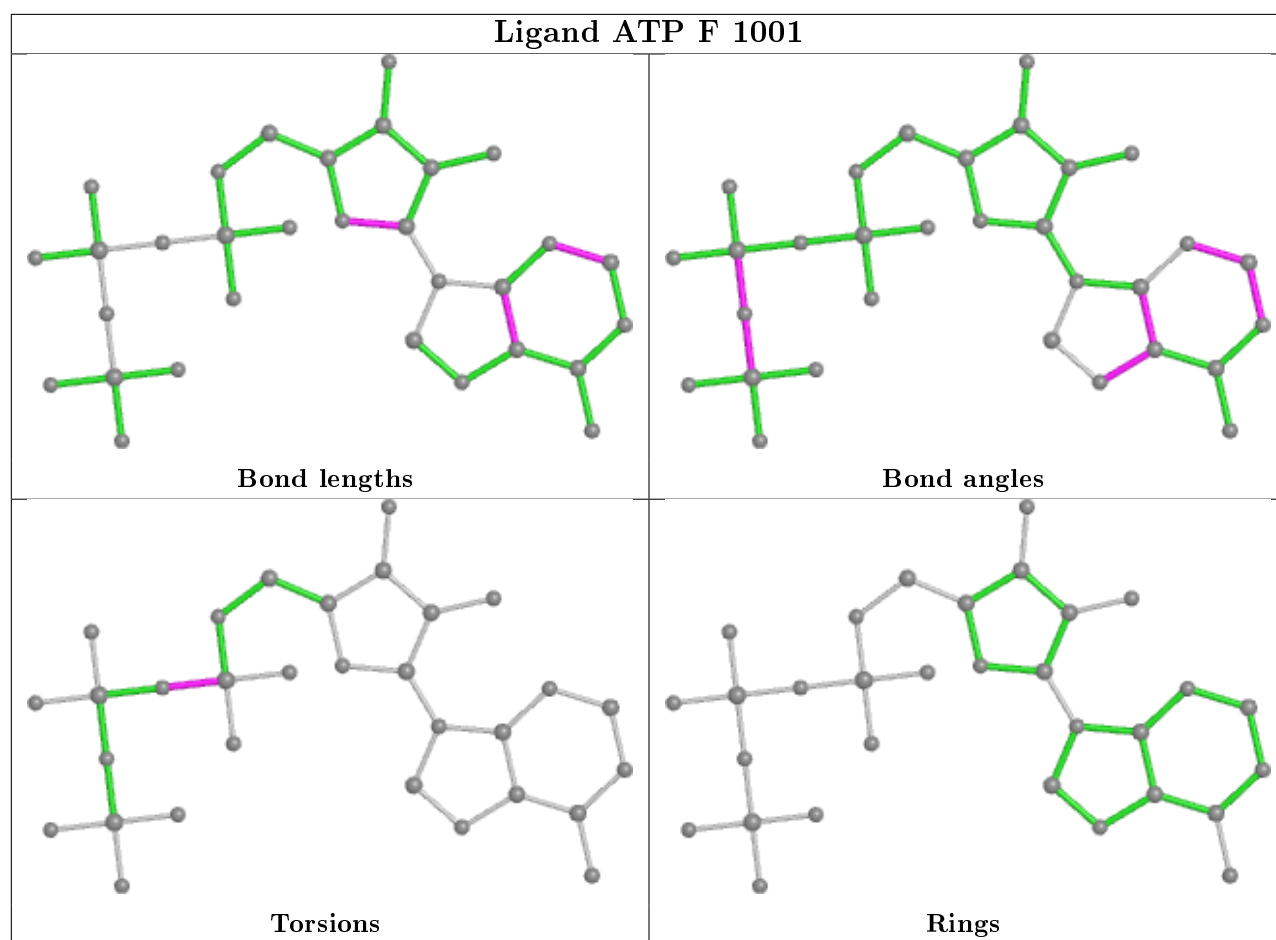
## Ligand FDP E 700



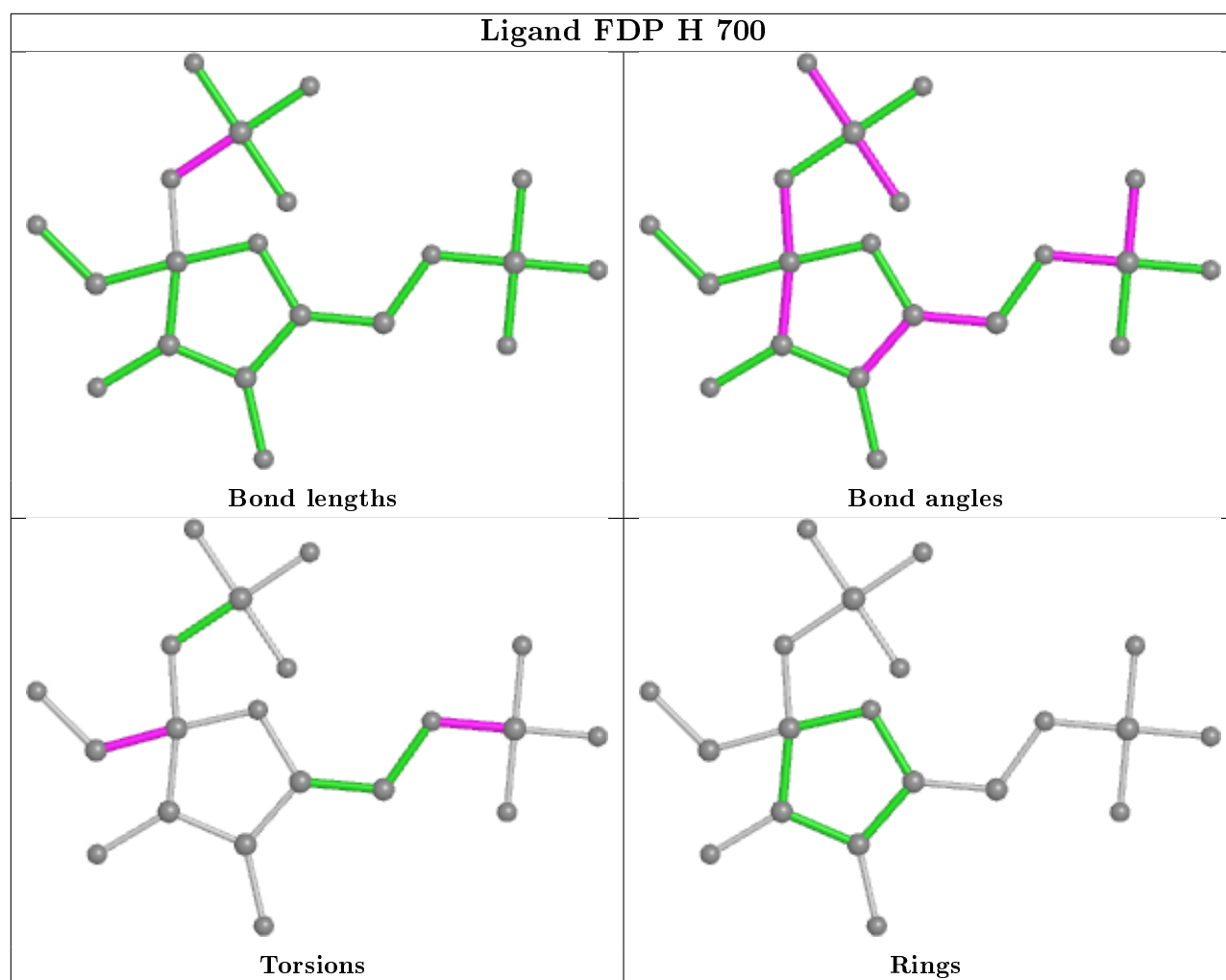


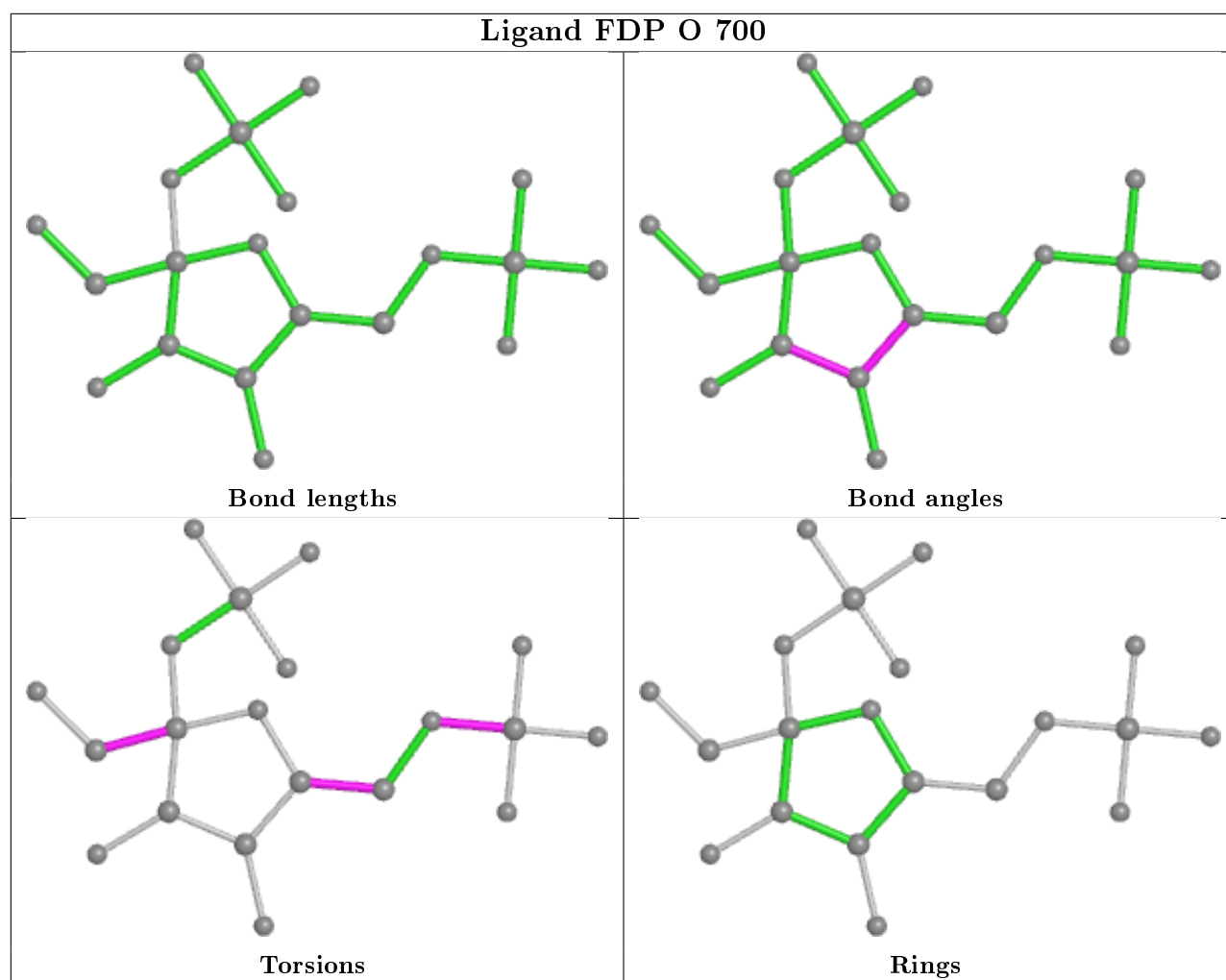


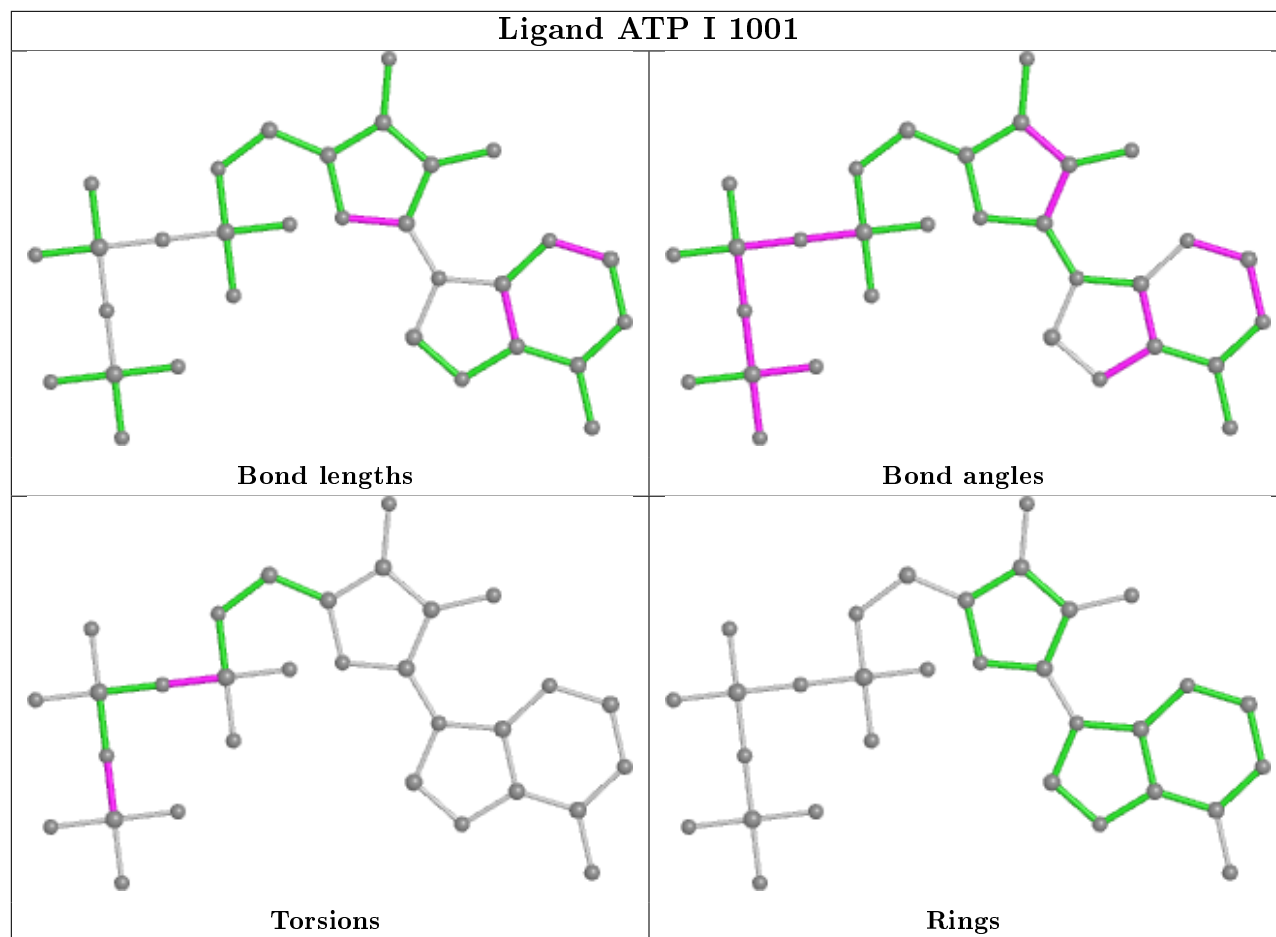


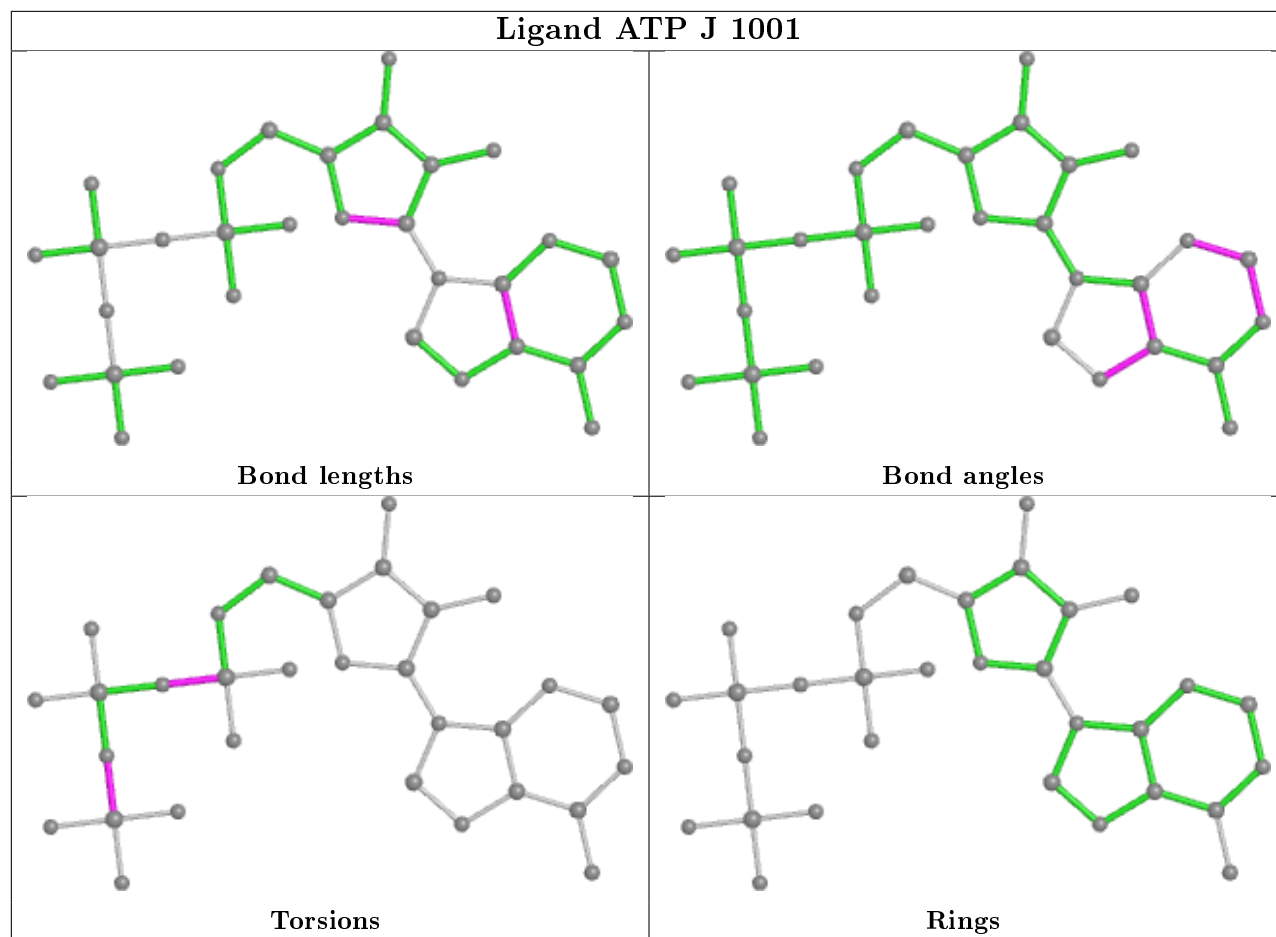


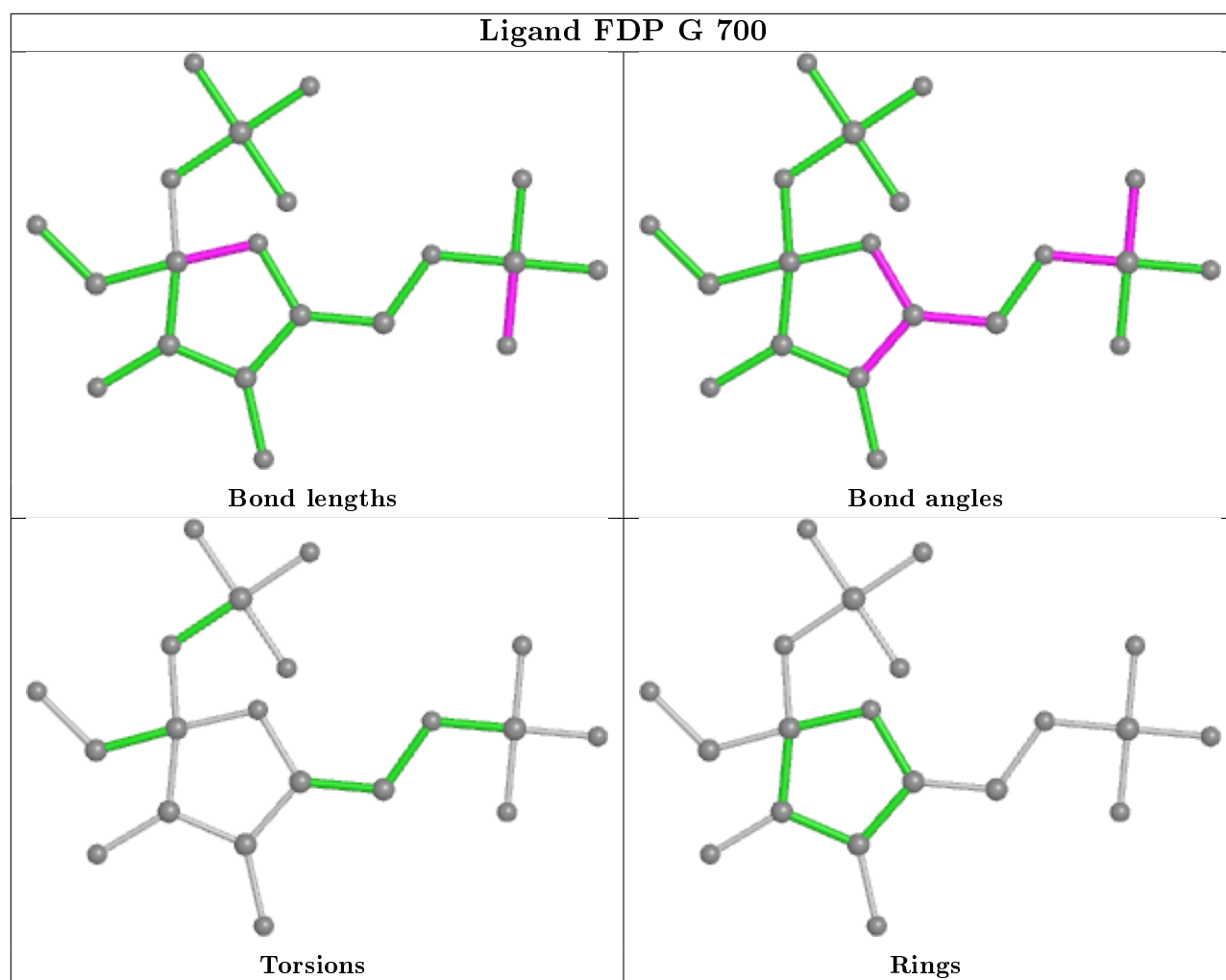


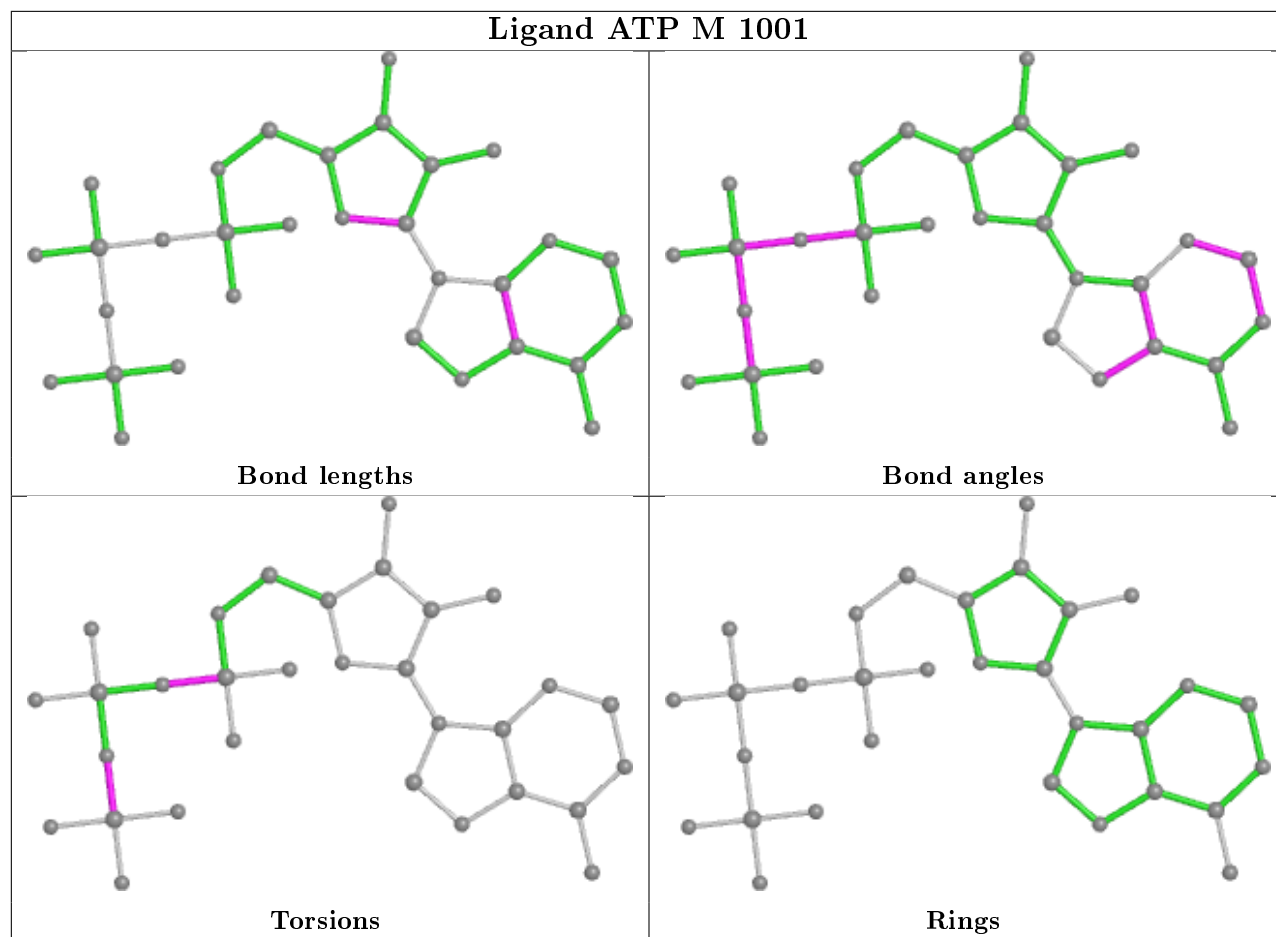


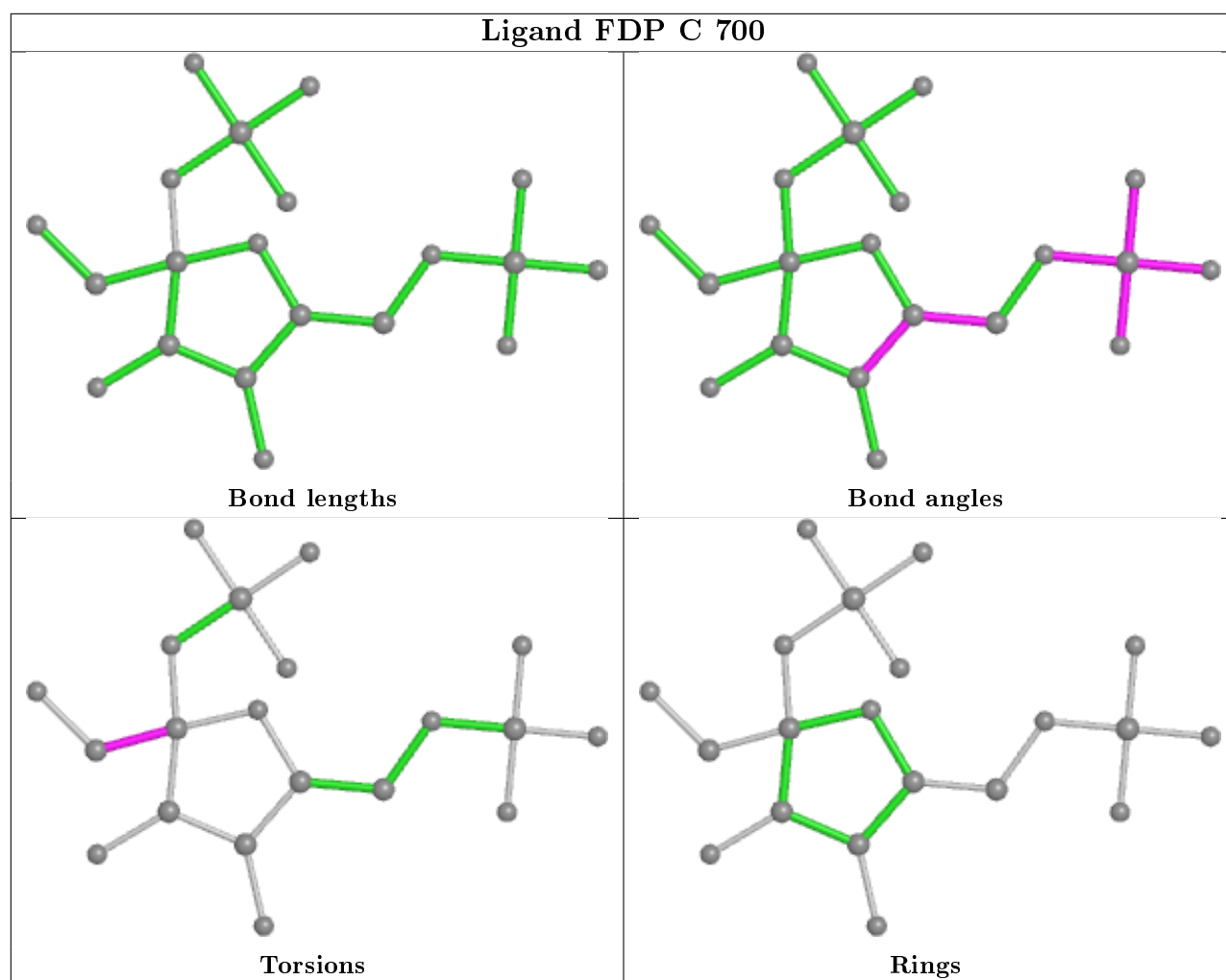


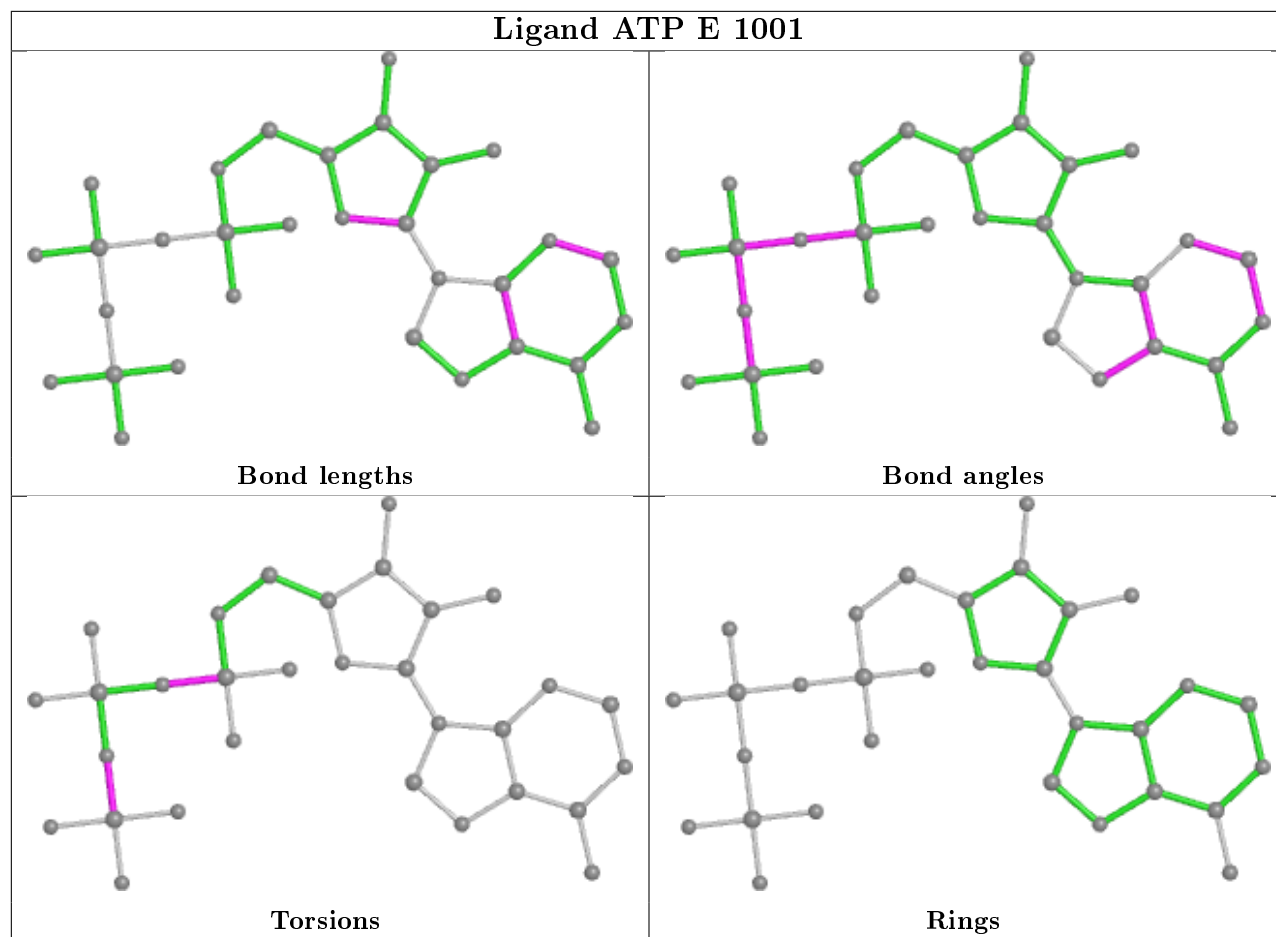




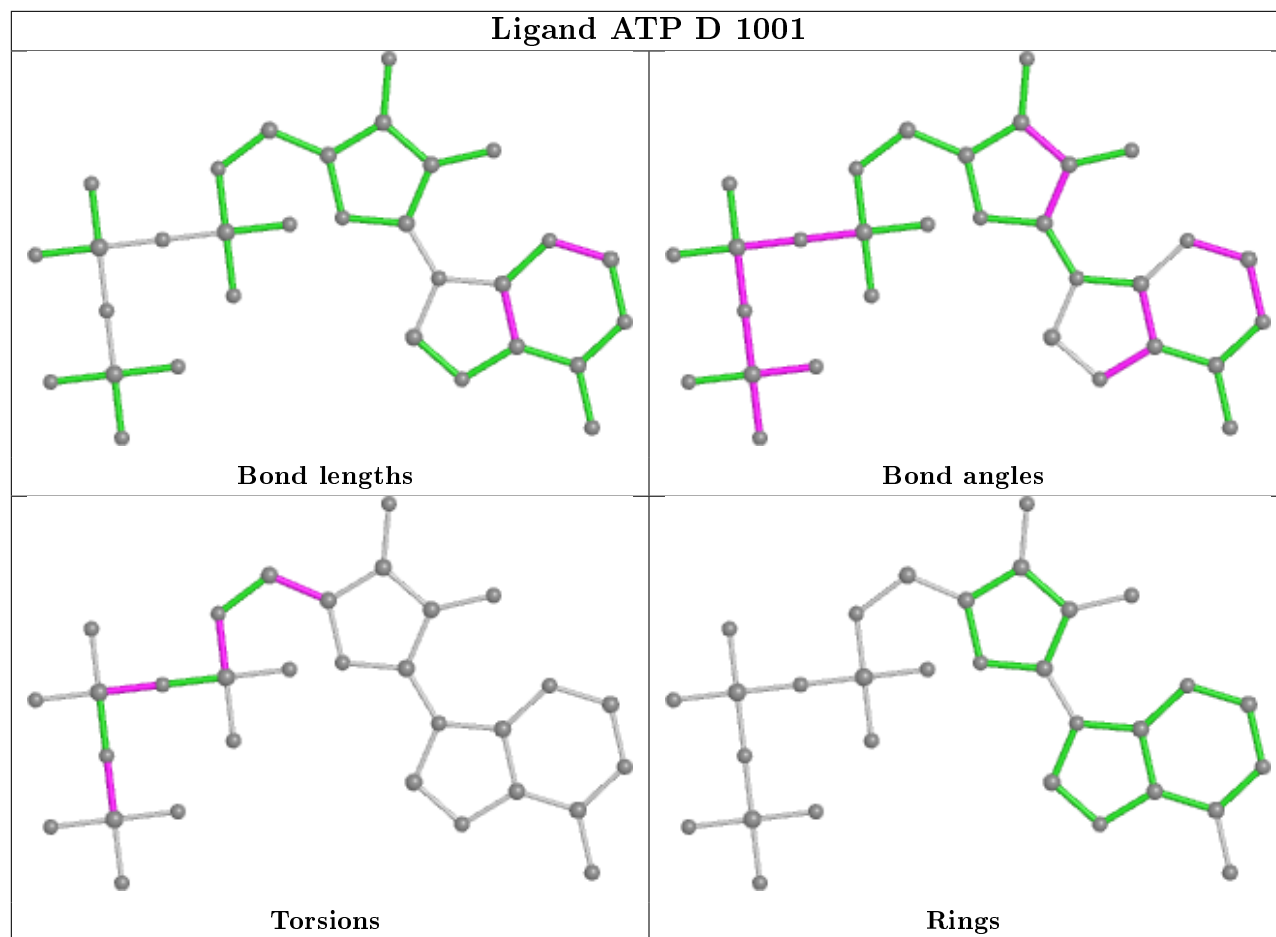


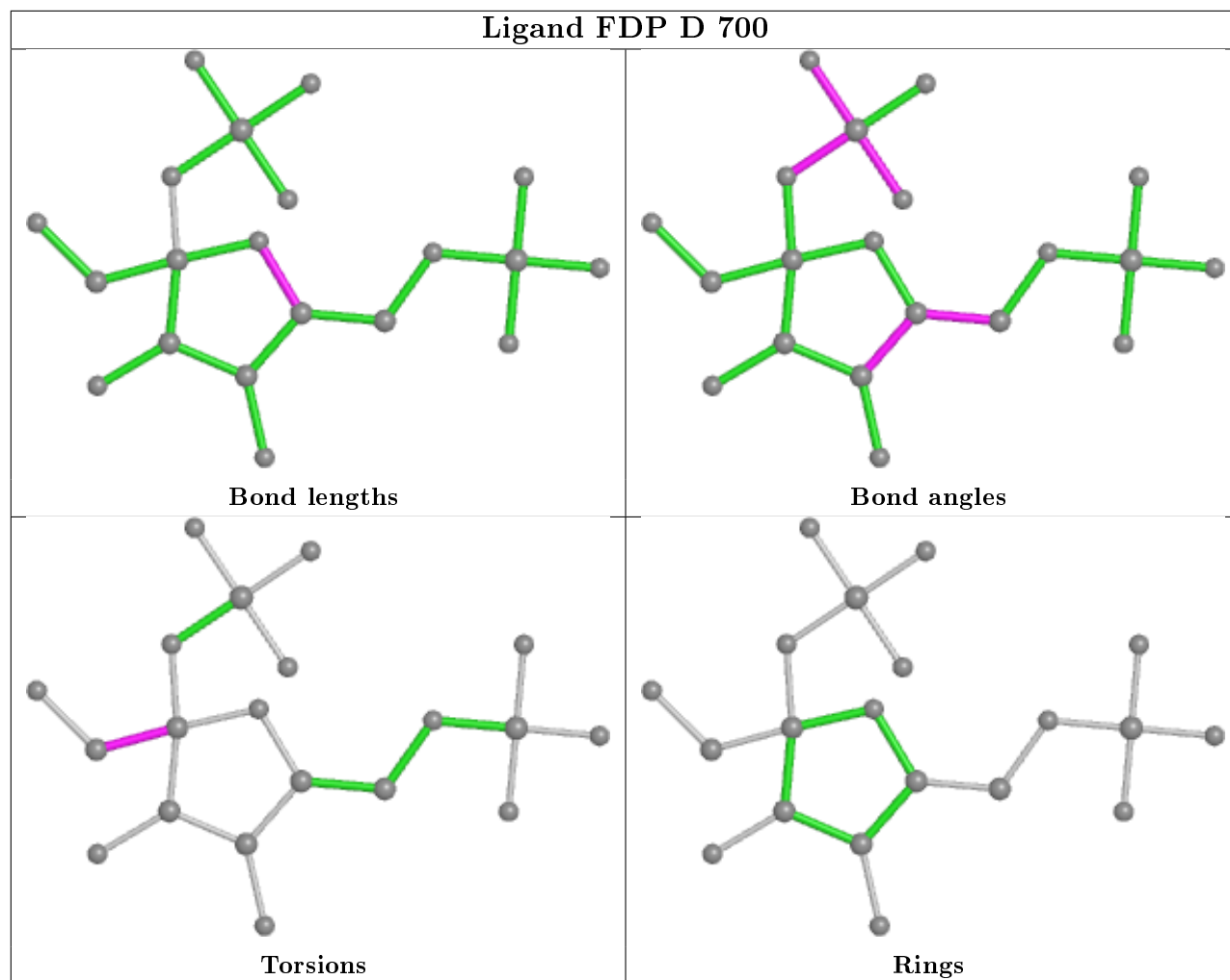


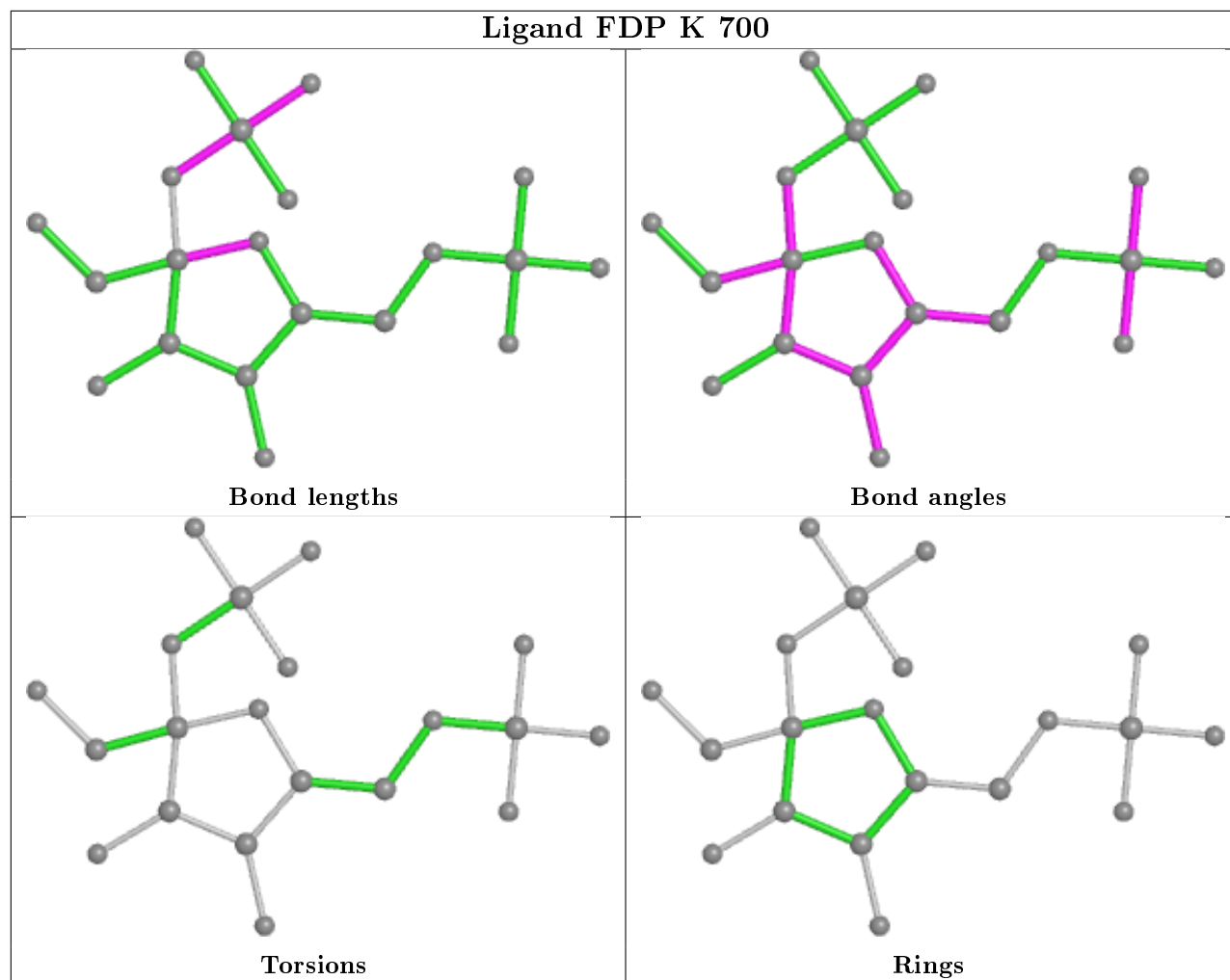


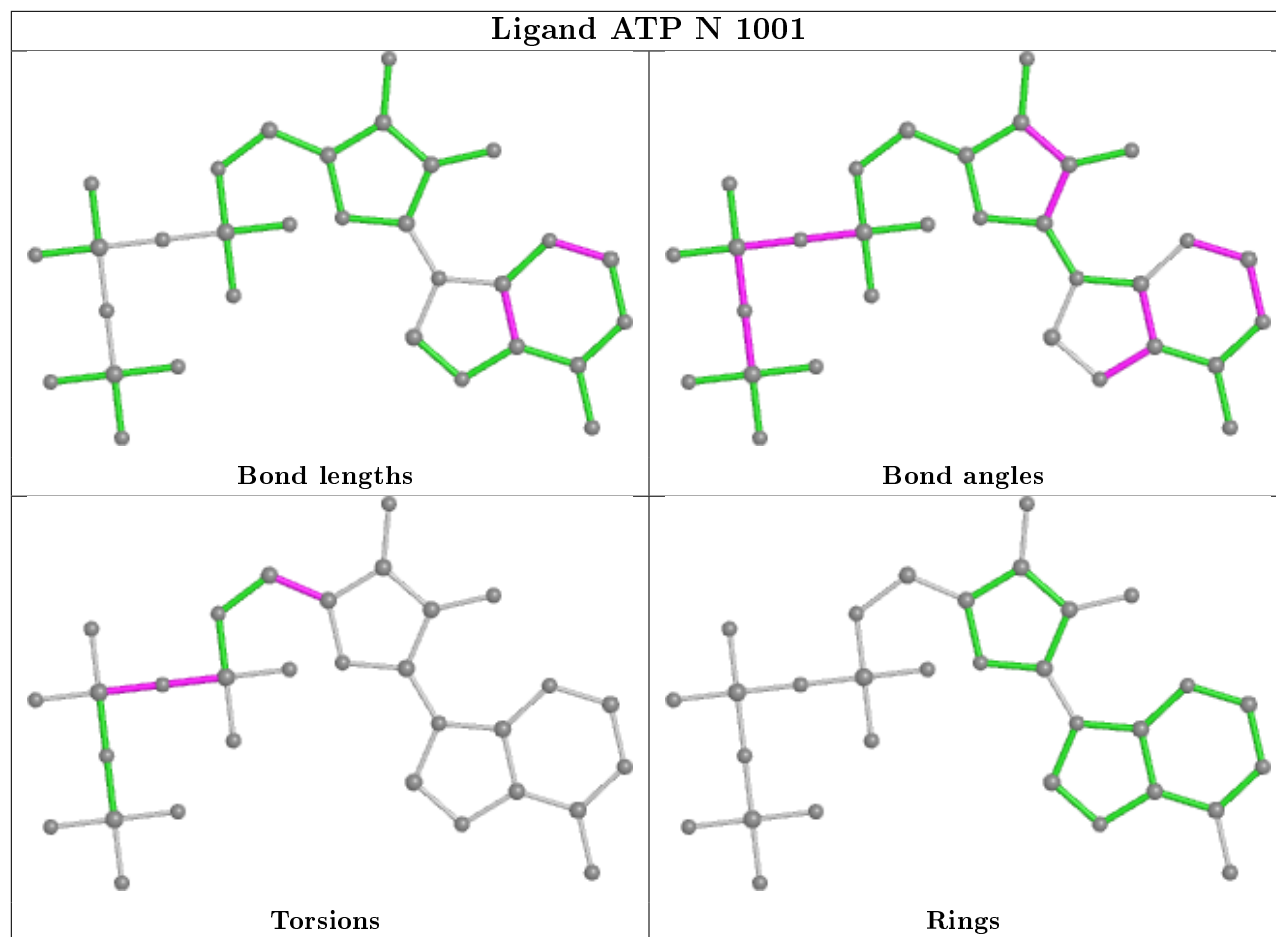


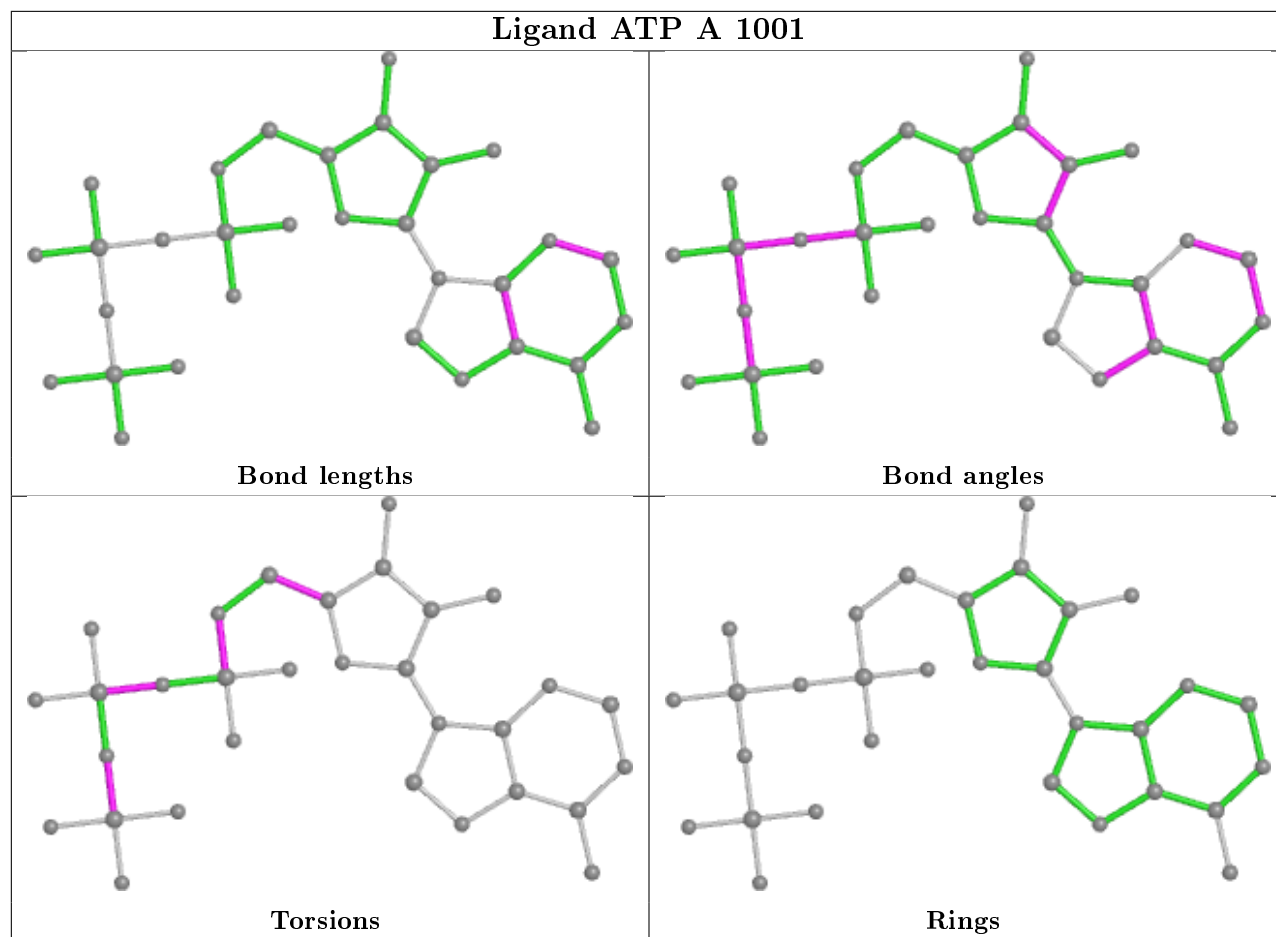


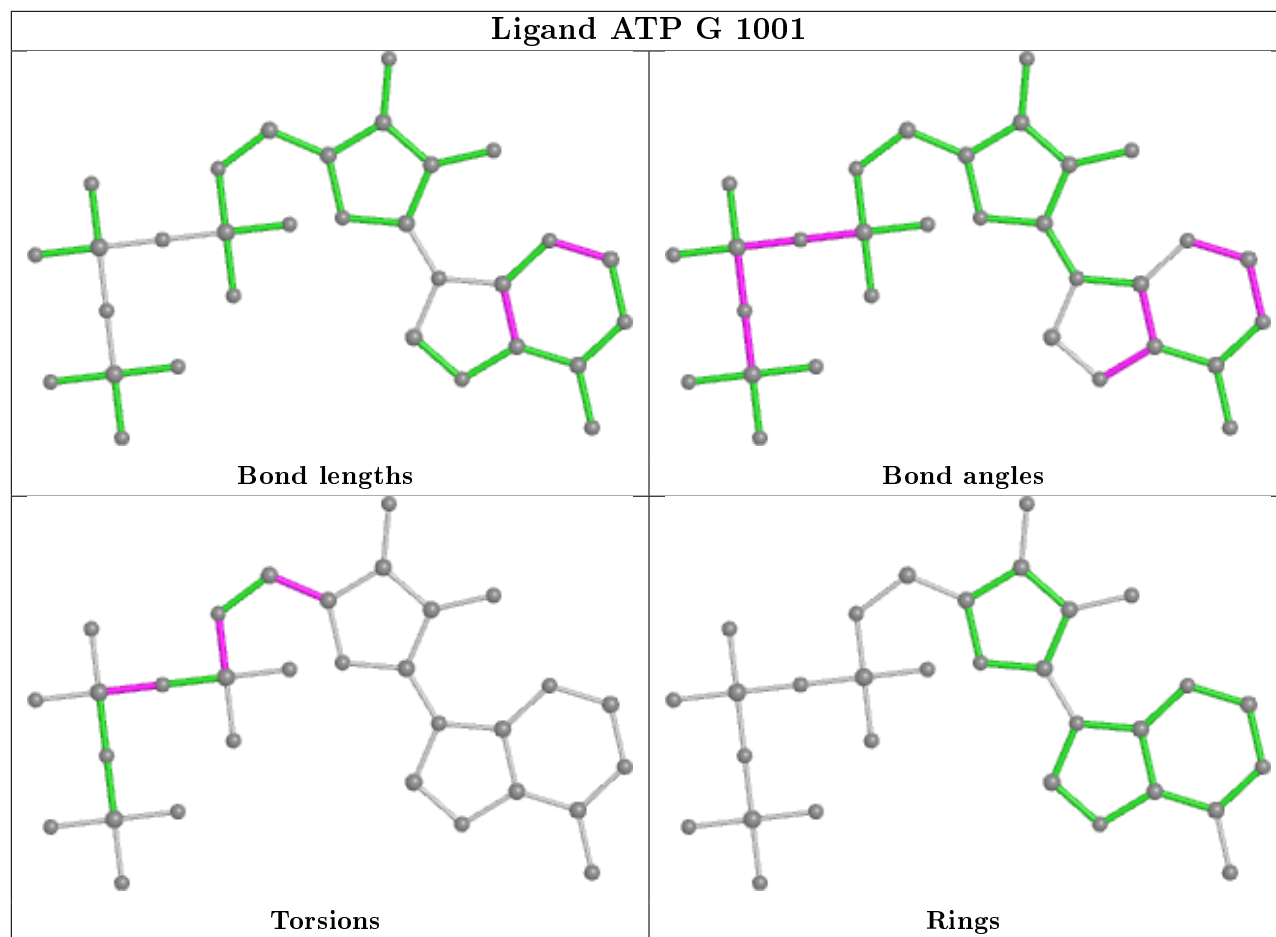




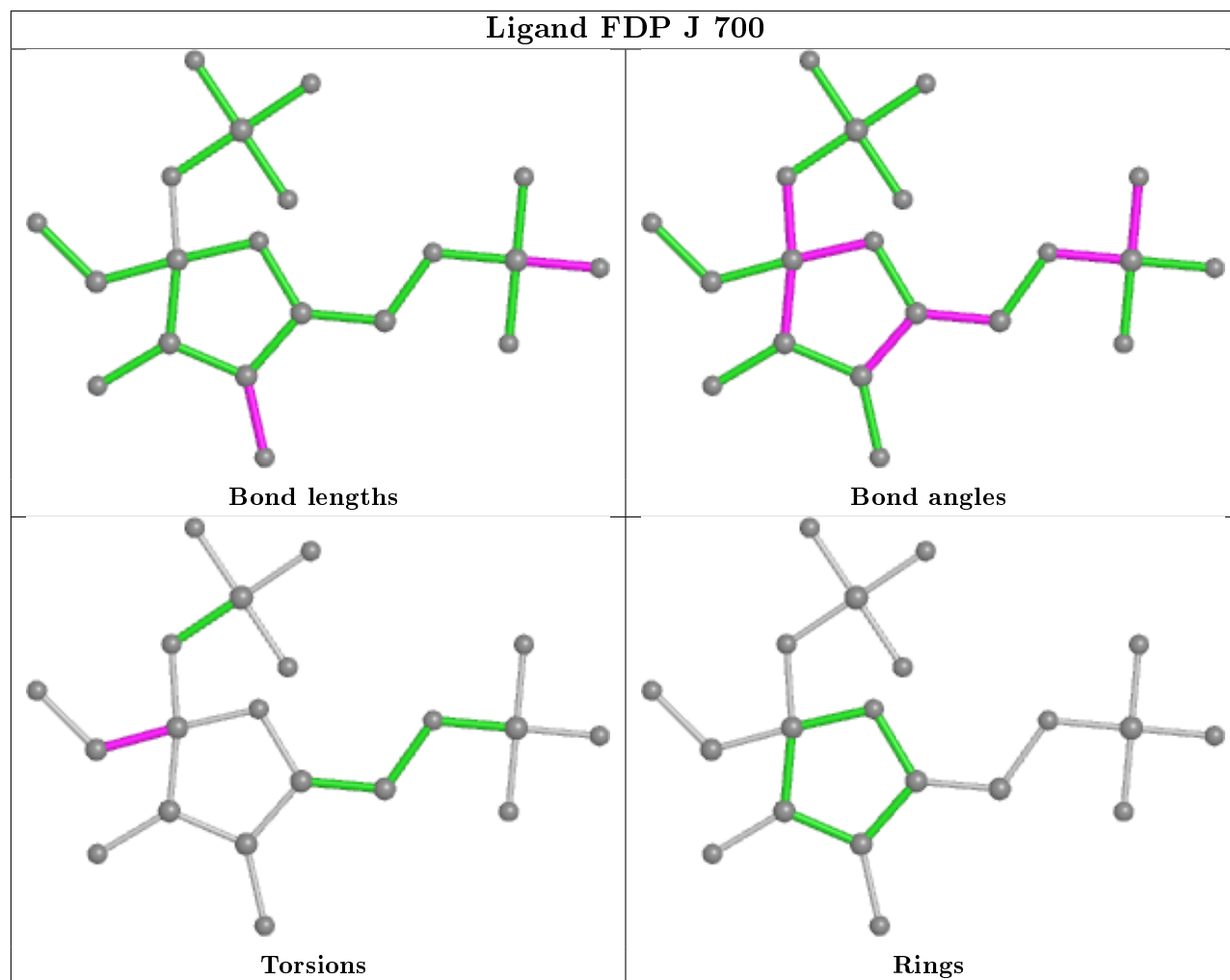




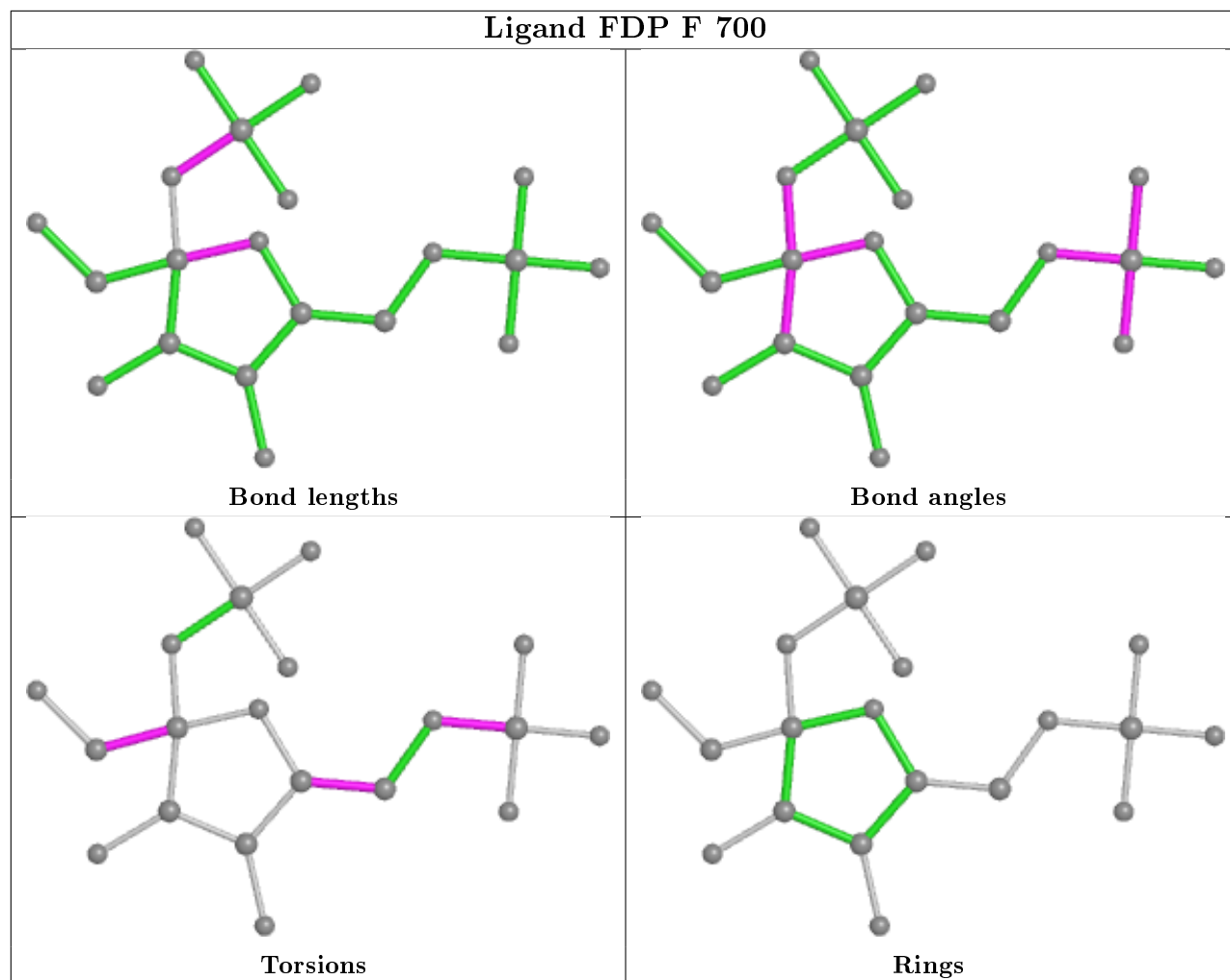




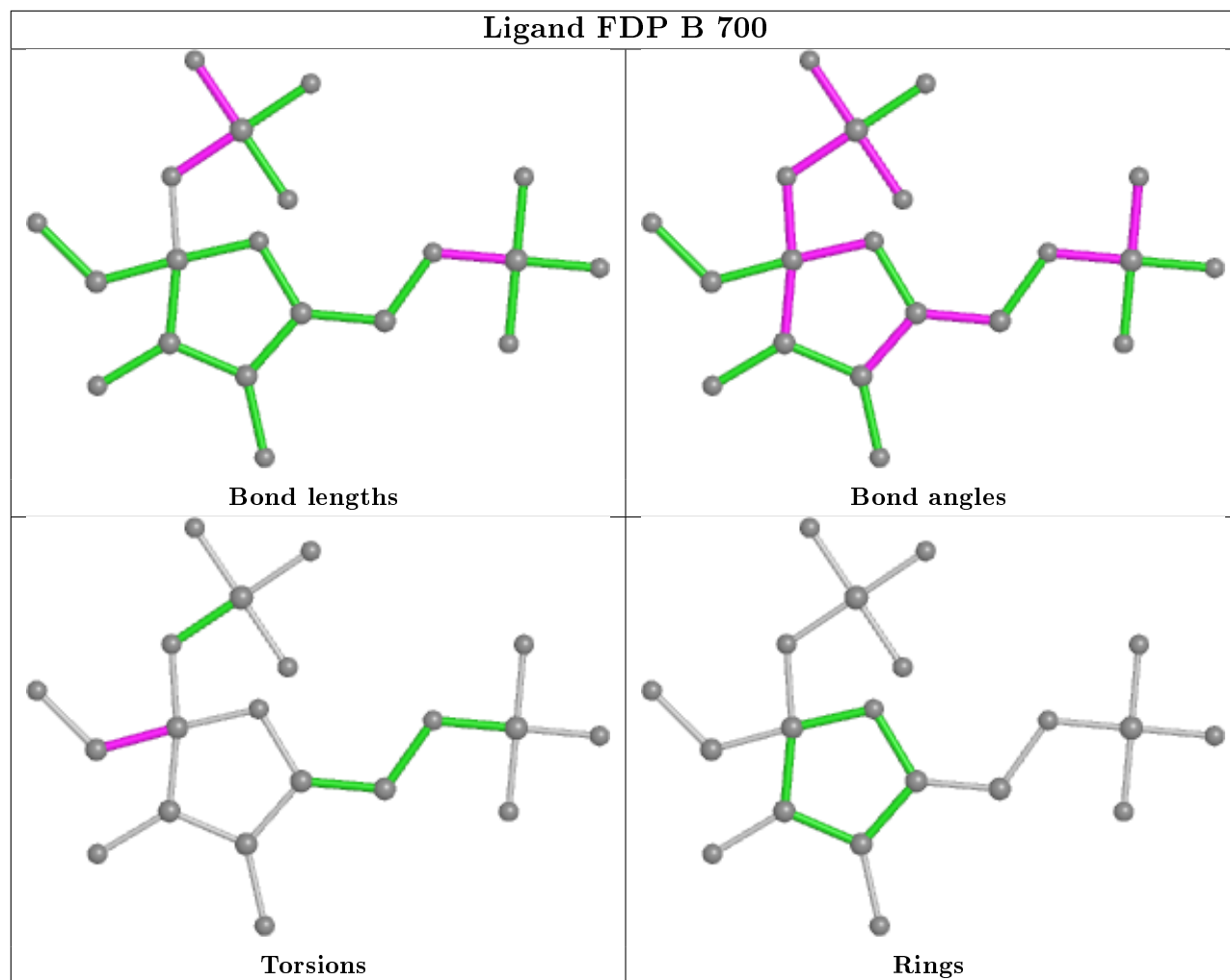
## Ligand FDP J 700

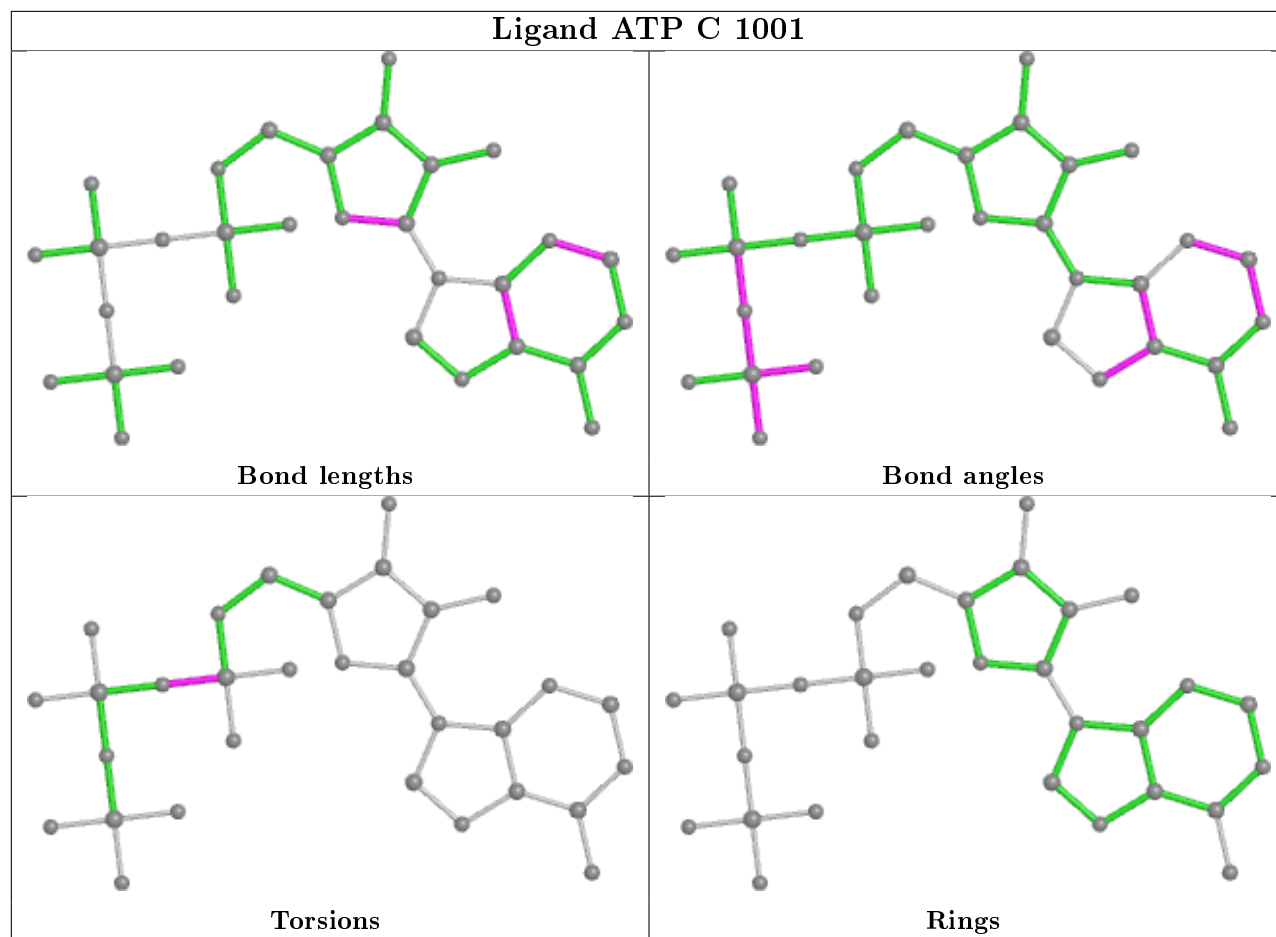


## Ligand FDP F 700

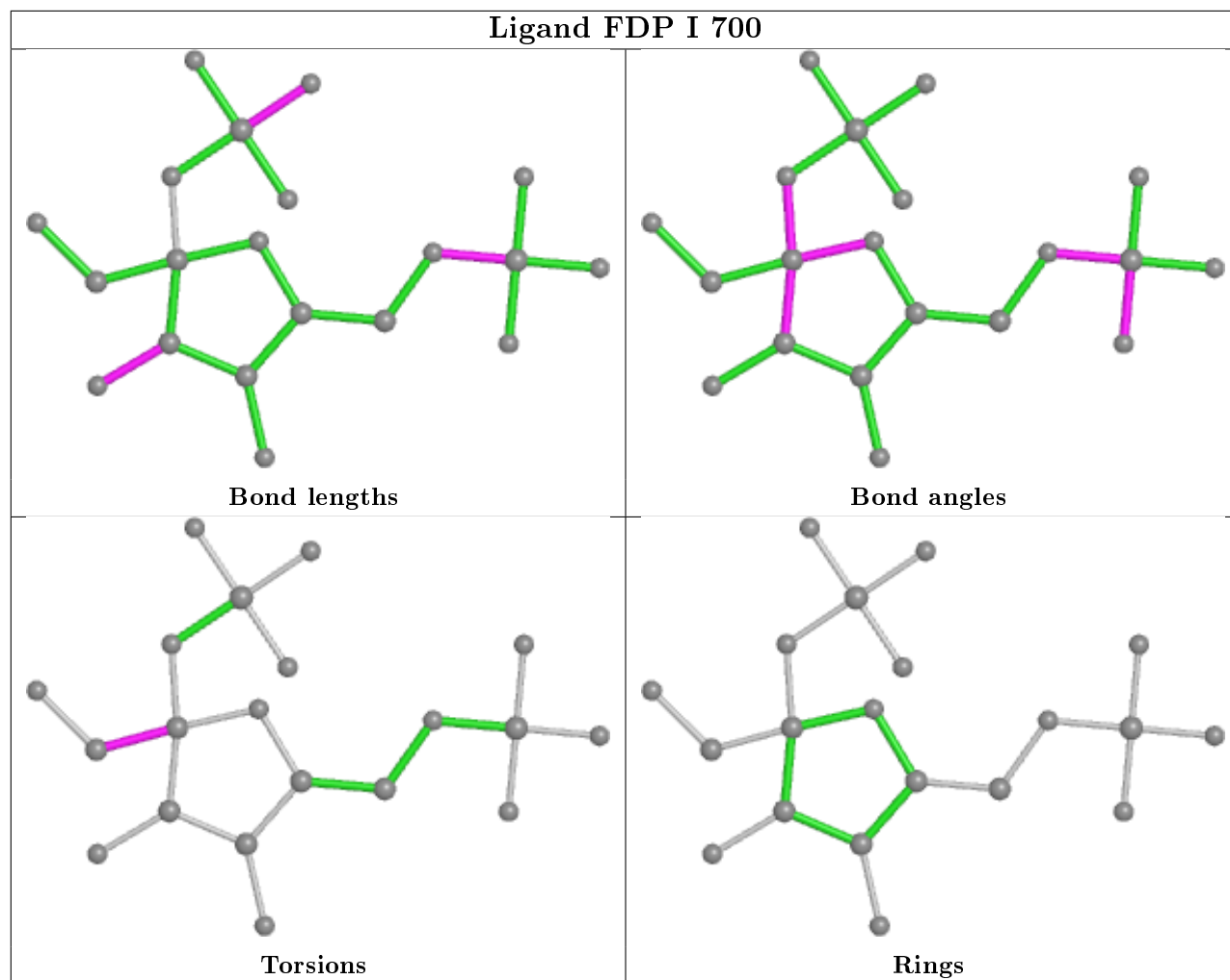




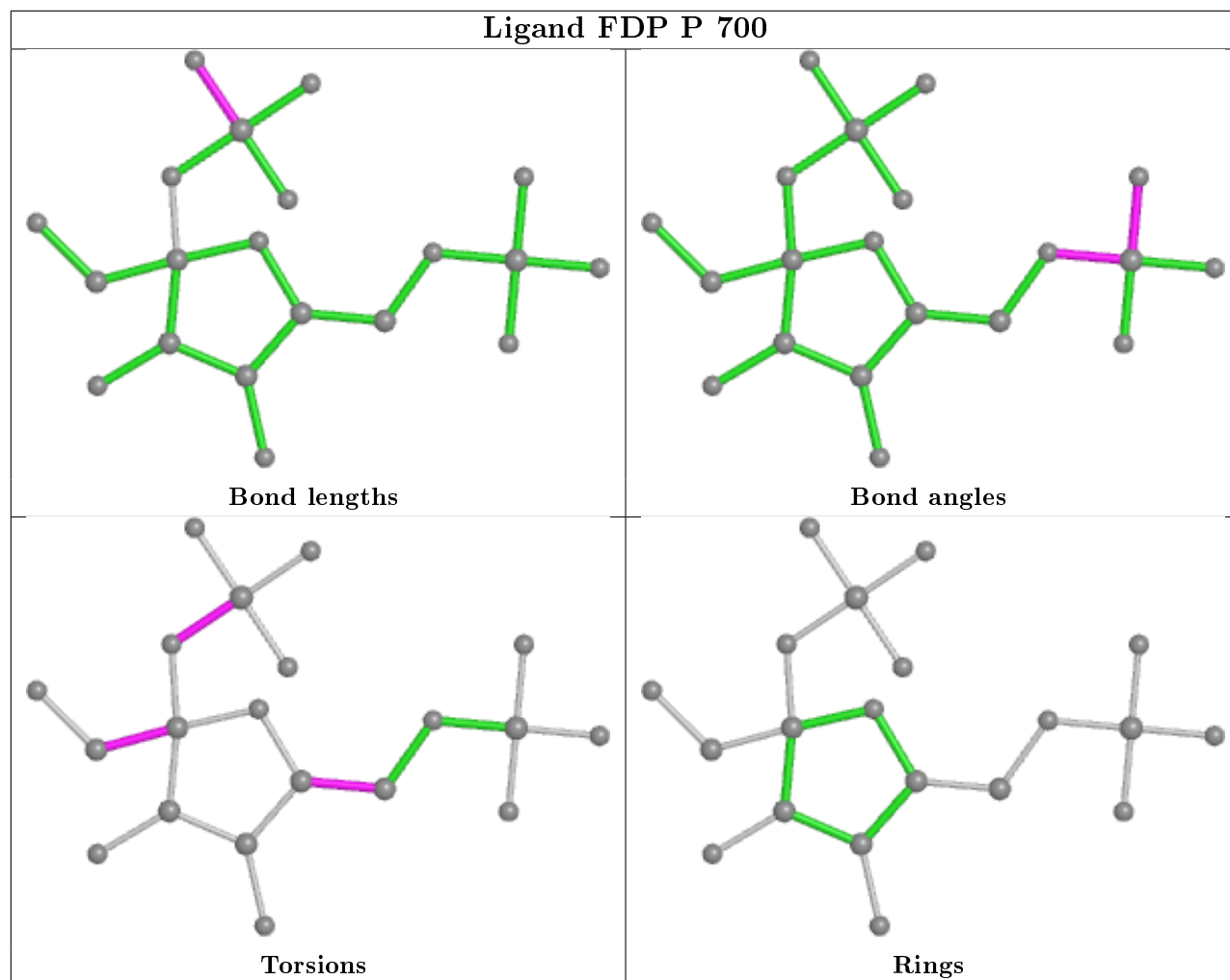


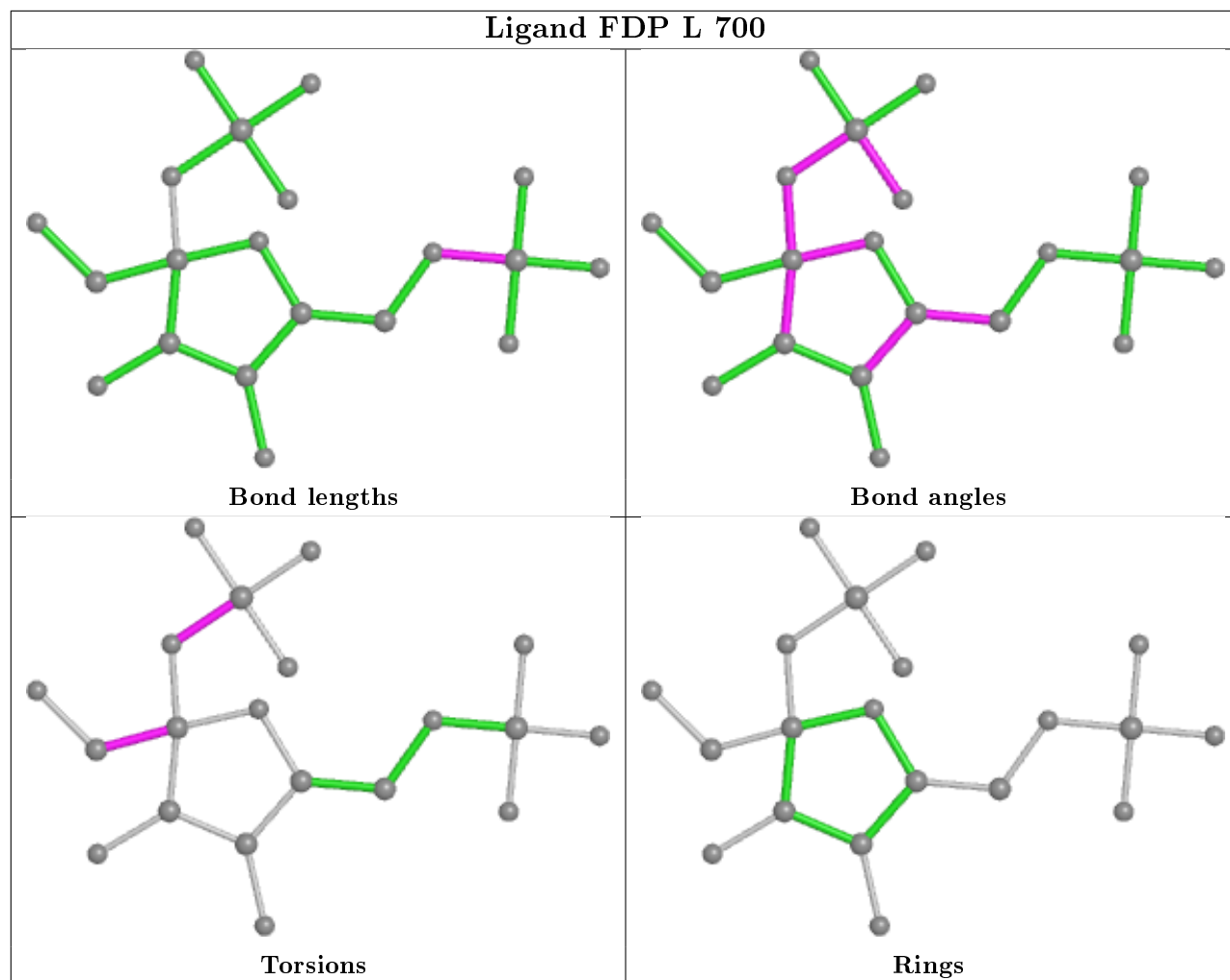


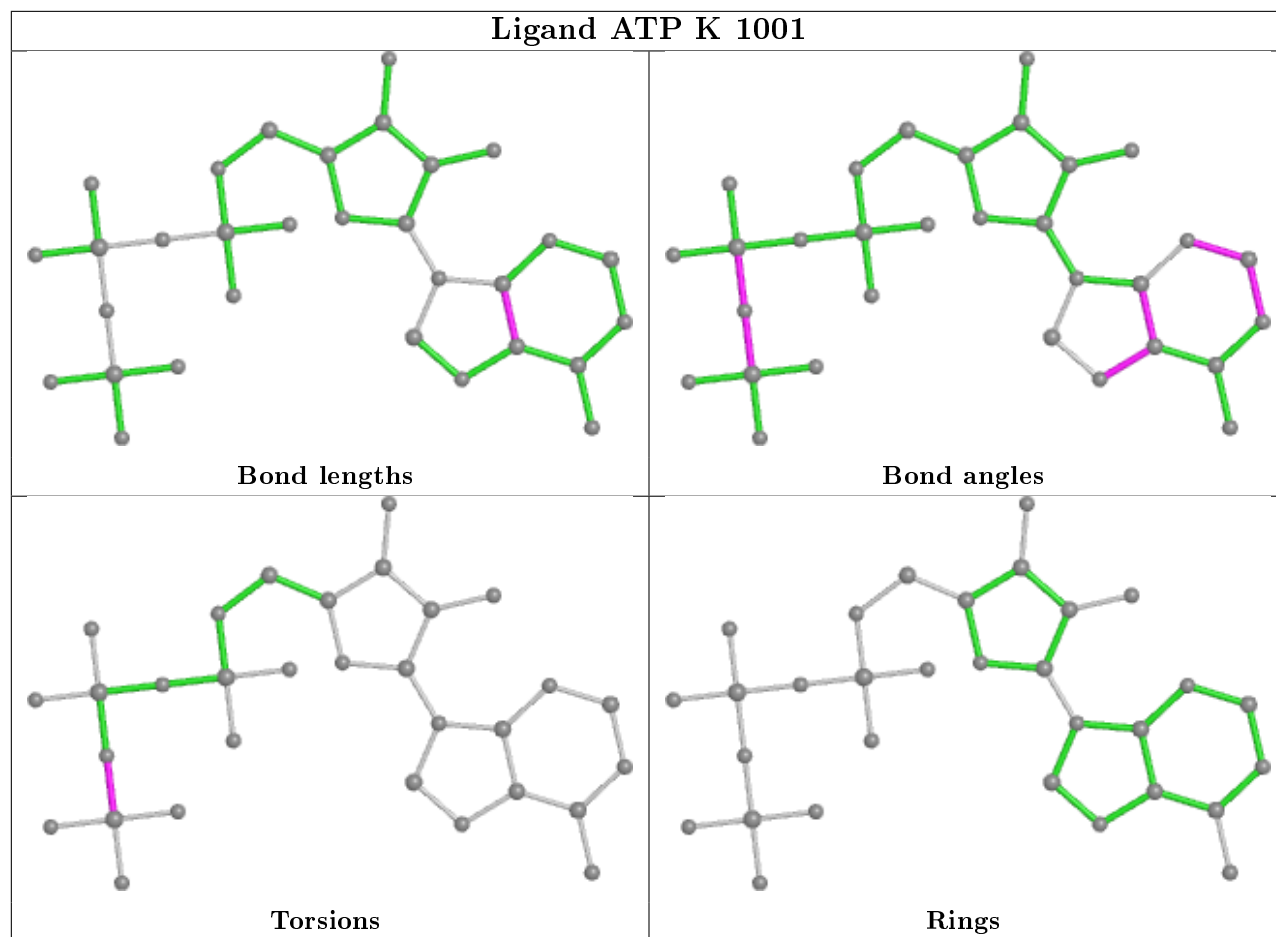
## Ligand FDP I 700



## Ligand FDP P 700







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

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

All (1566) RSRZ outliers are listed below:

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	431	LEU	9.0
1	N	195	VAL	8.6
1	O	113	PRO	8.5
1	P	496	LEU	7.9
1	O	120	THR	7.7
1	N	259	MET	7.7
1	O	447	LEU	7.6
1	O	132	SER	7.5
1	O	433	ILE	7.4
1	P	444	ALA	7.4
1	N	444	ALA	7.4
1	P	446	LYS	7.2
1	N	115	PHE	7.1
1	O	442	PHE	7.1
1	P	209	PHE	7.0
1	N	153	GLN	6.9
1	P	114	ALA	6.9
1	N	74	LEU	6.9
1	O	496	LEU	6.9
1	P	100	VAL	6.8
1	P	135	VAL	6.8
1	O	163	CYS	6.7
1	P	134	VAL	6.7
1	O	134	VAL	6.6
1	O	140	TYR	6.6
1	P	158	GLU	6.6
1	H	118	LYS	6.6
1	N	14	PRO	6.5
1	P	12	PHE	6.5
1	P	447	LEU	6.5
1	G	108	TYR	6.5
1	O	488	TYR	6.5
1	P	470	VAL	6.5
1	P	101	MET	6.5
1	P	191	ALA	6.4
1	N	163	CYS	6.4
1	M	118	LYS	6.4
1	O	156	GLU	6.4
1	M	108	TYR	6.4
1	G	198	GLN	6.3
1	P	125	TYR	6.3
1	M	104	GLY	6.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	34	VAL	6.3
1	P	113	PRO	6.2
1	N	97	GLY	6.2
1	P	108	TYR	6.2
1	N	260	VAL	6.1
1	O	108	TYR	6.1
1	O	224	LYS	6.1
1	N	24	ILE	6.1
1	O	151	GLN	6.1
1	P	14	PRO	6.1
1	O	74	LEU	6.1
1	N	108	TYR	6.1
1	P	118	LYS	6.1
1	O	119	GLY	6.0
1	N	105	ALA	6.0
1	O	209	PHE	6.0
1	P	131	LEU	6.0
1	G	24	ILE	6.0
1	O	449	HIS	6.0
1	O	157	ASP	5.9
1	O	472	THR	5.9
1	A	152	VAL	5.9
1	P	153	GLN	5.9
1	P	472	THR	5.9
1	O	102	GLU	5.9
1	O	135	VAL	5.8
1	P	238	LYS	5.8
1	O	105	ALA	5.8
1	O	455	HIS	5.8
1	P	129	GLN	5.8
1	N	448	GLY	5.8
1	A	209	PHE	5.7
1	O	12	PHE	5.7
1	E	118	LYS	5.7
1	N	214	ARG	5.7
1	P	498	GLU	5.7
1	P	154	SER	5.7
1	O	137	PRO	5.7
1	O	39	GLY	5.7
1	O	99	ALA	5.7
1	N	449	HIS	5.7
1	P	150	LEU	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	431	LEU	5.7
1	O	187	PRO	5.6
1	O	448	GLY	5.6
1	P	106	THR	5.6
1	N	247	ASN	5.6
1	P	229	LYS	5.6
1	P	449	HIS	5.6
1	G	96	GLY	5.6
1	O	38	LYS	5.6
1	G	189	VAL	5.5
1	P	137	PRO	5.5
1	P	107	CYS	5.5
1	N	104	GLY	5.5
1	P	443	ASP	5.5
1	O	481	ALA	5.5
1	P	445	ASP	5.5
1	P	227	GLY	5.4
1	P	433	ILE	5.4
1	H	293	ILE	5.4
1	P	39	GLY	5.4
1	M	120	THR	5.4
1	O	445	ASP	5.4
1	G	163	CYS	5.4
1	F	293	ILE	5.3
1	O	458	ALA	5.3
1	G	12	PHE	5.3
1	H	115	PHE	5.3
1	N	100	VAL	5.3
1	H	157	ASP	5.3
1	O	31	THR	5.2
1	O	434	THR	5.2
1	O	220	GLY	5.2
1	P	115	PHE	5.2
1	A	95	VAL	5.2
1	O	133	LYS	5.2
1	G	294	CYS	5.2
1	P	195	VAL	5.2
1	P	434	THR	5.1
1	O	131	LEU	5.1
1	G	327	VAL	5.1
1	P	165	VAL	5.1
1	M	115	PHE	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	187	PRO	5.1
1	P	132	SER	5.1
1	N	148	LEU	5.1
1	H	100	VAL	5.1
1	N	216	ALA	5.1
1	N	8	THR	5.1
1	O	129	GLN	5.1
1	P	451	GLU	5.1
1	N	107	CYS	5.1
1	G	124	PHE	5.1
1	P	82	LEU	5.0
1	H	497	VAL	5.0
1	A	108	TYR	5.0
1	O	106	THR	5.0
1	N	225	ALA	5.0
1	I	134	VAL	5.0
1	O	436	GLY	5.0
1	G	118	LYS	5.0
1	O	124	PHE	5.0
1	G	120	THR	5.0
1	M	182	CYS	5.0
1	M	156	GLU	5.0
1	N	166	THR	5.0
1	P	110	THR	5.0
1	M	100	VAL	4.9
1	O	221	ASP	4.9
1	A	24	ILE	4.9
1	E	177	VAL	4.9
1	O	125	TYR	4.9
1	N	251	ILE	4.9
1	H	12	PHE	4.9
1	P	128	TYR	4.9
1	O	441	PHE	4.9
1	M	293	ILE	4.9
1	M	294	CYS	4.9
1	O	118	LYS	4.9
1	O	139	ASN	4.9
1	O	154	SER	4.8
1	A	293	ILE	4.8
1	G	293	ILE	4.8
1	P	105	ALA	4.8
1	P	228	PRO	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	158	GLU	4.8
1	N	103	ARG	4.8
1	O	471	GLN	4.8
1	G	47	VAL	4.8
1	P	83	ASP	4.8
1	P	199	PHE	4.8
1	N	12	PHE	4.7
1	N	154	SER	4.7
1	O	443	ASP	4.7
1	K	293	ILE	4.7
1	N	102	GLU	4.7
1	N	185	ASP	4.7
1	N	258	ILE	4.7
1	P	187	PRO	4.7
1	P	72	ALA	4.7
1	O	468	GLY	4.7
1	P	471	GLN	4.7
1	N	209	PHE	4.7
1	N	176	GLY	4.7
1	O	469	TYR	4.7
1	O	182	CYS	4.7
1	N	164	THR	4.7
1	G	116	ALA	4.7
1	O	70	ALA	4.7
1	O	130	ASN	4.6
1	F	433	ILE	4.6
1	G	228	PRO	4.6
1	P	11	ILE	4.6
1	P	306	PRO	4.6
1	M	295	ALA	4.6
1	P	207	MET	4.6
1	G	107	CYS	4.6
1	C	293	ILE	4.6
1	E	176	GLY	4.6
1	P	136	ARG	4.6
1	M	158	GLU	4.6
1	O	13	ASP	4.6
1	P	10	SER	4.6
1	A	155	HIS	4.6
1	P	95	VAL	4.6
1	N	329	LEU	4.6
1	P	448	GLY	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	24	ILE	4.6
1	G	48	ALA	4.6
1	P	466	SER	4.6
1	N	95	VAL	4.6
1	O	14	PRO	4.6
1	M	135	VAL	4.6
1	P	37	LEU	4.6
1	N	145	ASP	4.6
1	N	129	GLN	4.5
1	E	12	PHE	4.5
1	G	152	VAL	4.5
1	N	188	ALA	4.5
1	L	115	PHE	4.5
1	P	103	ARG	4.5
1	P	74	LEU	4.5
1	N	98	ASP	4.5
1	N	160	THR	4.5
1	O	107	CYS	4.5
1	O	35	GLU	4.5
1	P	17	ASN	4.5
1	P	483	HIS	4.5
1	O	114	ALA	4.5
1	N	293	ILE	4.5
1	O	404	ARG	4.5
1	G	326	CYS	4.5
1	M	96	GLY	4.5
1	O	152	VAL	4.5
1	M	121	LYS	4.5
1	N	94	PHE	4.5
1	N	139	ASN	4.5
1	P	124	PHE	4.4
1	A	133	LYS	4.4
1	P	293	ILE	4.4
1	G	115	PHE	4.4
1	N	189	VAL	4.4
1	G	224	LYS	4.4
1	O	136	ARG	4.4
1	H	160	THR	4.4
1	O	164	THR	4.4
1	O	67	VAL	4.4
1	P	75	GLY	4.4
1	A	118	LYS	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	446	LYS	4.4
1	M	12	PHE	4.4
1	O	94	PHE	4.4
1	M	292	VAL	4.4
1	M	185	ASP	4.4
1	N	162	GLU	4.4
1	O	228	PRO	4.4
1	G	95	VAL	4.4
1	M	328	MET	4.4
1	N	133	LYS	4.4
1	M	433	ILE	4.3
1	E	108	TYR	4.3
1	A	228	PRO	4.3
1	E	14	PRO	4.3
1	G	137	PRO	4.3
1	N	69	GLN	4.3
1	M	95	VAL	4.3
1	P	394	LYS	4.3
1	P	102	GLU	4.3
1	N	372	ILE	4.3
1	G	74	LEU	4.3
1	G	292	VAL	4.3
1	O	287	VAL	4.3
1	C	433	ILE	4.3
1	D	293	ILE	4.3
1	P	236	ILE	4.3
1	A	449	HIS	4.3
1	G	295	ALA	4.3
1	F	12	PHE	4.3
1	N	226	LEU	4.3
1	A	156	GLU	4.3
1	O	470	VAL	4.3
1	O	236	ILE	4.3
1	G	259	MET	4.3
1	J	295	ALA	4.3
1	P	198	GLN	4.3
1	G	94	PHE	4.3
1	F	24	ILE	4.2
1	M	326	CYS	4.2
1	O	92	GLY	4.2
1	A	183	ASP	4.2
1	F	112	ASP	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	94	PHE	4.2
1	G	258	ILE	4.2
1	G	153	GLN	4.2
1	O	435	GLN	4.2
1	L	12	PHE	4.2
1	N	261	ALA	4.2
1	O	81	ALA	4.2
1	N	124	PHE	4.2
1	F	326	CYS	4.2
1	N	140	TYR	4.2
1	C	259	MET	4.1
1	O	451	GLU	4.1
1	M	145	ASP	4.1
1	P	89	ILE	4.1
1	A	434	THR	4.1
1	P	120	THR	4.1
1	M	134	VAL	4.1
1	P	488	TYR	4.1
1	P	99	ALA	4.1
1	K	433	ILE	4.1
1	N	217	GLU	4.1
1	O	173	ASP	4.1
1	N	132	SER	4.1
1	G	262	ARG	4.1
1	P	295	ALA	4.1
1	N	264	ASP	4.1
1	A	259	MET	4.1
1	O	227	GLY	4.1
1	N	330	SER	4.1
1	O	371	HIS	4.1
1	O	483	HIS	4.1
1	A	433	ILE	4.1
1	G	209	PHE	4.1
1	F	47	VAL	4.0
1	H	123	LYS	4.0
1	O	73	GLU	4.0
1	N	135	VAL	4.0
1	N	228	PRO	4.0
1	O	165	VAL	4.0
1	N	246	GLN	4.0
1	N	328	MET	4.0
1	A	326	CYS	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	155	HIS	4.0
1	G	223	ARG	4.0
1	P	475	TYR	4.0
1	P	441	PHE	4.0
1	O	204	GLY	4.0
1	G	296	THR	4.0
1	P	168	SER	4.0
1	P	96	GLY	4.0
1	M	103	ARG	4.0
1	M	437	VAL	4.0
1	O	158	GLU	4.0
1	O	207	MET	4.0
1	N	151	GLN	4.0
1	P	130	ASN	4.0
1	J	293	ILE	3.9
1	O	304	TYR	3.9
1	O	168	SER	3.9
1	N	433	ILE	3.9
1	P	372	ILE	3.9
1	O	487	GLY	3.9
1	N	125	TYR	3.9
1	O	59	TYR	3.9
1	N	295	ALA	3.9
1	G	260	VAL	3.9
1	O	98	ASP	3.9
1	P	22	ARG	3.9
1	N	465	LYS	3.9
1	G	226	LEU	3.9
1	H	108	TYR	3.9
1	C	260	VAL	3.9
1	A	328	MET	3.9
1	F	291	PRO	3.9
1	N	451	GLU	3.9
1	O	72	ALA	3.9
1	C	327	VAL	3.9
1	M	34	VAL	3.9
1	M	372	ILE	3.9
1	P	152	VAL	3.9
1	A	327	VAL	3.9
1	M	165	VAL	3.9
1	N	219	VAL	3.9
1	N	327	VAL	3.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	93	GLN	3.9
1	N	161	LEU	3.9
1	O	111	THR	3.8
1	H	470	VAL	3.8
1	P	455	HIS	3.8
1	M	9	LEU	3.8
1	O	110	THR	3.8
1	P	473	GLY	3.8
1	H	156	GLU	3.8
1	L	449	HIS	3.8
1	N	240	GLU	3.8
1	P	156	GLU	3.8
1	N	294	CYS	3.8
1	P	176	GLY	3.8
1	P	487	GLY	3.8
1	E	115	PHE	3.8
1	N	446	LYS	3.8
1	A	236	ILE	3.8
1	J	24	ILE	3.8
1	G	49	ARG	3.8
1	J	294	CYS	3.8
1	O	369	LEU	3.8
1	P	133	LYS	3.8
1	C	24	ILE	3.8
1	N	263	GLY	3.8
1	A	120	THR	3.8
1	O	112	ASP	3.8
1	P	432	ASN	3.8
1	M	159	GLN	3.8
1	P	181	GLY	3.8
1	A	292	VAL	3.8
1	E	295	ALA	3.8
1	F	221	ASP	3.8
1	J	260	VAL	3.8
1	M	410	ALA	3.8
1	O	191	ALA	3.8
1	B	326	CYS	3.8
1	C	294	CYS	3.8
1	E	136	ARG	3.8
1	O	432	ASN	3.8
1	C	238	LYS	3.8
1	A	12	PHE	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	191	ALA	3.7
1	N	120	THR	3.7
1	P	160	THR	3.7
1	O	32	GLN	3.7
1	O	161	LEU	3.7
1	H	132	SER	3.7
1	D	292	VAL	3.7
1	M	11	ILE	3.7
1	N	47	VAL	3.7
1	N	109	VAL	3.7
1	O	123	LYS	3.7
1	P	84	THR	3.7
1	N	199	PHE	3.7
1	P	93	GLN	3.7
1	G	433	ILE	3.7
1	G	185	ASP	3.7
1	M	183	ASP	3.7
1	L	158	GLU	3.7
1	H	129	GLN	3.7
1	C	326	CYS	3.7
1	N	114	ALA	3.7
1	G	187	PRO	3.7
1	G	447	LEU	3.7
1	N	224	LYS	3.7
1	O	170	THR	3.7
1	N	121	LYS	3.7
1	H	294	CYS	3.7
1	P	161	LEU	3.7
1	M	304	TYR	3.7
1	O	198	GLN	3.7
1	P	468	GLY	3.7
1	E	158	GLU	3.6
1	J	47	VAL	3.7
1	P	9	LEU	3.6
1	N	118	LYS	3.6
1	N	106	THR	3.6
1	P	162	GLU	3.6
1	G	109	VAL	3.6
1	M	418	ILE	3.6
1	O	326	CYS	3.6
1	P	73	GLU	3.6
1	A	160	THR	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	238	LYS	3.6
1	N	13	ASP	3.6
1	M	153	GLN	3.6
1	N	238	LYS	3.6
1	P	85	LYS	3.6
1	N	183	ASP	3.6
1	P	178	ASN	3.6
1	M	498	GLU	3.6
1	H	159	GLN	3.6
1	O	142	TYR	3.6
1	M	155	HIS	3.6
1	A	294	CYS	3.6
1	F	228	PRO	3.6
1	O	115	PHE	3.6
1	C	328	MET	3.6
1	F	226	LEU	3.6
1	M	496	LEU	3.6
1	N	59	TYR	3.6
1	O	409	VAL	3.6
1	O	56	SER	3.6
1	A	291	PRO	3.6
1	C	210	ALA	3.6
1	M	4	ALA	3.6
1	P	210	ALA	3.6
1	E	326	CYS	3.6
1	G	155	HIS	3.6
1	H	259	MET	3.6
1	P	242	HIS	3.6
1	A	98	ASP	3.6
1	O	103	ARG	3.6
1	P	173	ASP	3.6
1	G	114	ALA	3.5
1	M	114	ALA	3.5
1	P	36	ALA	3.5
1	H	445	ASP	3.5
1	N	64	ILE	3.5
1	N	178	ASN	3.5
1	O	82	LEU	3.5
1	O	122	ASP	3.5
1	O	231	ARG	3.5
1	E	293	ILE	3.5
1	O	219	VAL	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	408	LEU	3.5
1	O	475	TYR	3.5
1	A	103	ARG	3.5
1	N	117	ASP	3.5
1	J	326	CYS	3.5
1	P	123	LYS	3.5
1	G	98	ASP	3.5
1	O	128	TYR	3.5
1	O	338	TYR	3.5
1	P	304	TYR	3.5
1	F	181	GLY	3.5
1	M	436	GLY	3.5
1	N	156	GLU	3.5
1	O	75	GLY	3.5
1	O	479	ILE	3.5
1	P	49	ARG	3.5
1	F	261	ALA	3.5
1	G	261	ALA	3.5
1	N	194	ARG	3.5
1	O	234	MET	3.5
1	P	117	ASP	3.5
1	P	259	MET	3.5
1	J	433	ILE	3.5
1	P	8	THR	3.5
1	H	295	ALA	3.5
1	J	48	ALA	3.5
1	J	81	ALA	3.5
1	M	324	ALA	3.5
1	P	13	ASP	3.5
1	O	339	PRO	3.4
1	G	236	ILE	3.4
1	O	372	ILE	3.4
1	A	135	VAL	3.4
1	L	118	LYS	3.4
1	D	324	ALA	3.4
1	K	295	ALA	3.4
1	P	371	HIS	3.4
1	N	168	SER	3.4
1	G	237	CYS	3.4
1	O	229	LYS	3.4
1	A	92	GLY	3.4
1	D	24	ILE	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	89	ILE	3.4
1	F	197	LEU	3.4
1	G	138	GLY	3.4
1	G	431	LEU	3.4
1	O	149	ILE	3.4
1	O	418	ILE	3.4
1	I	295	ALA	3.4
1	E	160	THR	3.4
1	A	444	ALA	3.4
1	P	43	SER	3.4
1	L	95	VAL	3.4
1	M	15	VAL	3.4
1	N	443	ASP	3.4
1	P	34	VAL	3.4
1	P	76	VAL	3.4
1	O	340	ASN	3.4
1	K	259	MET	3.4
1	P	145	ASP	3.4
1	C	261	ALA	3.4
1	C	295	ALA	3.4
1	B	409	VAL	3.4
1	H	292	VAL	3.4
1	N	338	TYR	3.4
1	O	373	PRO	3.4
1	D	296	THR	3.4
1	M	259	MET	3.4
1	O	8	THR	3.4
1	A	447	LEU	3.4
1	N	150	LEU	3.4
1	O	162	GLU	3.4
1	P	212	PHE	3.4
1	F	134	VAL	3.4
1	O	474	ASP	3.4
1	E	140	TYR	3.4
1	G	434	THR	3.4
1	M	105	ALA	3.4
1	N	72	ALA	3.4
1	O	437	VAL	3.3
1	O	457	VAL	3.3
1	G	119	GLY	3.3
1	P	185	ASP	3.3
1	P	88	GLU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	424	ARG	3.3
1	C	258	ILE	3.3
1	D	158	GLU	3.3
1	O	117	ASP	3.3
1	D	294	CYS	3.3
1	E	137	PRO	3.3
1	M	176	GLY	3.3
1	M	164	THR	3.3
1	O	160	THR	3.3
1	E	324	ALA	3.3
1	F	225	ALA	3.3
1	P	116	ALA	3.3
1	O	150	LEU	3.3
1	A	258	ILE	3.3
1	G	176	GLY	3.3
1	P	104	GLY	3.3
1	A	229	LYS	3.3
1	E	133	LYS	3.3
1	N	155	HIS	3.3
1	O	424	ARG	3.3
1	N	25	CYS	3.3
1	N	211	SER	3.3
1	O	33	SER	3.3
1	P	163	CYS	3.3
1	G	162	GLU	3.3
1	P	4	ALA	3.3
1	O	495	LEU	3.3
1	G	171	ILE	3.3
1	O	104	GLY	3.3
1	H	95	VAL	3.3
1	O	183	ASP	3.3
1	O	450	ASP	3.3
1	P	391	THR	3.3
1	O	97	GLY	3.3
1	B	24	ILE	3.3
1	D	433	ILE	3.3
1	E	154	SER	3.3
1	A	47	VAL	3.3
1	N	177	VAL	3.3
1	I	13	ASP	3.3
1	O	325	ASP	3.3
1	E	296	THR	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	21	ALA	3.3
1	A	81	ALA	3.3
1	M	102	GLU	3.3
1	N	326	CYS	3.3
1	P	462	GLU	3.3
1	A	207	MET	3.3
1	N	483	HIS	3.3
1	F	431	LEU	3.3
1	N	250	SER	3.3
1	I	12	PHE	3.3
1	M	157	ASP	3.3
1	P	138	GLY	3.2
1	G	59	TYR	3.2
1	P	338	TYR	3.2
1	G	23	ILE	3.2
1	O	171	ILE	3.2
1	L	159	GLN	3.2
1	F	295	ALA	3.2
1	O	406	ALA	3.2
1	M	3	LEU	3.2
1	G	182	CYS	3.2
1	A	224	LYS	3.2
1	N	245	VAL	3.2
1	O	47	VAL	3.2
1	P	497	VAL	3.2
1	I	324	ALA	3.2
1	F	14	PRO	3.2
1	N	262	ARG	3.2
1	O	405	SER	3.2
1	M	471	GLN	3.2
1	O	430	GLN	3.2
1	D	326	CYS	3.2
1	A	130	ASN	3.2
1	D	260	VAL	3.2
1	G	165	VAL	3.2
1	P	58	GLU	3.2
1	P	90	ARG	3.2
1	N	113	PRO	3.2
1	L	433	ILE	3.2
1	C	12	PHE	3.2
1	C	449	HIS	3.2
1	E	292	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	327	VAL	3.2
1	O	201	VAL	3.2
1	O	419	VAL	3.2
1	A	238	LYS	3.2
1	P	81	ALA	3.2
1	C	236	ILE	3.2
1	G	52	PHE	3.2
1	A	109	VAL	3.2
1	D	380	VAL	3.2
1	G	100	VAL	3.2
1	A	163	CYS	3.2
1	N	1	SER	3.2
1	O	420	CYS	3.2
1	P	336	GLY	3.2
1	F	23	ILE	3.1
1	N	254	GLU	3.1
1	H	94	PHE	3.1
1	N	10	SER	3.1
1	P	18	TYR	3.1
1	F	409	VAL	3.1
1	A	137	PRO	3.1
1	F	183	ASP	3.1
1	M	17	ASN	3.1
1	N	65	ASN	3.1
1	P	186	LEU	3.1
1	N	170	THR	3.1
1	F	209	PHE	3.1
1	G	154	SER	3.1
1	P	211	SER	3.1
1	P	442	PHE	3.1
1	N	222	VAL	3.1
1	P	15	VAL	3.1
1	L	295	ALA	3.1
1	P	183	ASP	3.1
1	O	93	GLN	3.1
1	N	131	LEU	3.1
1	D	479	ILE	3.1
1	I	183	ASP	3.1
1	O	185	ASP	3.1
1	D	409	VAL	3.1
1	E	152	VAL	3.1
1	O	477	VAL	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	177	VAL	3.1
1	F	224	LYS	3.1
1	O	9	LEU	3.1
1	E	434	THR	3.1
1	N	445	ASP	3.1
1	J	23	ILE	3.1
1	M	169	HIS	3.1
1	O	57	HIS	3.1
1	N	157	ASP	3.1
1	O	190	SER	3.1
1	P	298	MET	3.1
1	G	129	GLN	3.1
1	J	89	ILE	3.1
1	J	236	ILE	3.1
1	N	257	GLY	3.1
1	B	260	VAL	3.1
1	C	292	VAL	3.1
1	G	102	GLU	3.1
1	G	195	VAL	3.1
1	O	189	VAL	3.1
1	P	189	VAL	3.1
1	G	31	THR	3.1
1	G	82	LEU	3.1
1	A	231	ARG	3.1
1	H	384	ALA	3.1
1	B	327	VAL	3.0
1	N	371	HIS	3.0
1	M	133	LYS	3.0
1	O	465	LYS	3.0
1	G	249	ASP	3.0
1	H	155	HIS	3.0
1	G	243	GLN	3.0
1	L	177	VAL	3.0
1	O	486	LYS	3.0
1	L	156	GLU	3.0
1	G	186	LEU	3.0
1	N	230	GLY	3.0
1	O	49	ARG	3.0
1	P	7	LEU	3.0
1	G	121	LYS	3.0
1	N	235	ILE	3.0
1	O	253	GLU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	209	PHE	3.0
1	N	215	SER	3.0
1	O	205	VAL	3.0
1	F	434	THR	3.0
1	A	157	ASP	3.0
1	D	329	LEU	3.0
1	N	143	ILE	3.0
1	H	39	GLY	3.0
1	M	14	PRO	3.0
1	F	207	MET	3.0
1	F	449	HIS	3.0
1	A	295	ALA	3.0
1	D	236	ILE	3.0
1	E	168	SER	3.0
1	P	494	ILE	3.0
1	H	119	GLY	3.0
1	N	152	VAL	3.0
1	P	184	VAL	3.0
1	P	436	GLY	3.0
1	I	185	ASP	3.0
1	M	296	THR	3.0
1	P	170	THR	3.0
1	H	326	CYS	3.0
1	D	295	ALA	3.0
1	O	36	ALA	3.0
1	B	479	ILE	3.0
1	O	58	GLU	3.0
1	F	227	GLY	3.0
1	L	97	GLY	3.0
1	I	177	VAL	3.0
1	K	292	VAL	3.0
1	C	237	CYS	2.9
1	A	235	ILE	2.9
1	O	52	PHE	2.9
1	O	121	LYS	2.9
1	O	401	ASN	2.9
1	P	38	LYS	2.9
1	D	437	VAL	2.9
1	N	34	VAL	2.9
1	A	69	GLN	2.9
1	P	40	LEU	2.9
1	H	114	ALA	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	434	THR	2.9
1	J	292	VAL	2.9
1	P	157	ASP	2.9
1	M	101	MET	2.9
1	E	261	ALA	2.9
1	M	261	ALA	2.9
1	O	66	ASN	2.9
1	P	141	ILE	2.9
1	P	339	PRO	2.9
1	A	124	PHE	2.9
1	G	437	VAL	2.9
1	L	134	VAL	2.9
1	L	183	ASP	2.9
1	N	123	LYS	2.9
1	O	498	GLU	2.9
1	A	431	LEU	2.9
1	A	436	GLY	2.9
1	O	138	GLY	2.9
1	F	188	ALA	2.9
1	F	406	ALA	2.9
1	H	11	ILE	2.9
1	O	293	ILE	2.9
1	M	472	THR	2.9
1	N	35[A]	GLU	2.9
1	A	184	VAL	2.9
1	F	223	ARG	2.9
1	P	220	GLY	2.9
1	C	265	LEU	2.9
1	F	114	ALA	2.9
1	P	430	GLN	2.9
1	P	59	TYR	2.9
1	F	13	ASP	2.9
1	G	339	PRO	2.9
1	N	11	ILE	2.9
1	O	141	ILE	2.9
1	N	136	ARG	2.9
1	P	423	THR	2.9
1	G	211	SER	2.9
1	H	154	SER	2.9
1	B	47	VAL	2.9
1	D	95	VAL	2.9
1	I	326	CYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	94	PHE	2.9
1	M	380	VAL	2.9
1	D	328	MET	2.9
1	F	100	VAL	2.8
1	F	158	GLU	2.8
1	O	15	VAL	2.8
1	I	294	CYS	2.8
1	K	294	CYS	2.8
1	M	99	ALA	2.8
1	M	140	TYR	2.8
1	H	64	ILE	2.8
1	I	293	ILE	2.8
1	O	43	SER	2.8
1	G	17	ASN	2.8
1	P	454	GLU	2.8
1	C	209	PHE	2.8
1	G	15	VAL	2.8
1	N	101	MET	2.8
1	H	158	GLU	2.8
1	P	230	GLY	2.8
1	H	433	ILE	2.8
1	D	12	PHE	2.8
1	G	177	VAL	2.8
1	I	327	VAL	2.8
1	D	261	ALA	2.8
1	E	102	GLU	2.8
1	I	81	ALA	2.8
1	K	263	GLY	2.8
1	F	296	THR	2.8
1	P	171	ILE	2.8
1	J	12	PHE	2.8
1	D	135	VAL	2.8
1	F	292	VAL	2.8
1	P	243	GLN	2.8
1	L	21	ALA	2.8
1	A	161	LEU	2.8
1	N	49	ARG	2.8
1	A	237	CYS	2.8
1	C	84	THR	2.8
1	N	182	CYS	2.8
1	G	105	ALA	2.8
1	M	319	ALA	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	340	ASN	2.8
1	C	185	ASP	2.8
1	G	443	ASP	2.8
1	J	259	MET	2.8
1	A	62	THR	2.8
1	P	69	GLN	2.8
1	E	126	ILE	2.8
1	A	324	ALA	2.7
1	G	291	PRO	2.7
1	N	58	GLU	2.8
1	O	83	ASP	2.7
1	L	96	GLY	2.7
1	O	222	VAL	2.7
1	B	259	MET	2.7
1	N	9	LEU	2.7
1	N	207	MET	2.7
1	A	84	THR	2.7
1	G	26	THR	2.7
1	O	492	THR	2.7
1	B	433	ILE	2.7
1	H	162	GLU	2.7
1	I	433	ILE	2.7
1	J	49	ARG	2.7
1	H	112	ASP	2.7
1	L	113	PRO	2.7
1	M	291	PRO	2.7
1	G	191	ALA	2.7
1	K	261	ALA	2.7
1	N	191	ALA	2.7
1	N	227	GLY	2.7
1	F	327	VAL	2.7
1	I	209	PHE	2.7
1	K	260	VAL	2.7
1	L	437	VAL	2.7
1	O	159	GLN	2.7
1	P	435	GLN	2.7
1	N	110	THR	2.7
1	J	258	ILE	2.7
1	L	293	ILE	2.7
1	O	248	ILE	2.7
1	F	257	GLY	2.7
1	G	46	SER	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	70	ALA	2.7
1	D	327	VAL	2.7
1	F	118	LYS	2.7
1	L	47	VAL	2.7
1	P	421	VAL	2.7
1	O	423	THR	2.7
1	E	130	ASN	2.7
1	G	173	ASP	2.7
1	O	172	SER	2.7
1	P	202	GLU	2.7
1	E	135	VAL	2.7
1	P	287	VAL	2.7
1	N	450	ASP	2.7
1	P	305	ASN	2.7
1	C	228	PRO	2.7
1	G	80	ILE	2.7
1	M	113	PRO	2.7
1	H	72	ALA	2.7
1	I	261	ALA	2.7
1	I	384	ALA	2.7
1	J	327	VAL	2.7
1	A	102	GLU	2.7
1	C	434	THR	2.7
1	I	296	THR	2.7
1	P	234	MET	2.7
1	N	175	ARG	2.7
1	A	116	ALA	2.7
1	B	13	ASP	2.7
1	P	16	ALA	2.7
1	K	177	VAL	2.7
1	P	148	LEU	2.7
1	P	226	LEU	2.7
1	M	107	CYS	2.6
1	O	232	ASP	2.6
1	O	24	ILE	2.6
1	G	81	ALA	2.6
1	D	134	VAL	2.6
1	G	328	MET	2.6
1	M	97	GLY	2.6
1	P	92	GLY	2.6
1	G	133	LYS	2.6
1	P	112	ASP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	51	ASN	2.6
1	P	159	GLN	2.6
1	P	237	CYS	2.6
1	H	116	ALA	2.6
1	J	21	ALA	2.6
1	N	149	ILE	2.6
1	O	48	ALA	2.6
1	O	210	ALA	2.6
1	O	407	ARG	2.6
1	B	158	GLU	2.6
1	A	134	VAL	2.6
1	F	15	VAL	2.6
1	F	177	VAL	2.6
1	P	201	VAL	2.6
1	F	98	ASP	2.6
1	O	10	SER	2.6
1	O	439	SER	2.6
1	P	33	SER	2.6
1	O	223	ARG	2.6
1	G	202	GLU	2.6
1	F	55	GLY	2.6
1	A	111	THR	2.6
1	P	91	THR	2.6
1	O	145	ASP	2.6
1	A	100	VAL	2.6
1	D	316	VAL	2.6
1	H	330	SER	2.6
1	I	292	VAL	2.6
1	M	209	PHE	2.6
1	N	442	PHE	2.6
1	O	179	LEU	2.6
1	O	197	LEU	2.6
1	P	61	GLN	2.6
1	P	485	VAL	2.6
1	L	137	PRO	2.6
1	B	295	ALA	2.6
1	D	319	ALA	2.6
1	G	324	ALA	2.6
1	H	71	ALA	2.6
1	M	449	HIS	2.6
1	C	23	ILE	2.6
1	F	258	ILE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	75	GLY	2.6
1	A	182	CYS	2.6
1	L	326	CYS	2.6
1	N	198	GLN	2.6
1	N	434	THR	2.6
1	G	190	SER	2.6
1	M	130	ASN	2.6
1	N	167	ASN	2.6
1	A	74	LEU	2.6
1	A	150	LEU	2.6
1	P	495	LEU	2.6
1	I	437	VAL	2.6
1	J	328	MET	2.6
1	O	440	VAL	2.6
1	P	219	VAL	2.6
1	D	384	ALA	2.6
1	F	384	ALA	2.6
1	A	239	ILE	2.6
1	F	236	ILE	2.6
1	P	64	ILE	2.6
1	A	132	SER	2.6
1	P	164	THR	2.6
1	A	223	ARG	2.6
1	N	237	CYS	2.6
1	A	115	PHE	2.6
1	E	100	VAL	2.6
1	I	135	VAL	2.6
1	P	109	VAL	2.6
1	N	122	ASP	2.6
1	A	119	GLY	2.6
1	A	220	GLY	2.6
1	D	418	ILE	2.6
1	E	106	THR	2.5
1	N	296	THR	2.5
1	O	1	SER	2.5
1	A	187	PRO	2.5
1	E	259	MET	2.5
1	K	326	CYS	2.5
1	H	409	VAL	2.5
1	N	212	PHE	2.5
1	M	13	ASP	2.5
1	M	35	GLU	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	O	360	TYR	2.5
1	P	486	LYS	2.5
1	C	384	ALA	2.5
1	A	168	SER	2.5
1	B	236	ILE	2.5
1	G	330	SER	2.5
1	M	171	ILE	2.5
1	P	250	SER	2.5
1	I	434	THR	2.5
1	N	62	THR	2.5
1	N	265	LEU	2.5
1	F	328	MET	2.5
1	B	294	CYS	2.5
1	H	104	GLY	2.5
1	H	263	GLY	2.5
1	G	338	TYR	2.5
1	N	130	ASN	2.5
1	B	261	ALA	2.5
1	M	10	SER	2.5
1	O	466	SER	2.5
1	E	433	ILE	2.5
1	L	160	THR	2.5
1	M	122	ASP	2.5
1	N	137	PRO	2.5
1	P	35	GLU	2.5
1	A	446	LYS	2.5
1	L	157	ASP	2.5
1	I	431	LEU	2.5
1	M	131	LEU	2.5
1	P	369	LEU	2.5
1	D	398	VAL	2.5
1	L	292	VAL	2.5
1	M	94	PHE	2.5
1	P	437	VAL	2.5
1	J	25	CYS	2.5
1	J	444	ALA	2.5
1	N	48	ALA	2.5
1	O	217	GLU	2.5
1	P	53	SER	2.5
1	P	341	GLU	2.5
1	M	117	ASP	2.5
1	M	325	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	418	ILE	2.5
1	O	41	ILE	2.5
1	O	96	GLY	2.5
1	L	447	LEU	2.5
1	A	165	VAL	2.5
1	G	219	VAL	2.5
1	N	441	PHE	2.5
1	A	117	ASP	2.5
1	M	445	ASP	2.5
1	K	14	PRO	2.5
1	L	24	ILE	2.5
1	M	479	ILE	2.5
1	N	126	ILE	2.5
1	N	171	ILE	2.5
1	P	239	ILE	2.5
1	M	129	GLN	2.5
1	E	132	SER	2.5
1	K	209	PHE	2.5
1	M	116	ALA	2.5
1	O	356	ALA	2.5
1	G	231	ARG	2.5
1	E	345	TYR	2.5
1	I	14	PRO	2.5
1	J	291	PRO	2.5
1	P	31	THR	2.5
1	P	166	THR	2.5
1	A	483[A]	HIS	2.5
1	L	448	GLY	2.5
1	O	428	CYS	2.5
1	P	86	GLY	2.5
1	P	97	GLY	2.5
1	K	47	VAL	2.4
1	L	477	VAL	2.4
1	O	184	VAL	2.4
1	G	217	GLU	2.4
1	B	434	THR	2.4
1	G	14	PRO	2.4
1	H	296	THR	2.4
1	K	296	THR	2.4
1	O	17	ASN	2.4
1	J	449	HIS	2.4
1	N	236	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	P	126	ILE	2.4
1	A	22	ARG	2.4
1	C	211	SER	2.4
1	G	136	ARG	2.4
1	K	49	ARG	2.4
1	I	259	MET	2.4
1	F	437	VAL	2.4
1	G	444	ALA	2.4
1	H	34	VAL	2.4
1	O	51	ASN	2.4
1	P	167	ASN	2.4
1	E	436	GLY	2.4
1	O	344	GLN	2.4
1	P	62	THR	2.4
1	M	98	ASP	2.4
1	M	112	ASP	2.4
1	I	236	ILE	2.4
1	L	418	ILE	2.4
1	O	484	LYS	2.4
1	G	21	ALA	2.4
1	G	225	ALA	2.4
1	M	216	ALA	2.4
1	H	397	VAL	2.4
1	N	15	VAL	2.4
1	O	42	GLN	2.4
1	O	478	VAL	2.4
1	E	264	ASP	2.4
1	G	103	ARG	2.4
1	O	249	ASP	2.4
1	P	307	ARG	2.4
1	M	128	TYR	2.4
1	N	142	TYR	2.4
1	A	154	SER	2.4
1	A	211	SER	2.4
1	F	10	SER	2.4
1	L	261	ALA	2.4
1	N	4	ALA	2.4
1	A	112	ASP	2.4
1	C	437	VAL	2.4
1	E	183	ASP	2.4
1	L	291	PRO	2.4
1	M	177	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	292	VAL	2.4
1	M	154	SER	2.4
1	A	171	ILE	2.4
1	I	479	ILE	2.4
1	N	128	TYR	2.4
1	B	498	GLU	2.4
1	G	197	LEU	2.4
1	I	446	LYS	2.4
1	M	263	GLY	2.4
1	N	220	GLY	2.4
1	P	224	LYS	2.4
1	L	259	MET	2.4
1	P	328	MET	2.4
1	F	260	VAL	2.4
1	I	316	VAL	2.4
1	C	239	ILE	2.4
1	N	141	ILE	2.4
1	P	469	TYR	2.4
1	H	122	ASP	2.4
1	M	22	ARG	2.4
1	E	138	GLY	2.4
1	E	155	HIS	2.4
1	E	263	GLY	2.4
1	F	447	LEU	2.4
1	A	225	ALA	2.4
1	G	50	MET	2.4
1	O	101	MET	2.4
1	C	296	THR	2.4
1	J	209	PHE	2.4
1	E	178	ASN	2.4
1	G	241	ASN	2.4
1	H	178	ASN	2.4
1	C	444	ALA	2.3
1	A	409	VAL	2.3
1	C	177	VAL	2.3
1	F	22	ARG	2.3
1	P	98	ASP	2.3
1	G	220	GLY	2.3
1	G	149	ILE	2.3
1	I	24	ILE	2.3
1	O	494	ILE	2.3
1	A	329	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	324	ALA	2.3
1	F	410	ALA	2.3
1	H	99	ALA	2.3
1	M	7	LEU	2.3
1	M	74	LEU	2.3
1	C	432	ASN	2.3
1	H	26	THR	2.3
1	J	296	THR	2.3
1	P	493	ARG	2.3
1	D	330	SER	2.3
1	J	46	SER	2.3
1	D	34	VAL	2.3
1	E	477	VAL	2.3
1	P	292	VAL	2.3
1	I	263	GLY	2.3
1	K	176	GLY	2.3
1	A	169	HIS	2.3
1	N	93	GLN	2.3
1	P	258	ILE	2.3
1	F	82	LEU	2.3
1	G	22	ARG	2.3
1	B	328	MET	2.3
1	E	157	ASP	2.3
1	G	183	ASP	2.3
1	G	193	ASP	2.3
1	P	474	ASP	2.3
1	G	156	GLU	2.3
1	D	238	LYS	2.3
1	I	260	VAL	2.3
1	L	152	VAL	2.3
1	M	477	VAL	2.3
1	H	181	GLY	2.3
1	N	452	GLY	2.3
1	N	231	ARG	2.3
1	E	105	ALA	2.3
1	D	259	MET	2.3
1	F	259	MET	2.3
1	G	97	GLY	2.3
1	I	398[A]	VAL	2.3
1	O	22	ARG	2.3
1	C	158	GLU	2.3
1	A	113	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	17	ASN	2.3
1	B	23	ILE	2.3
1	O	410	ALA	2.3
1	O	459	ALA	2.3
1	H	423	THR	2.3
1	D	159	GLN	2.3
1	N	266	GLY	2.3
1	C	22	ARG	2.3
1	L	451	GLU	2.3
1	P	217	GLU	2.3
1	B	209	PHE	2.3
1	O	397	VAL	2.3
1	L	185	ASP	2.3
1	N	173	ASP	2.3
1	J	410	ALA	2.3
1	N	99	ALA	2.3
1	O	269	ILE	2.3
1	D	26	THR	2.2
1	J	431	LEU	2.2
1	D	396	MET	2.2
1	A	337	LYS	2.2
1	A	13	ASP	2.2
1	O	167	ASN	2.2
1	O	482	ASP	2.2
1	I	47	VAL	2.2
1	L	209	PHE	2.2
1	M	260	VAL	2.2
1	C	198	GLN	2.2
1	M	132	SER	2.2
1	A	23	ILE	2.2
1	I	80	ILE	2.2
1	M	162	GLU	2.2
1	J	22	ARG	2.2
1	A	227	GLY	2.2
1	J	434	THR	2.2
1	M	8	THR	2.2
1	E	13	ASP	2.2
1	F	445	ASP	2.2
1	P	139	ASN	2.2
1	N	243	GLN	2.2
1	N	158	GLU	2.2
1	P	342	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	2.2
1	C	224	LYS	2.2
1	F	21	ALA	2.2
1	M	444	ALA	2.2
1	O	453	LYS	2.2
1	P	368	LYS	2.2
1	G	110	THR	2.2
1	M	24	ILE	2.2
1	A	173	ASP	2.2
1	B	265	LEU	2.2
1	C	178	ASN	2.2
1	G	122	ASP	2.2
1	H	101	MET	2.2
1	G	58	GLU	2.2
1	N	253	GLU	2.2
1	N	339	PRO	2.2
1	K	316	VAL	2.2
1	L	294	CYS	2.2
1	M	497	VAL	2.2
1	M	448	GLY	2.2
1	E	145	ASP	2.2
1	G	117	ASP	2.2
1	N	324	ALA	2.2
1	A	178	ASN	2.2
1	M	178	ASN	2.2
1	N	84	THR	2.2
1	N	208	ILE	2.2
1	P	80	ILE	2.2
1	P	233	ILE	2.2
1	D	435	GLN	2.2
1	L	431	LEU	2.2
1	M	431	LEU	2.2
1	N	431	LEU	2.2
1	G	101	MET	2.2
1	G	234	MET	2.2
1	B	137	PRO	2.2
1	B	292	VAL	2.2
1	C	478	VAL	2.2
1	A	325	ASP	2.2
1	F	117	ASP	2.2
1	O	460	GLY	2.2
1	B	381	CYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	163	CYS	2.2
1	B	406	ALA	2.2
1	D	81	ALA	2.2
1	G	69	GLN	2.2
1	I	21	ALA	2.2
1	I	311	ALA	2.2
1	O	235	ILE	2.2
1	F	408	LEU	2.2
1	O	351	LEU	2.2
1	C	14	PRO	2.2
1	L	14	PRO	2.2
1	G	35	GLU	2.2
1	N	221	ASP	2.2
1	H	437	VAL	2.2
1	G	199	PHE	2.2
1	K	51	ASN	2.2
1	M	93	GLN	2.2
1	M	139	ASN	2.2
1	B	324	ALA	2.2
1	G	79	ALA	2.2
1	L	324	ALA	2.2
1	L	434	THR	2.2
1	P	48	ALA	2.2
1	P	214	ARG	2.2
1	F	80	ILE	2.2
1	K	236	ILE	2.2
1	A	240	GLU	2.2
1	E	162	GLU	2.2
1	M	451	GLU	2.2
1	A	185	ASP	2.2
1	L	198	GLN	2.2
1	O	178	ASN	2.1
1	O	467	LYS	2.1
1	A	125	TYR	2.1
1	H	140	TYR	2.1
1	B	398	VAL	2.1
1	H	134	VAL	2.1
1	I	477	VAL	2.1
1	K	327	VAL	2.1
1	M	262	ARG	2.1
1	F	115	PHE	2.1
1	H	444	ALA	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	79	ALA	2.1
1	N	73	GLU	2.1
1	K	23	ILE	2.1
1	F	46	SER	2.1
1	F	192	LYS	2.1
1	M	1	SER	2.1
1	F	230	GLY	2.1
1	A	49	ARG	2.1
1	D	477	VAL	2.1
1	P	254	GLU	2.1
1	A	199	PHE	2.1
1	H	8	THR	2.1
1	I	79	ALA	2.1
1	L	94	PHE	2.1
1	O	71	ALA	2.1
1	F	229	LYS	2.1
1	K	258	ILE	2.1
1	M	42	GLN	2.1
1	P	23	ILE	2.1
1	D	447	LEU	2.1
1	G	432	ASN	2.1
1	I	436	GLY	2.1
1	L	130	ASN	2.1
1	L	136	ARG	2.1
1	B	298	MET	2.1
1	I	328	MET	2.1
1	P	294	CYS	2.1
1	B	296	THR	2.1
1	E	410	ALA	2.1
1	F	189	VAL	2.1
1	F	216	ALA	2.1
1	F	444	ALA	2.1
1	G	34	VAL	2.1
1	H	406	ALA	2.1
1	H	472	THR	2.1
1	K	434	THR	2.1
1	L	84	THR	2.1
1	N	116	ALA	2.1
1	O	177	VAL	2.1
1	K	183	ASP	2.1
1	D	136	ARG	2.1
1	I	103	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	217	GLU	2.1
1	K	328	MET	2.1
1	P	467	LYS	2.1
1	O	69	GLN	2.1
1	O	377	ASP	2.1
1	A	385	VAL	2.1
1	B	316	VAL	2.1
1	D	21	ALA	2.1
1	G	134	VAL	2.1
1	H	135	VAL	2.1
1	K	21	ALA	2.1
1	L	296	THR	2.1
1	E	22	ARG	2.1
1	P	140	TYR	2.1
1	P	231	ARG	2.1
1	N	6	ASN	2.1
1	A	46	SER	2.1
1	E	10	SER	2.1
1	B	293	ILE	2.1
1	H	242	HIS	2.1
1	M	5	HIS	2.1
1	E	246	GLN	2.1
1	F	435	GLN	2.1
1	G	325	ASP	2.1
1	C	451[A]	GLU	2.1
1	E	381	CYS	2.1
1	A	210	ALA	2.1
1	B	20	ALA	2.1
1	E	384	ALA	2.1
1	H	188	ALA	2.1
1	M	106	THR	2.1
1	E	380	VAL	2.1
1	E	385	VAL	2.1
1	H	380	VAL	2.1
1	O	245	VAL	2.1
1	E	104	GLY	2.1
1	G	212	PHE	2.1
1	H	96	GLY	2.1
1	L	154	SER	2.1
1	P	28	GLY	2.1
1	H	431	LEU	2.1
1	M	371	HIS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	13	ASP	2.1
1	O	153	GLN	2.1
1	E	101	MET	2.1
1	O	175	ARG	2.1
1	O	310	ARG	2.1
1	J	84	THR	2.1
1	N	26	THR	2.1
1	E	21	ALA	2.1
1	F	79	ALA	2.1
1	K	79	ALA	2.1
1	A	107	CYS	2.1
1	C	46	SER	2.1
1	D	478	VAL	2.1
1	I	409	VAL	2.1
1	I	420	CYS	2.1
1	L	409	VAL	2.1
1	M	138	GLY	2.1
1	M	320	VAL	2.1
1	M	330	SER	2.1
1	O	250	SER	2.1
1	M	345	TYR	2.1
1	A	58	GLU	2.0
1	F	42	GLN	2.0
1	N	218	GLN	2.0
1	B	183	ASP	2.0
1	D	325	ASP	2.0
1	M	136	ARG	2.0
1	O	40	LEU	2.0
1	F	432	ASN	2.0
1	A	296	THR	2.0
1	C	492	THR	2.0
1	A	55	GLY	2.0
1	A	410	ALA	2.0
1	G	448	GLY	2.0
1	H	261	ALA	2.0
1	K	48	ALA	2.0
1	M	16	ALA	2.0
1	N	81	ALA	2.0
1	P	334	ALA	2.0
1	P	406	ALA	2.0
1	G	151	GLN	2.0
1	A	221	ASP	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	478	VAL	2.0
1	H	185	ASP	2.0
1	J	445	ASP	2.0
1	L	419	VAL	2.0
1	P	47	VAL	2.0
1	D	381	CYS	2.0
1	F	242	HIS	2.0
1	H	133	LYS	2.0
1	P	121	LYS	2.0
1	P	335	LYS	2.0
1	A	89	ILE	2.0
1	E	24	ILE	2.0
1	E	236	ILE	2.0
1	A	139	ASN	2.0
1	O	298	MET	2.0
1	F	35	GLU	2.0
1	H	217	GLU	2.0
1	A	79	ALA	2.0
1	A	435	GLN	2.0
1	M	84	THR	2.0
1	M	151	GLN	2.0
1	O	84	THR	2.0
1	G	458	ALA	2.0
1	O	116	ALA	2.0
1	P	151	GLN	2.0
1	P	261	ALA	2.0
1	K	185	ASP	2.0
1	P	221	ASP	2.0
1	A	189	VAL	2.0
1	C	409	VAL	2.0
1	K	238	LYS	2.0
1	L	135	VAL	2.0
1	O	199	PHE	2.0
1	M	125	TYR	2.0
1	P	420	CYS	2.0
1	C	479	ILE	2.0
1	O	233	ILE	2.0
1	H	328	MET	2.0
1	J	207	MET	2.0
1	L	436	GLY	2.0
1	O	473	GLY	2.0
1	P	203	GLN	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	136	ARG	2.0
1	G	145	ASP	2.0
1	H	63	THR	2.0
1	L	445	ASP	2.0
1	N	33	SER	2.0
1	O	166	THR	2.0
1	H	216	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	O	500	1/1	0.66	0.30	122,122,122,122	0
7	GOL	J	499	6/6	0.66	0.37	69,71,71,72	0
3	K	A	504	1/1	0.68	0.28	106,106,106,106	0
3	K	G	501	1/1	0.71	0.37	137,137,137,137	0
3	K	N	499	1/1	0.71	0.27	107,107,107,107	0
3	K	P	504	1/1	0.79	0.19	98,98,98,98	0
3	K	M	499	1/1	0.79	0.15	106,106,106,106	0
3	K	P	499	1/1	0.80	0.22	119,119,119,119	0
7	GOL	I	499	6/6	0.82	0.44	91,91,91,92	0
4	OXL	P	510	6/6	0.83	0.19	85,85,85,86	0
3	K	G	504	1/1	0.84	0.16	82,82,82,82	0
7	GOL	O	499	6/6	0.84	0.41	74,75,75,75	0
7	GOL	I	501	6/6	0.85	0.47	85,85,85,85	0
6	ATP	P	1001	31/31	0.86	0.20	132,134,134,134	0
2	MG	P	500	1/1	0.86	0.39	94,94,94,94	0
7	GOL	G	499	6/6	0.88	0.16	97,97,97,97	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	F	502	1/1	0.88	0.10	60,60,60,60	0
2	MG	P	502	1/1	0.89	0.07	64,64,64,64	0
5	FDP	P	700	20/20	0.89	0.15	110,115,119,119	0
3	K	F	499	1/1	0.89	0.09	85,85,85,85	0
2	MG	N	500	1/1	0.89	0.43	88,88,88,88	0
6	ATP	G	1001	31/31	0.90	0.18	77,97,101,101	0
3	K	N	504	1/1	0.90	0.20	84,84,84,84	0
4	OXL	M	510	6/6	0.90	0.16	64,66,67,67	0
4	OXL	N	510	6/6	0.90	0.15	77,79,80,80	0
2	MG	I	502	1/1	0.91	0.12	30,30,30,30	0
2	MG	N	502	1/1	0.91	0.20	76,76,76,76	0
4	OXL	A	510	6/6	0.91	0.14	63,65,66,66	0
4	OXL	F	510	6/6	0.91	0.26	83,83,83,83	0
2	MG	I	500	1/1	0.91	0.12	36,36,36,36	0
4	OXL	G	510	6/6	0.91	0.15	71,74,75,75	0
7	GOL	E	499	6/6	0.91	0.16	78,79,80,80	0
5	FDP	O	700	20/20	0.92	0.13	118,119,121,121	0
6	ATP	N	1001	31/31	0.92	0.12	83,94,95,95	0
2	MG	E	500	1/1	0.93	0.08	55,55,55,55	0
2	MG	H	500	1/1	0.93	0.14	63,63,63,63	0
3	K	C	504	1/1	0.94	0.13	56,56,56,56	0
6	ATP	A	1001	31/31	0.94	0.15	70,85,87,87	0
6	ATP	H	1001	31/31	0.94	0.12	62,69,72,72	0
3	K	F	504	1/1	0.94	0.07	69,69,69,69	0
6	ATP	M	1001	31/31	0.95	0.10	66,73,76,76	0
6	ATP	C	1001	31/31	0.95	0.11	43,52,54,54	0
2	MG	G	500	1/1	0.95	0.36	81,81,81,81	0
4	OXL	H	510	6/6	0.95	0.10	54,54,55,55	0
2	MG	L	500	1/1	0.95	0.07	46,46,46,46	0
6	ATP	F	1001	31/31	0.95	0.12	64,73,76,76	0
3	K	E	501	1/1	0.95	0.10	75,75,75,75	0
3	K	C	499	1/1	0.95	0.08	68,68,68,68	0
5	FDP	A	700	20/20	0.96	0.11	53,58,61,64	0
6	ATP	E	1001	31/31	0.96	0.10	52,58,63,63	0
2	MG	E	502	1/1	0.96	0.13	48,48,48,48	0
3	K	H	499	1/1	0.96	0.06	76,76,76,76	0
2	MG	M	500	1/1	0.96	0.14	69,69,69,69	0
3	K	O	501	1/1	0.96	0.42	30,30,30,30	0
2	MG	M	502	1/1	0.96	0.14	60,60,60,60	0
2	MG	H	502	1/1	0.96	0.31	61,61,61,61	0
6	ATP	L	1001	31/31	0.96	0.11	44,55,59,59	0
3	K	L	504	1/1	0.96	0.06	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

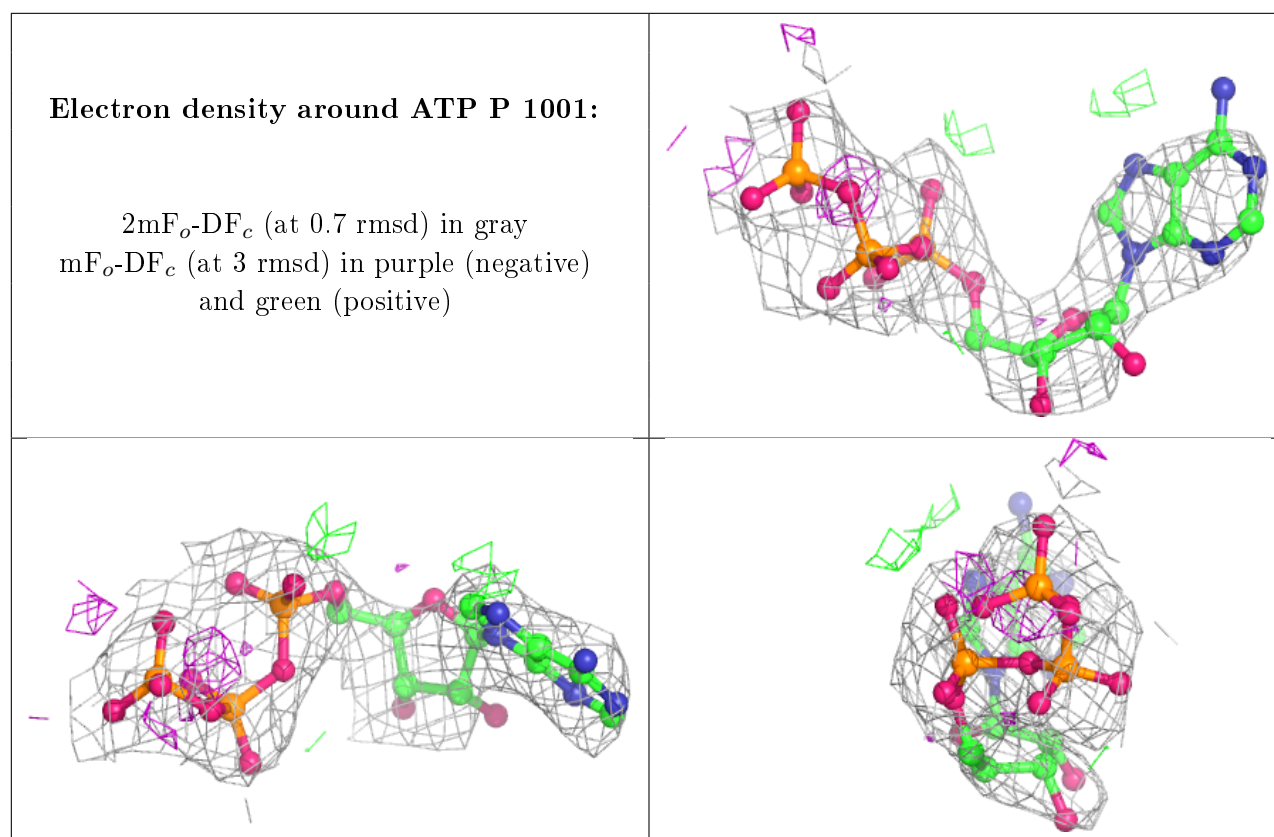
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	OXL	C	510	6/6	0.96	0.17	39,40,41,41	0
2	MG	J	502	1/1	0.97	0.07	26,26,26,26	0
6	ATP	I	1001	31/31	0.97	0.10	36,37,39,40	0
5	FDP	N	700	20/20	0.97	0.12	76,78,81,82	0
3	K	B	499	1/1	0.97	0.04	60,60,60,60	0
2	MG	G	502	1/1	0.97	0.20	66,66,66,66	0
4	OXL	L	510	6/6	0.97	0.10	37,38,38,39	0
3	K	H	504	1/1	0.97	0.07	59,59,59,59	0
2	MG	A	502	1/1	0.97	0.15	58,58,58,58	0
2	MG	C	500	1/1	0.97	0.18	45,45,45,45	0
2	MG	B	502	1/1	0.97	0.10	28,28,28,28	0
2	MG	C	502	1/1	0.97	0.14	38,38,38,38	0
5	FDP	G	700	20/20	0.97	0.09	69,74,75,75	0
2	MG	D	500	1/1	0.97	0.10	37,37,37,37	0
3	K	D	499	1/1	0.98	0.07	53,53,53,53	0
6	ATP	J	1001	31/31	0.98	0.11	26,34,36,36	0
5	FDP	H	700	20/20	0.98	0.10	54,57,59,60	0
5	FDP	C	700	20/20	0.98	0.09	36,45,48,50	0
5	FDP	F	700	20/20	0.98	0.07	48,53,55,56	0
5	FDP	L	700	20/20	0.98	0.08	37,41,43,43	0
3	K	M	504	1/1	0.98	0.04	61,61,61,61	0
2	MG	D	502	1/1	0.98	0.11	34,34,34,34	0
6	ATP	B	1001	31/31	0.98	0.10	31,35,39,40	0
5	FDP	D	700	20/20	0.98	0.07	32,40,43,45	0
6	ATP	D	1001	31/31	0.98	0.10	35,42,44,44	0
4	OXL	K	510	6/6	0.98	0.12	25,27,28,28	0
6	ATP	K	1001	31/31	0.98	0.14	28,31,37,38	0
2	MG	K	502	1/1	0.98	0.10	28,28,28,28	0
2	MG	K	500	1/1	0.98	0.11	29,29,29,29	0
2	MG	F	500	1/1	0.98	0.24	67,67,67,67	0
5	FDP	B	700	20/20	0.98	0.08	37,40,45,46	0
5	FDP	M	700	20/20	0.98	0.07	55,59,62,64	0
5	FDP	K	700	20/20	0.98	0.07	36,38,42,43	0
2	MG	A	500	1/1	0.98	0.19	77,77,77,77	0
4	OXL	E	510	6/6	0.98	0.15	48,49,49,50	0
3	K	A	499	1/1	0.98	0.12	60,60,60,60	0
3	K	K	499	1/1	0.98	0.13	52,52,52,52	0
2	MG	L	502	1/1	0.98	0.12	37,37,37,37	0
4	OXL	I	510	6/6	0.99	0.14	32,33,34,35	0
3	K	I	504	1/1	0.99	0.05	36,36,36,36	0
3	K	B	504	1/1	0.99	0.05	38,38,38,38	0
4	OXL	J	510	6/6	0.99	0.11	30,31,32,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	FDP	E	700	20/20	0.99	0.07	38,41,46,47	0
5	FDP	J	700	20/20	0.99	0.05	25,32,34,35	0
3	K	D	504	1/1	0.99	0.08	33,33,33,33	0
3	K	E	504	1/1	0.99	0.07	48,48,48,48	0
3	K	J	501	1/1	0.99	0.09	50,50,50,50	0
4	OXL	B	510	6/6	0.99	0.06	30,32,33,33	0
2	MG	J	500	1/1	0.99	0.12	27,27,27,27	0
4	OXL	D	510	6/6	0.99	0.10	37,38,39,39	0
3	K	I	503	1/1	0.99	0.12	47,47,47,47	0
3	K	L	499	1/1	0.99	0.04	47,47,47,47	0
5	FDP	I	700	20/20	0.99	0.07	29,32,34,35	0
3	K	J	504	1/1	0.99	0.07	35,35,35,35	0
2	MG	B	500	1/1	0.99	0.08	35,35,35,35	0
3	K	K	504	1/1	1.00	0.10	29,29,29,29	0

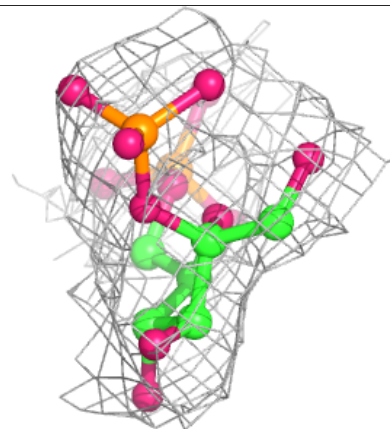
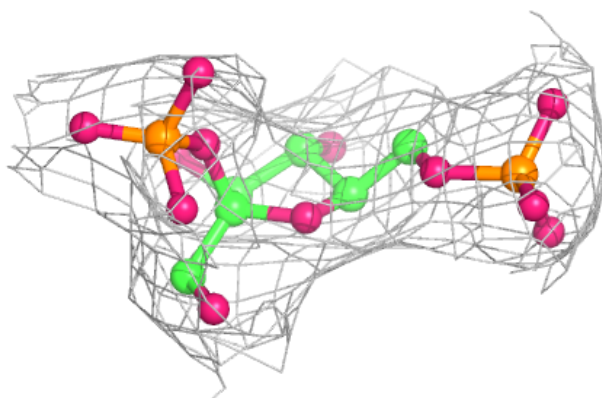
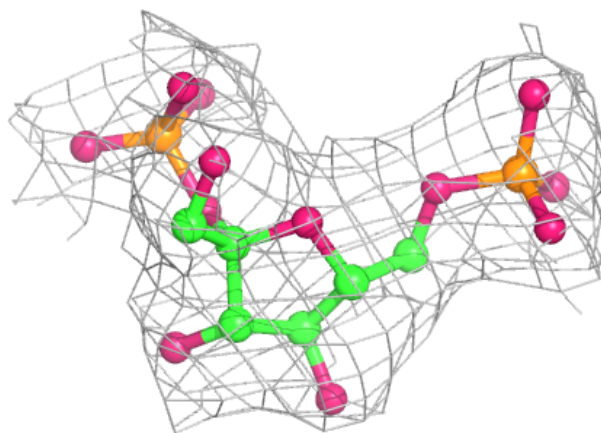
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



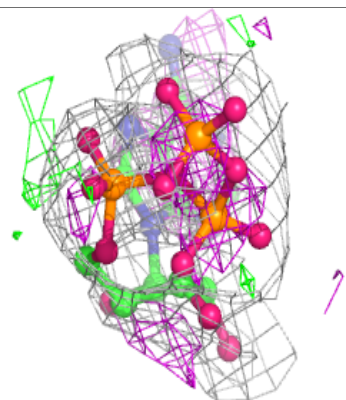
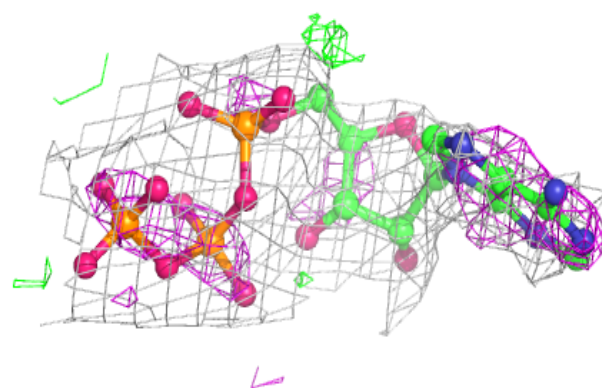
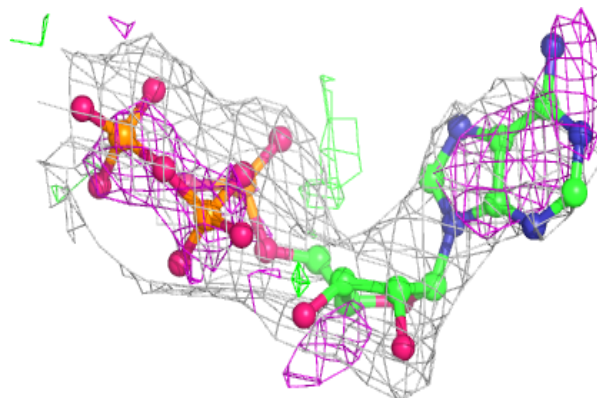


**Electron density around FDP P 700:**

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

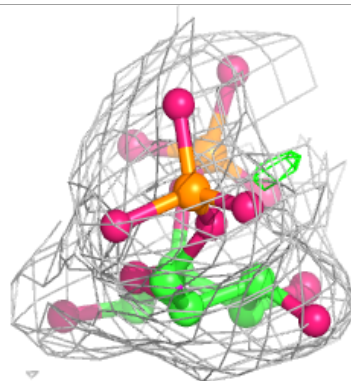
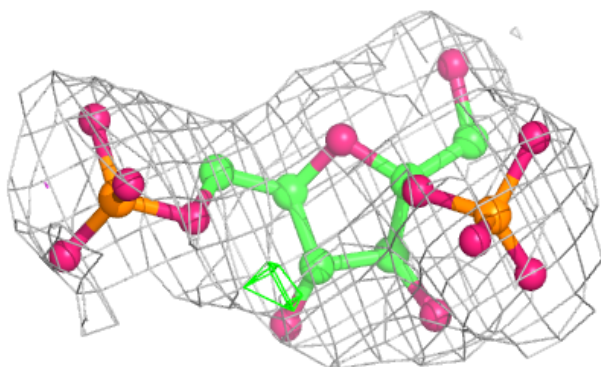
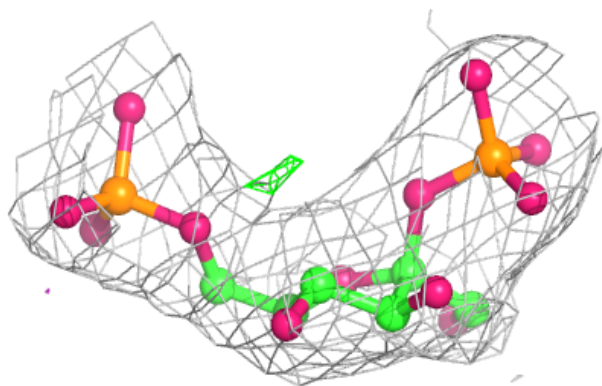
**Electron density around ATP G 1001:**

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

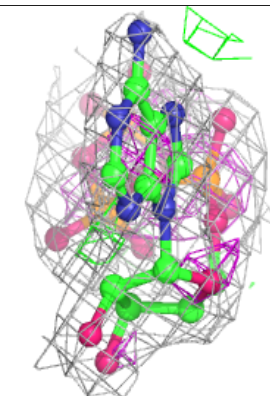
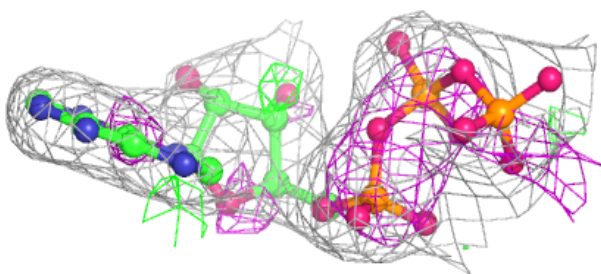
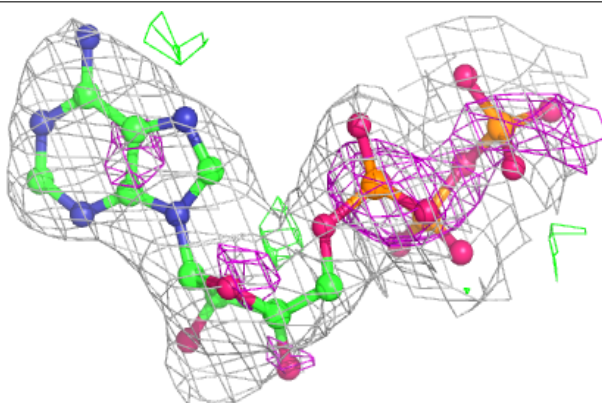


**Electron density around FDP O 700:**

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

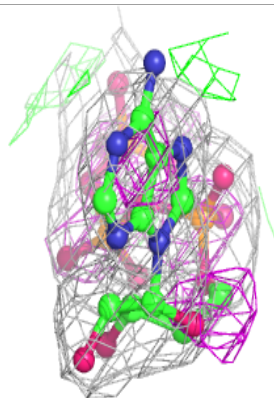
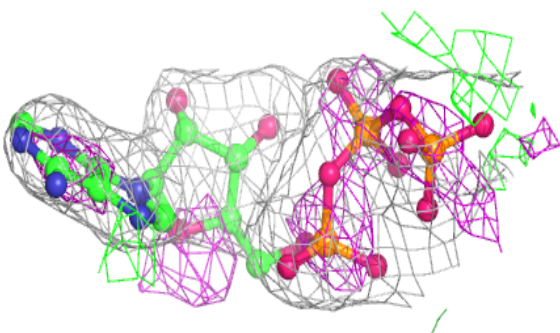
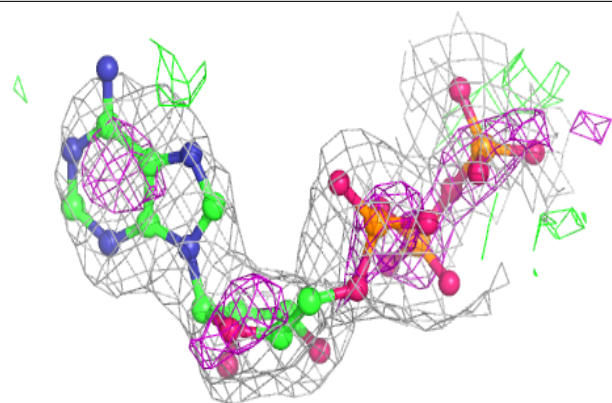
**Electron density around ATP N 1001:**

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

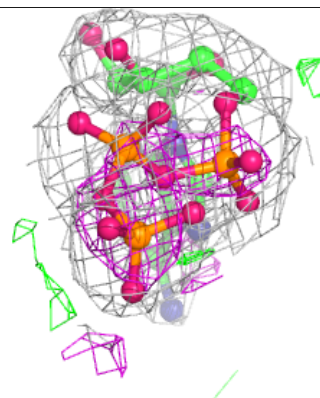
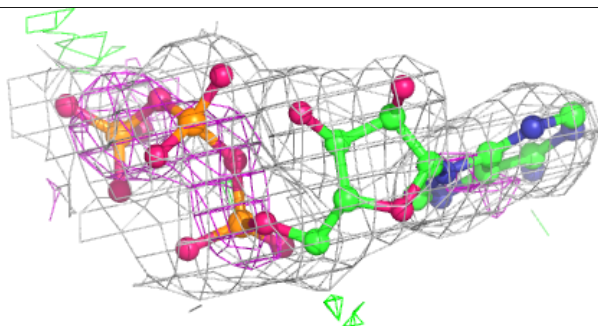
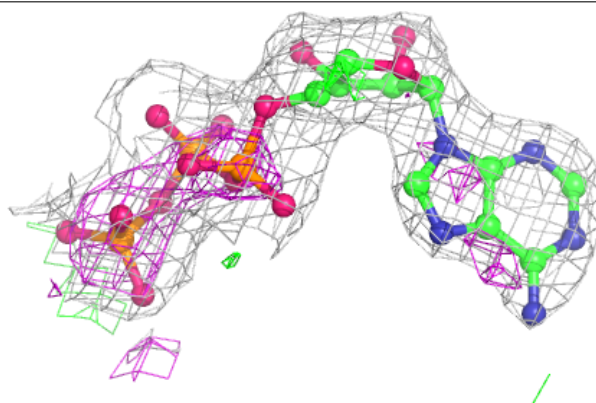


**Electron density around ATP A 1001:**

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

**Electron density around ATP H 1001:**

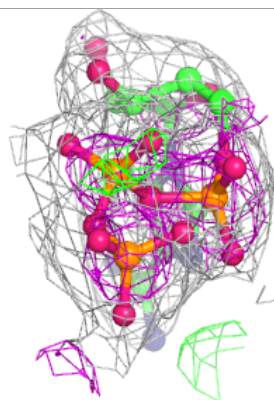
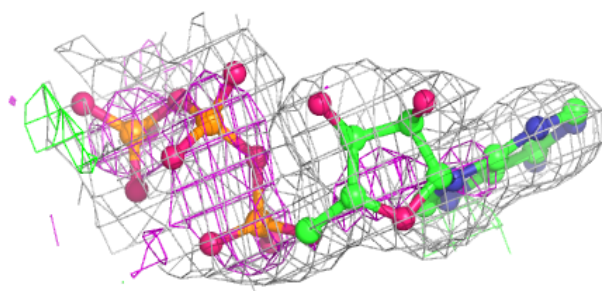
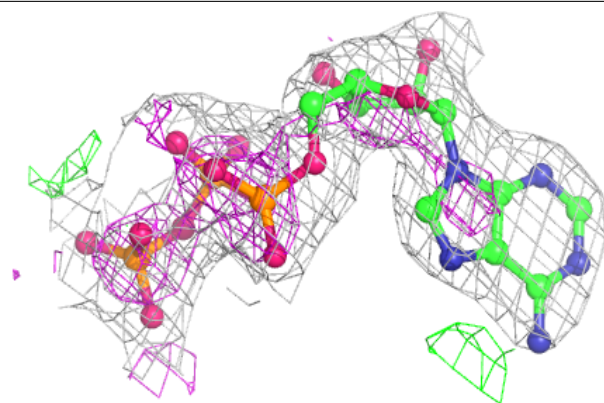
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



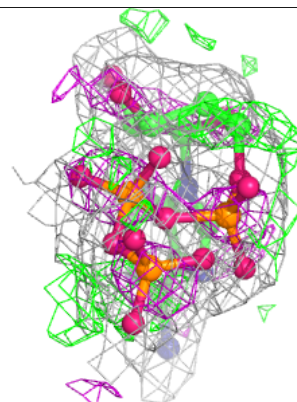
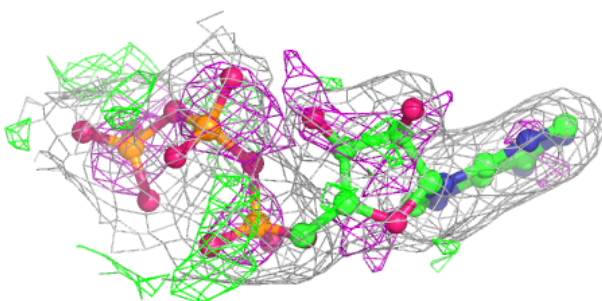
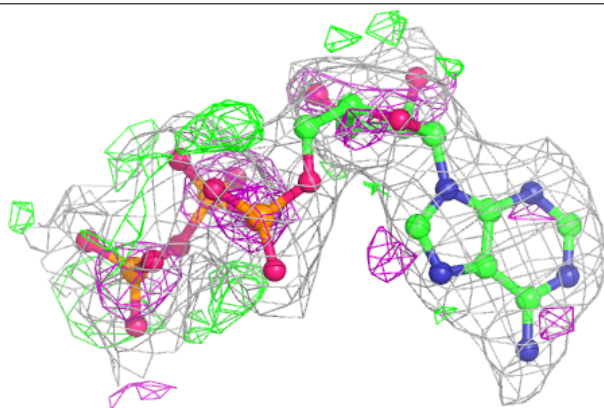


**Electron density around ATP M 1001:**

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

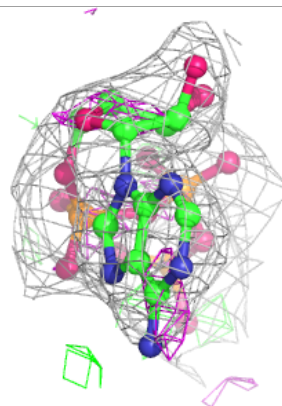
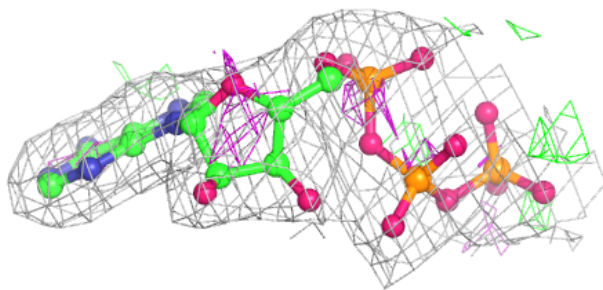
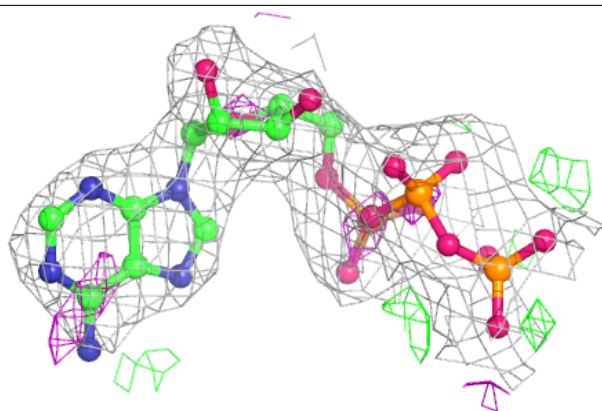
**Electron density around ATP C 1001:**

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

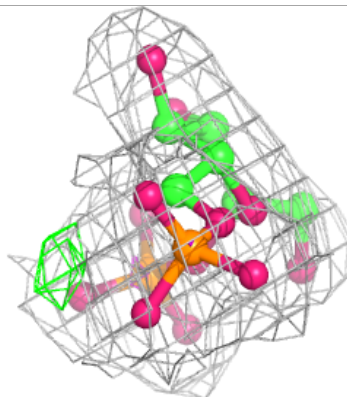
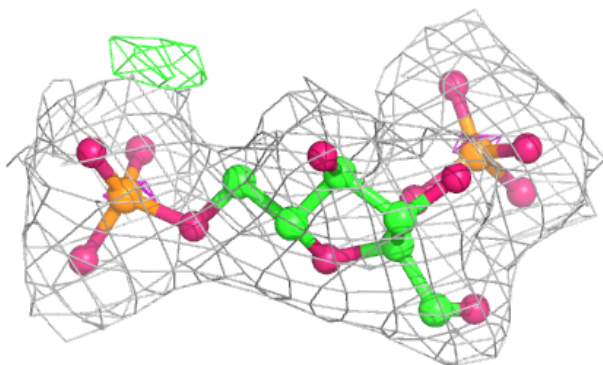
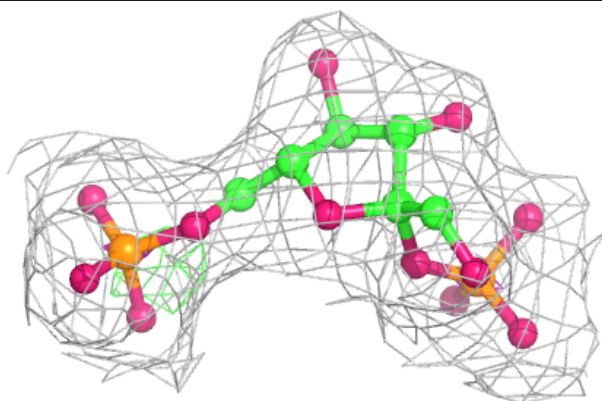


**Electron density around ATP F 1001:**

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

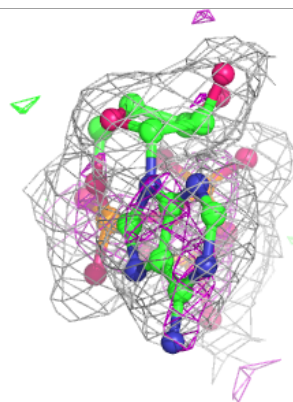
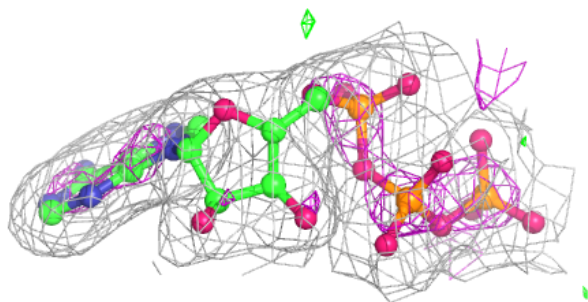
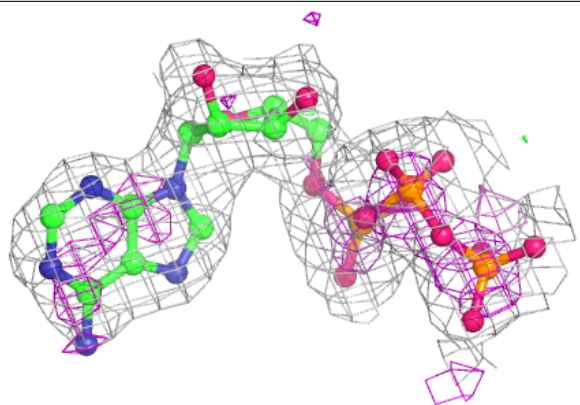
**Electron density around FDP A 700:**

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

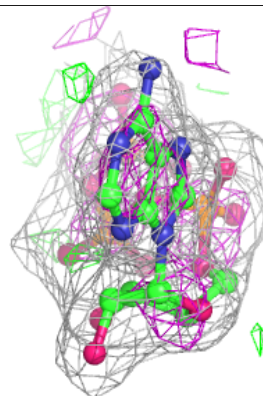
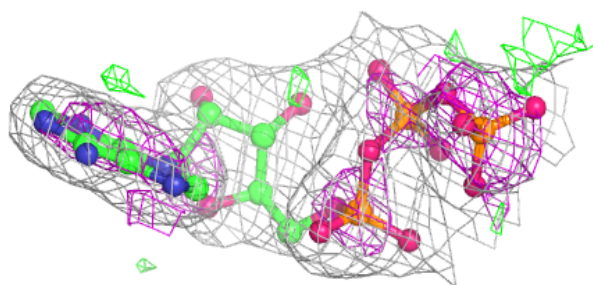
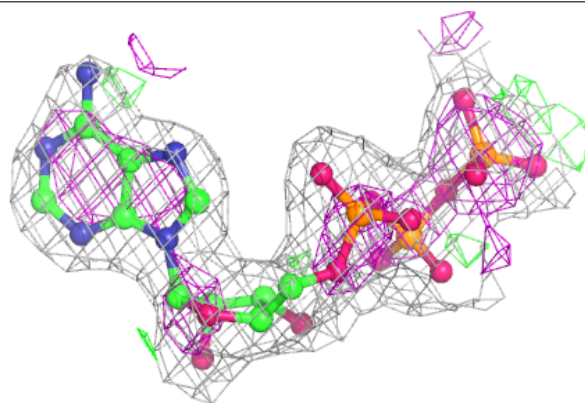


**Electron density around ATP E 1001:**

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

**Electron density around ATP L 1001:**

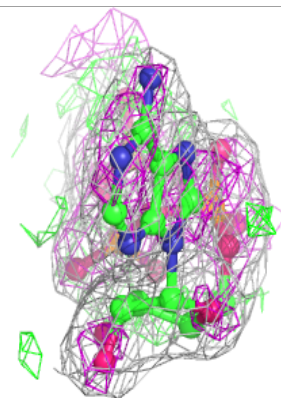
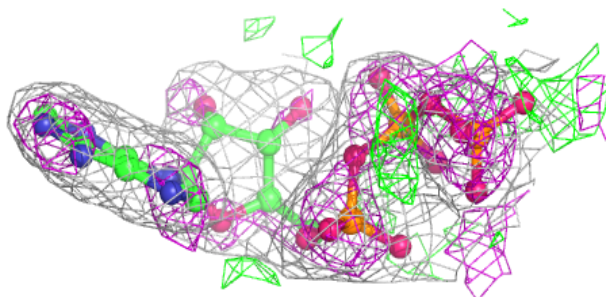
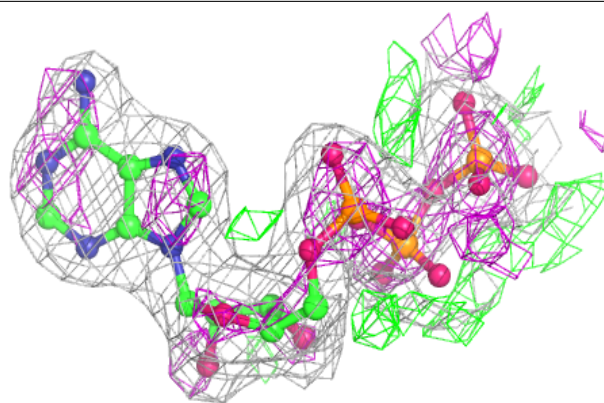
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



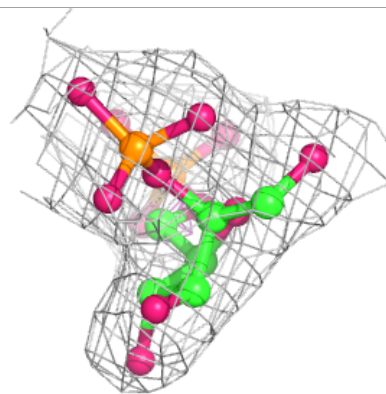
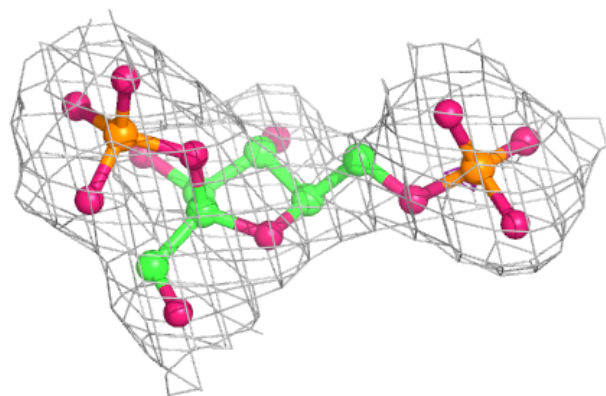
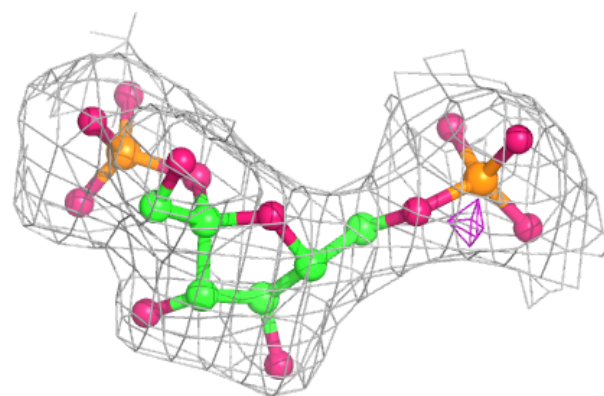


**Electron density around ATP I 1001:**

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

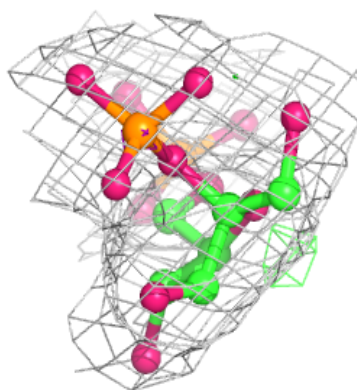
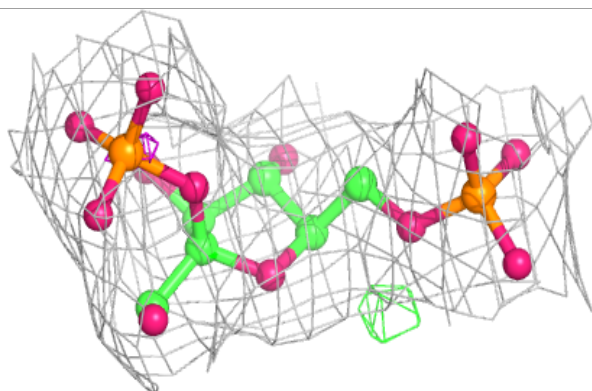
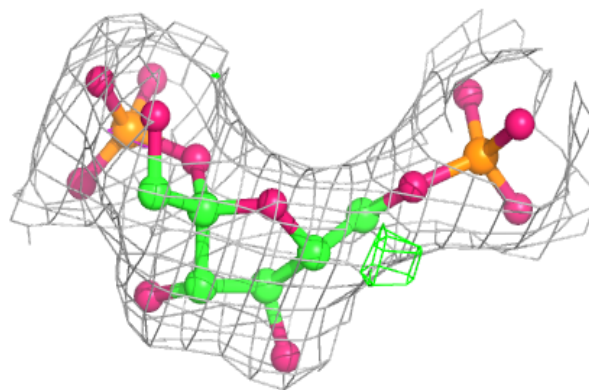
**Electron density around FDP N 700:**

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

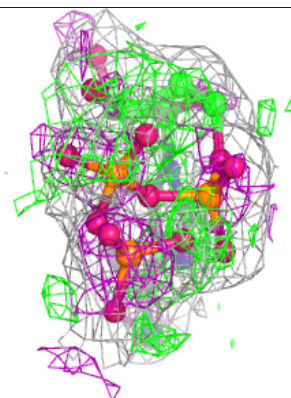
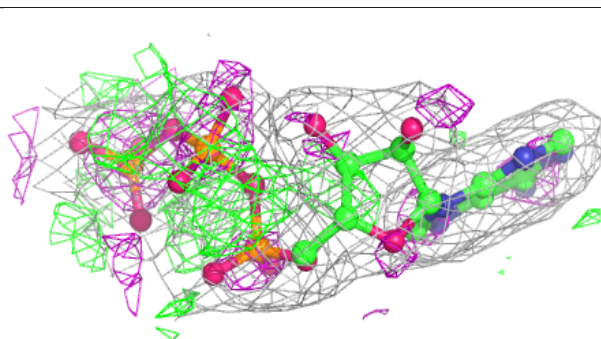
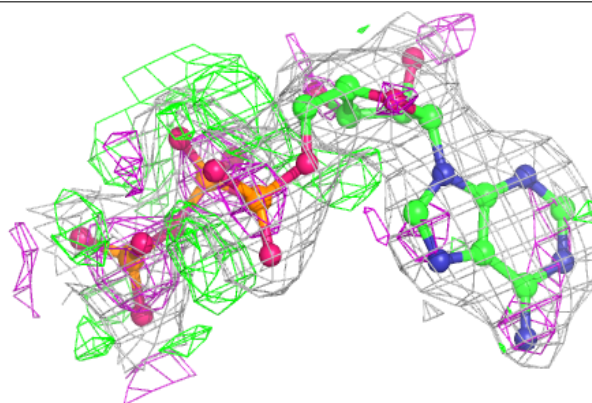


**Electron density around FDP G 700:**

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

**Electron density around ATP J 1001:**

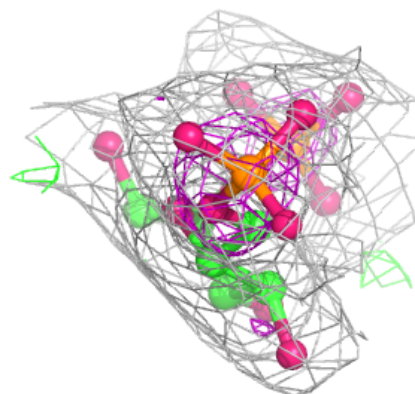
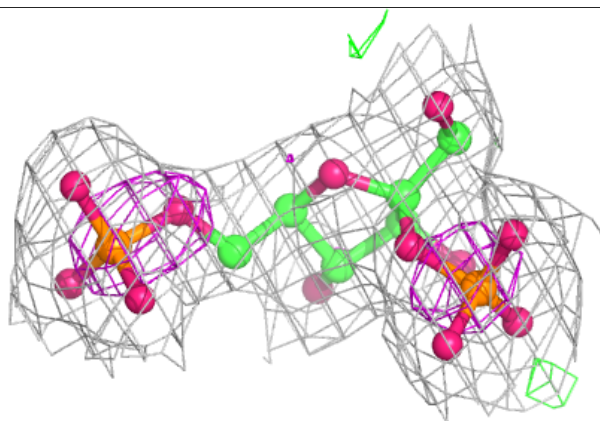
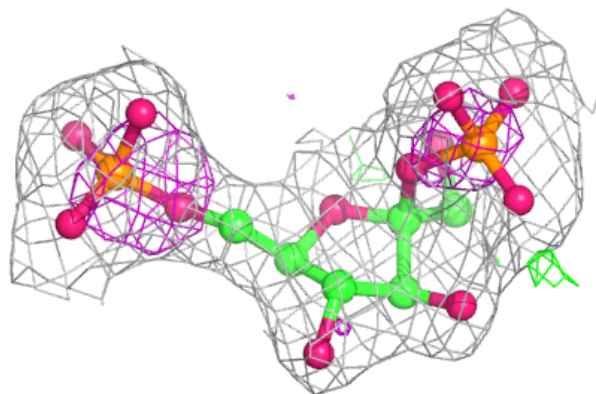
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



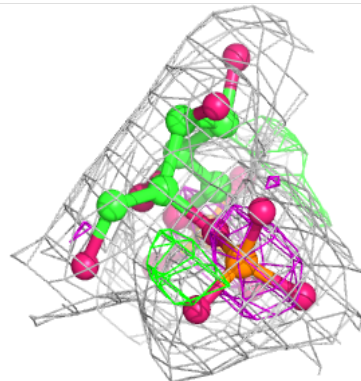
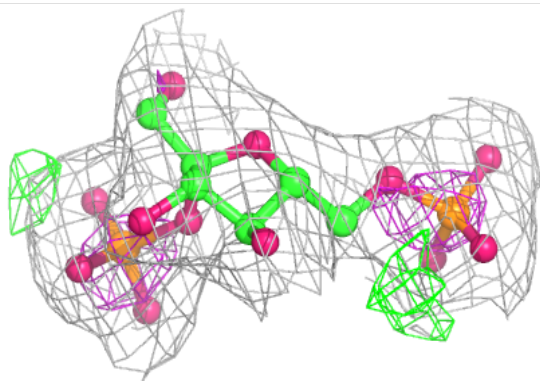
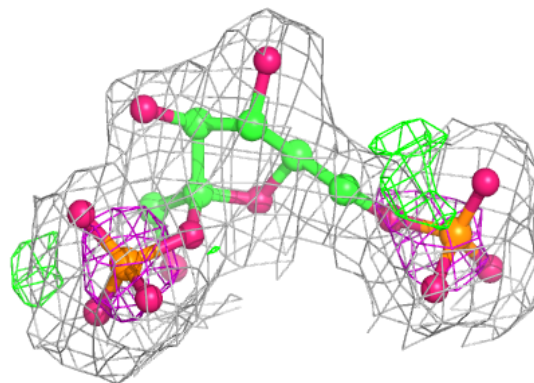


**Electron density around FDP H 700:**

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

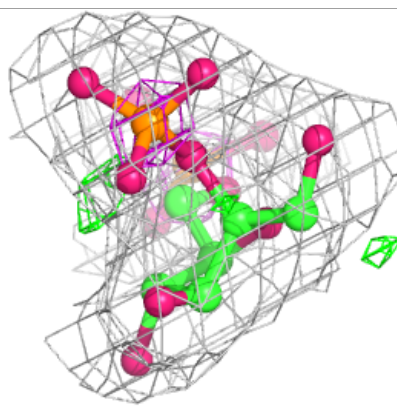
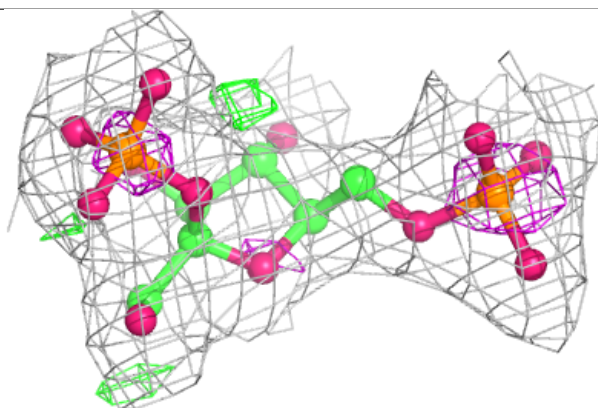
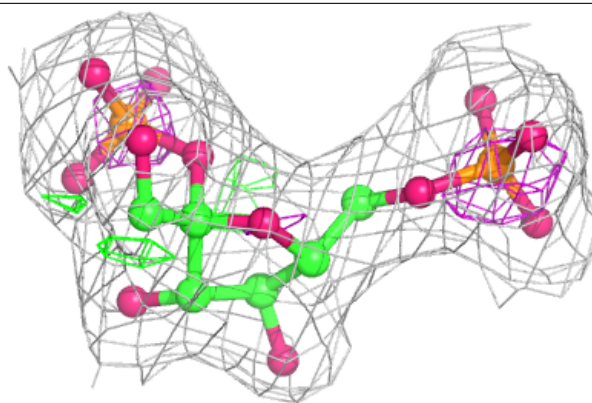
**Electron density around FDP C 700:**

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

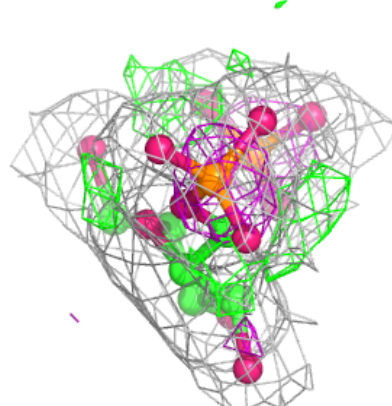
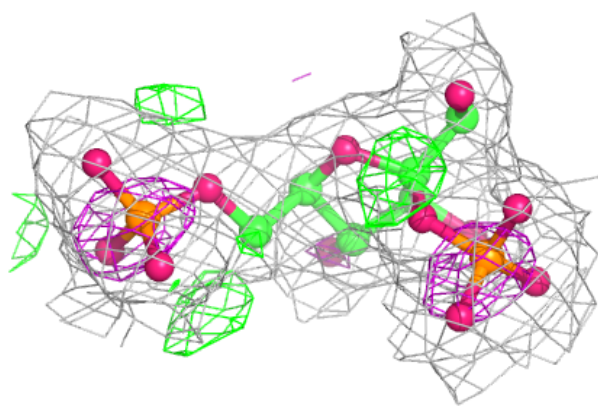
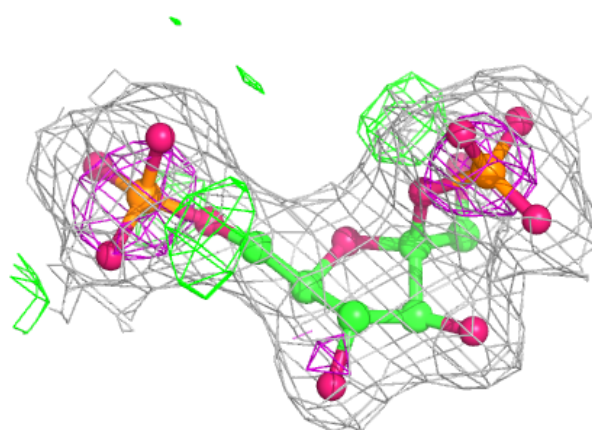


**Electron density around FDP F 700:**

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

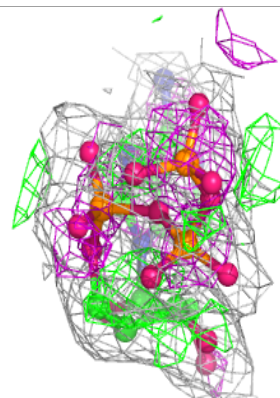
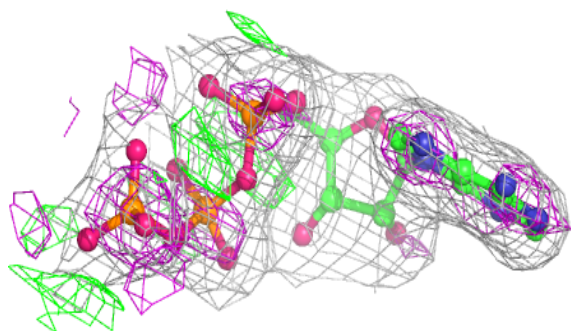
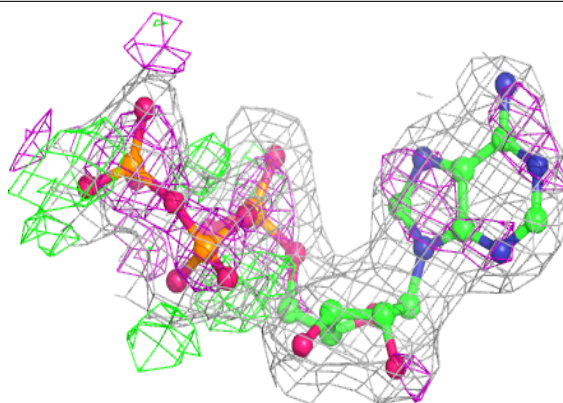
**Electron density around FDP L 700:**

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

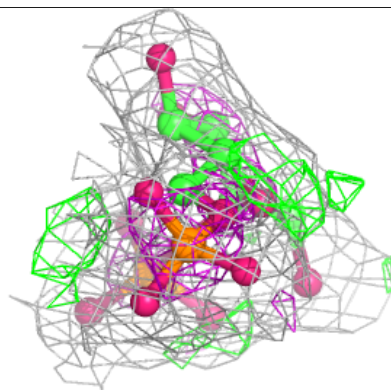
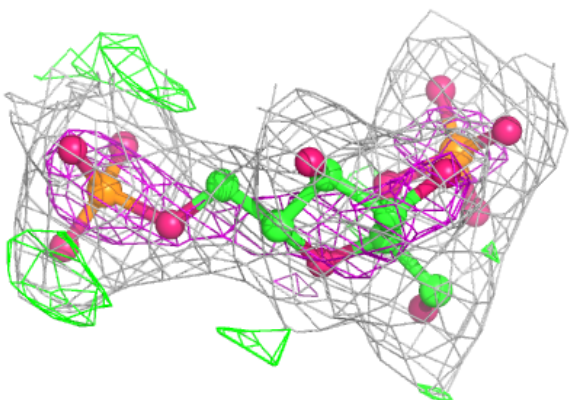
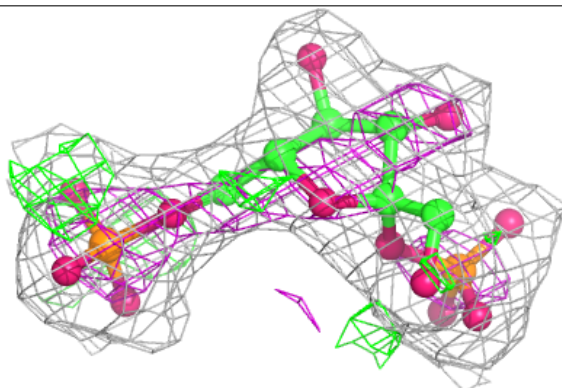


**Electron density around ATP B 1001:**

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

**Electron density around FDP D 700:**

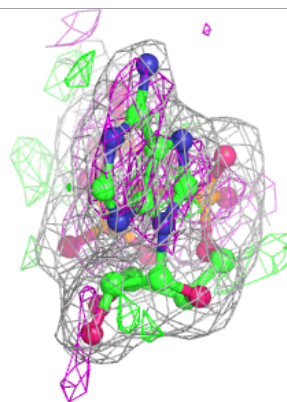
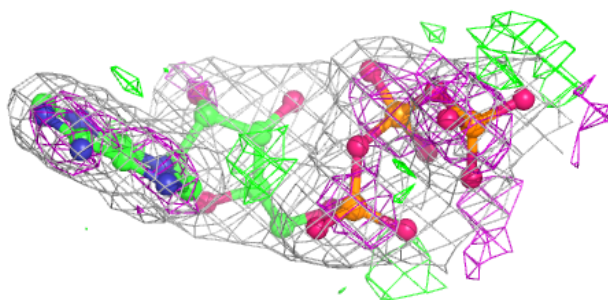
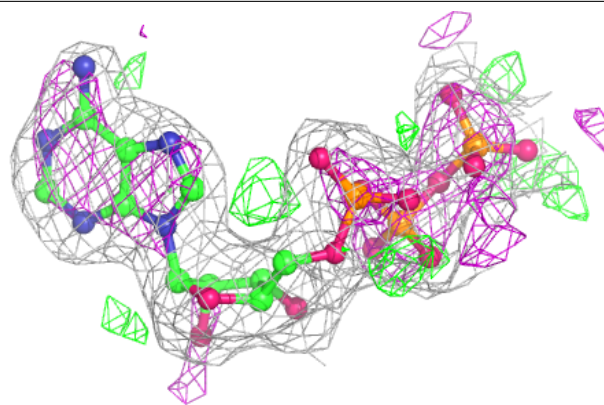
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



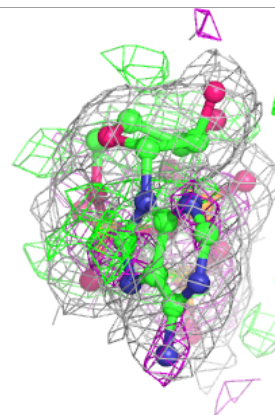
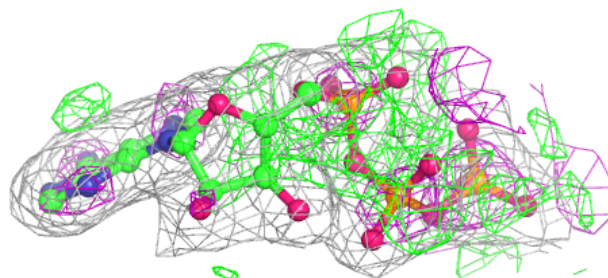
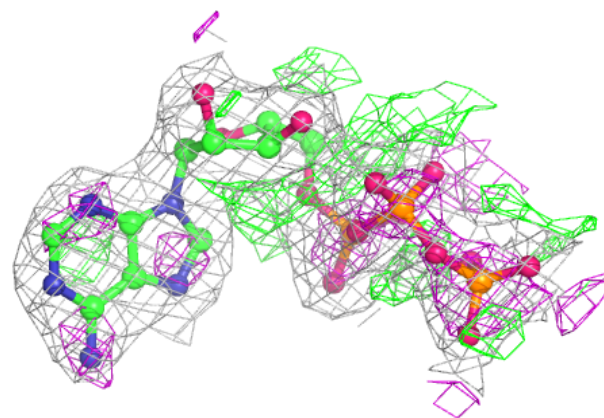


**Electron density around ATP D 1001:**

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

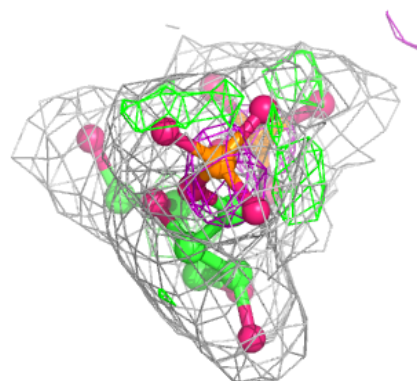
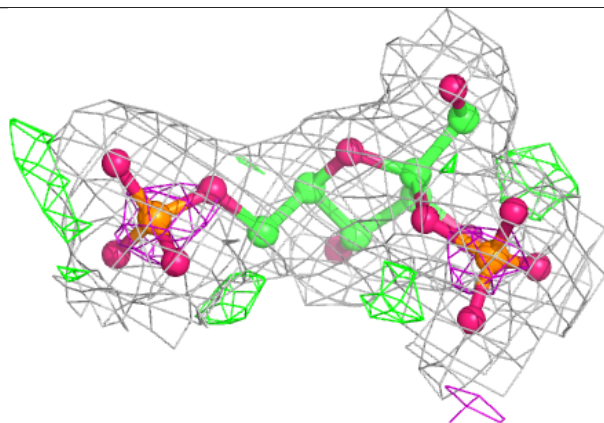
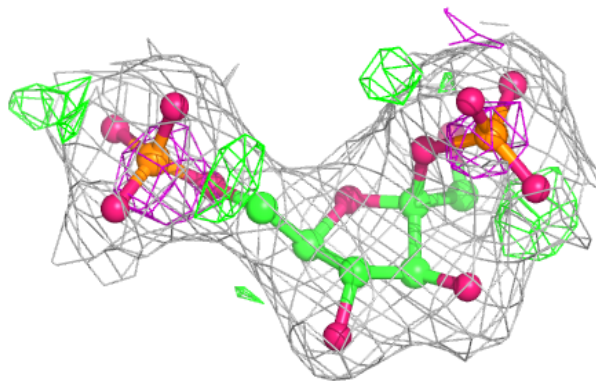
**Electron density around ATP K 1001:**

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

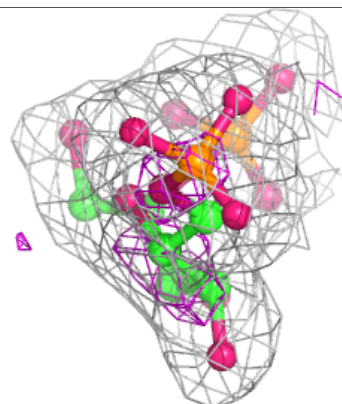
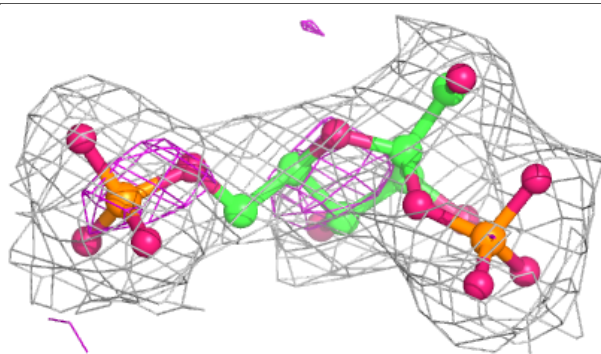
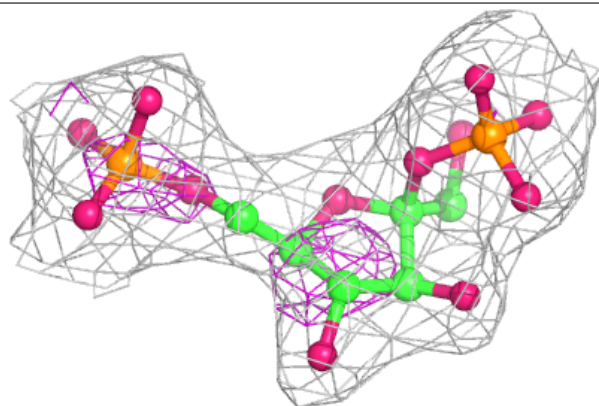


**Electron density around FDP B 700:**

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

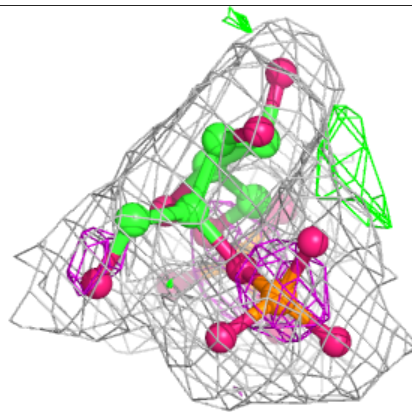
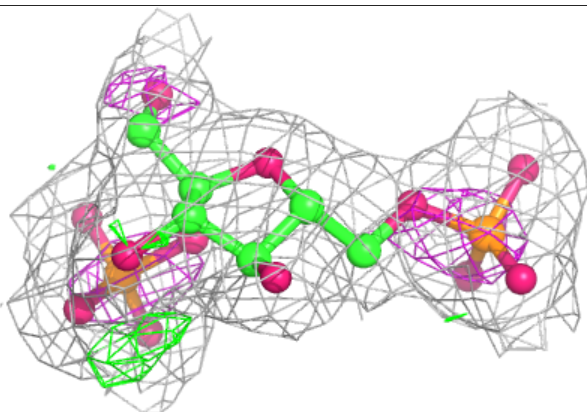
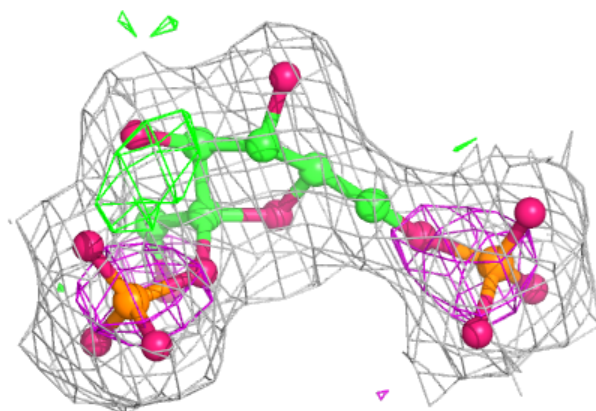
**Electron density around FDP M 700:**

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

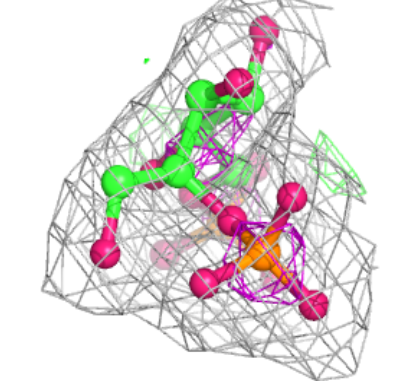
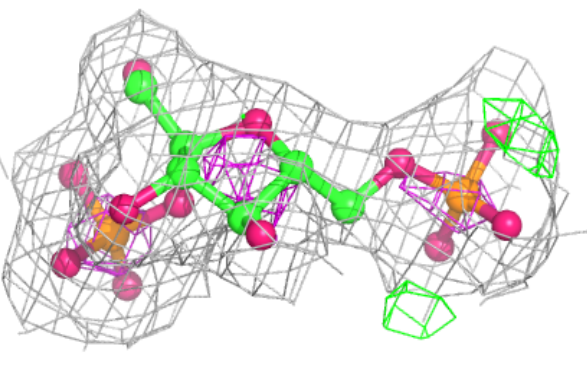
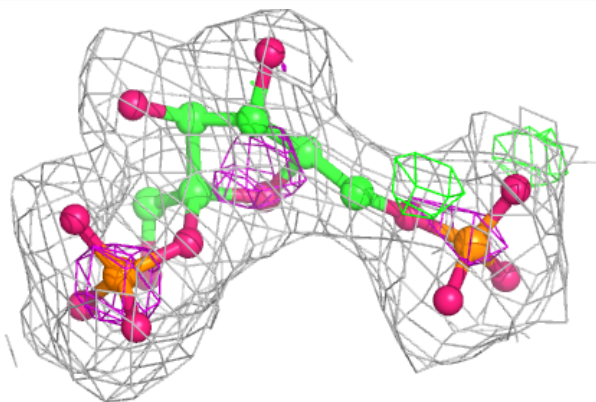


**Electron density around FDP K 700:**

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

**Electron density around FDP E 700:**

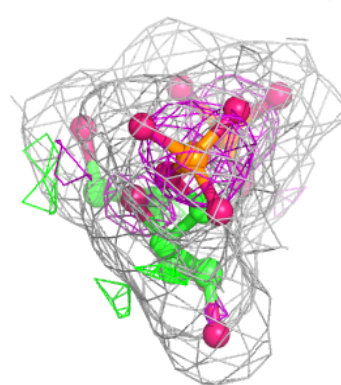
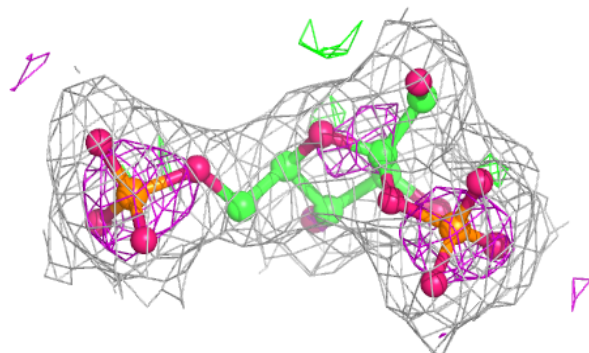
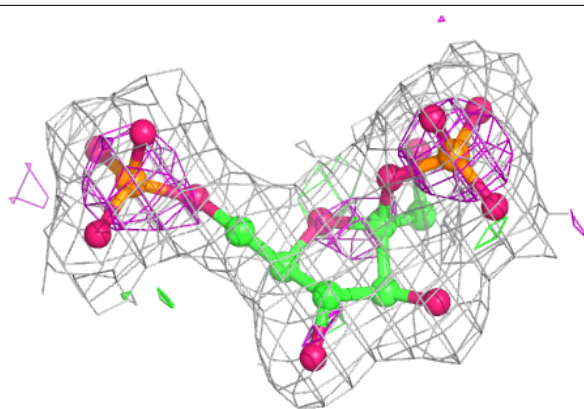
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



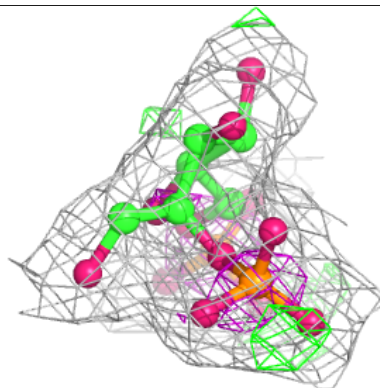
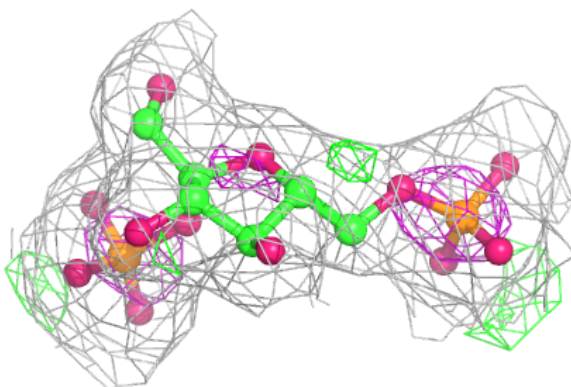
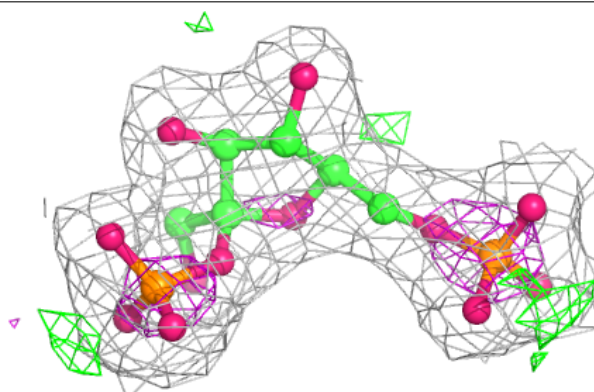


**Electron density around FDP J 700:**

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

**Electron density around FDP I 700:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.