



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:34 pm BST

PDB ID : 5MCP  
Title : Structure of IMP dehydrogenase from *Ashbya gossypii* bound to ATP  
Authors : Winter, G.; Fernandez-Justel, D.; de Pereda, J.M.; Revuelta, J.L.; Buey, R.M.  
Deposited on : 2016-11-10  
Resolution : 2.40 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

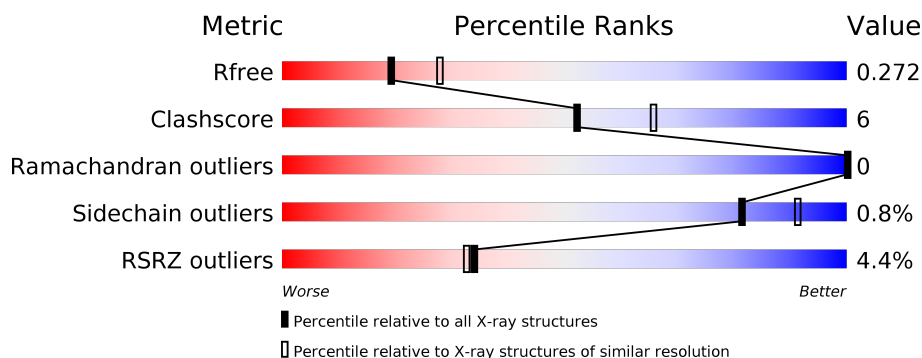
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 77%, yellow 77%, yellow 84%, grey 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>7%</span> <span>16%</span> </div> </div>
1	B	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 76%, yellow 76%, yellow 84%, grey 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>76%</span> <span>8%</span> <span>15%</span> </div> </div>
1	C	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 0%, green 79%, yellow 79%, yellow 85%, grey 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>79%</span> <span>6%</span> <span>15%</span> </div> </div>
1	D	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 76%, yellow 76%, yellow 85%, grey 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>76%</span> <span>9%</span> <span>15%</span> </div> </div>
1	E	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 66%, yellow 66%, yellow 74%, grey 74%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>66%</span> <span>8%</span> <span>26%</span> </div> </div>
1	F	523	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, orange 5%, orange 59%, yellow 59%, yellow 65%, grey 65%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>59%</span> <span>6%</span> <span>35%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	523	<div><div></div><div>7%</div><div>64%</div><div>9%</div><div>27%</div></div>
1	H	523	<div><div></div><div>8%</div><div>57%</div><div>5%</div><div>39%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45606 atoms, of which 21090 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	H	N	O	S	0	0	0
			6568	2057	3293	563	632	23			
1	B	444	Total	C	H	N	O	S	0	0	0
			6442	2039	3187	564	631	21			
1	C	446	Total	C	H	N	O	S	0	1	0
			6556	2068	3260	567	637	24			
1	D	443	Total	C	H	N	O	S	0	1	0
			6541	2060	3267	566	625	23			
1	E	387	Total	C	H	N	O	S	0	0	0
			5039	1659	2384	464	517	15			
1	F	342	Total	C	H	N	O	S	0	1	0
			4054	1379	1832	407	423	13			
1	G	382	Total	C	H	N	O	S	0	0	0
			4580	1561	2066	455	484	14			
1	H	321	Total	C	H	N	O	S	0	0	0
			3526	1225	1529	374	387	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q756Z6
B	0	HIS	-	expression tag	UNP Q756Z6
C	0	HIS	-	expression tag	UNP Q756Z6
D	0	HIS	-	expression tag	UNP Q756Z6
E	0	HIS	-	expression tag	UNP Q756Z6
F	0	HIS	-	expression tag	UNP Q756Z6
G	0	HIS	-	expression tag	UNP Q756Z6
H	0	HIS	-	expression tag	UNP Q756Z6

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	E	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	E	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0
2	F	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0
2	G	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	G	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	G	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0
2	H	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	H	1	Total	C	H	N	O	P	
			42	10	11	5	13	3	0
2	H	1	Total	C	H	N	O	P	
			43	10	12	5	13	3	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg		
			1	1	0	0
3	D	1	Total	Mg		
			1	1	0	0
3	E	2	Total	Mg		
			2	2	0	0
3	B	1	Total	Mg		
			1	1	0	0
3	C	2	Total	Mg		
			2	2	0	0
3	F	1	Total	Mg		
			1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O		
			277	277	0	0

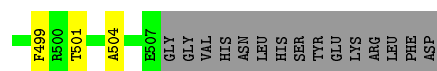
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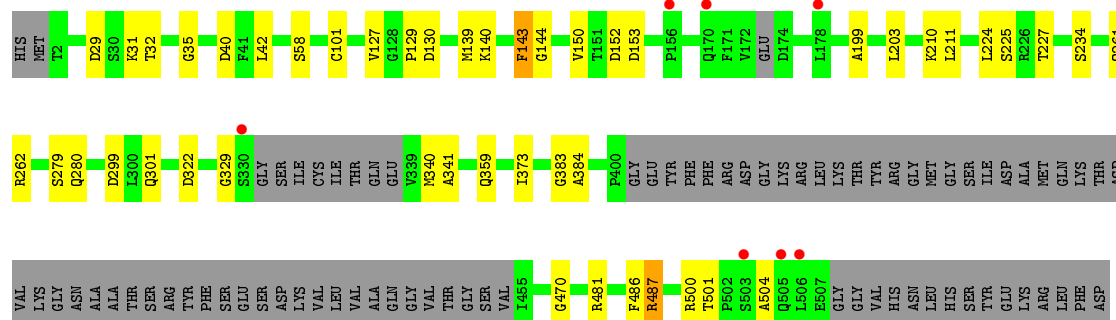
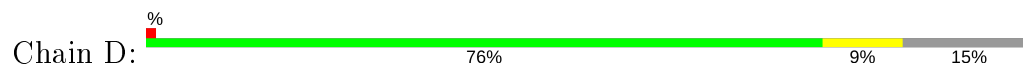
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	283	Total 283	O 283	0	0
4	C	301	Total 301	O 301	0	0
4	D	285	Total 285	O 285	0	0
4	E	51	Total 51	O 51	0	0
4	F	38	Total 38	O 38	0	0
4	G	24	Total 24	O 24	0	0
4	H	17	Total 17	O 17	0	0



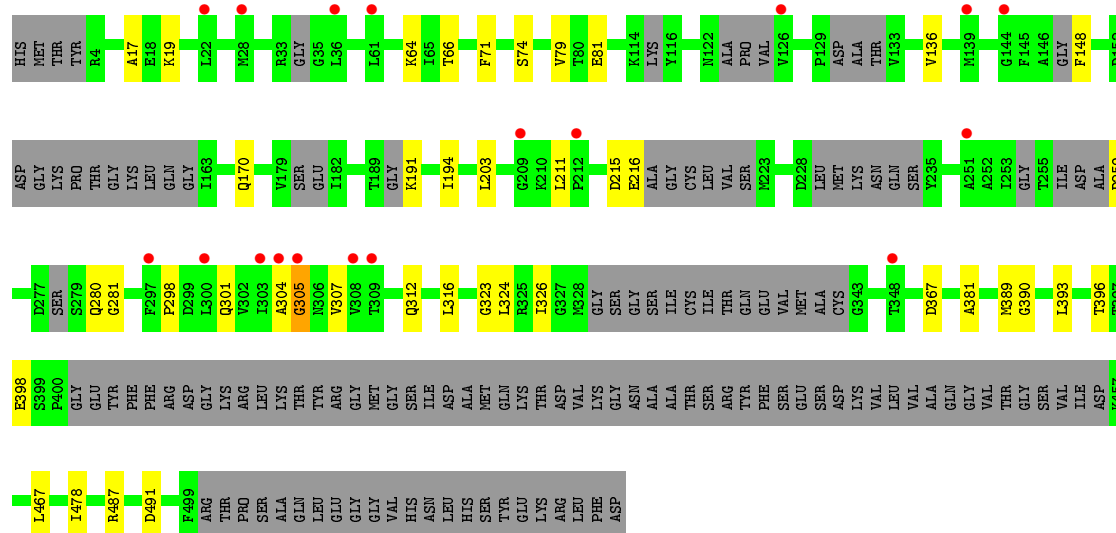




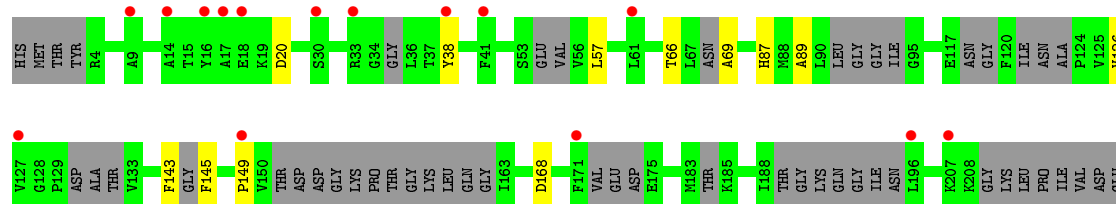
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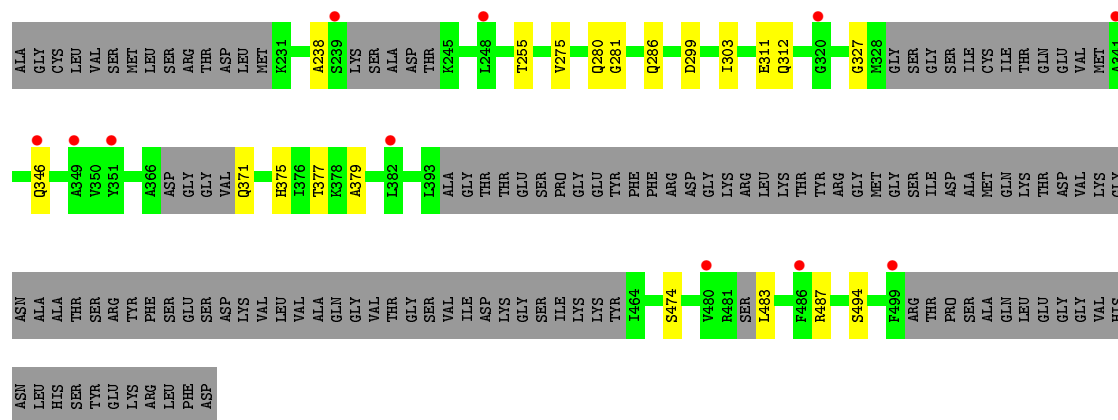


• Molecule 1: Inosine-5'-monophosphate dehydrogenase

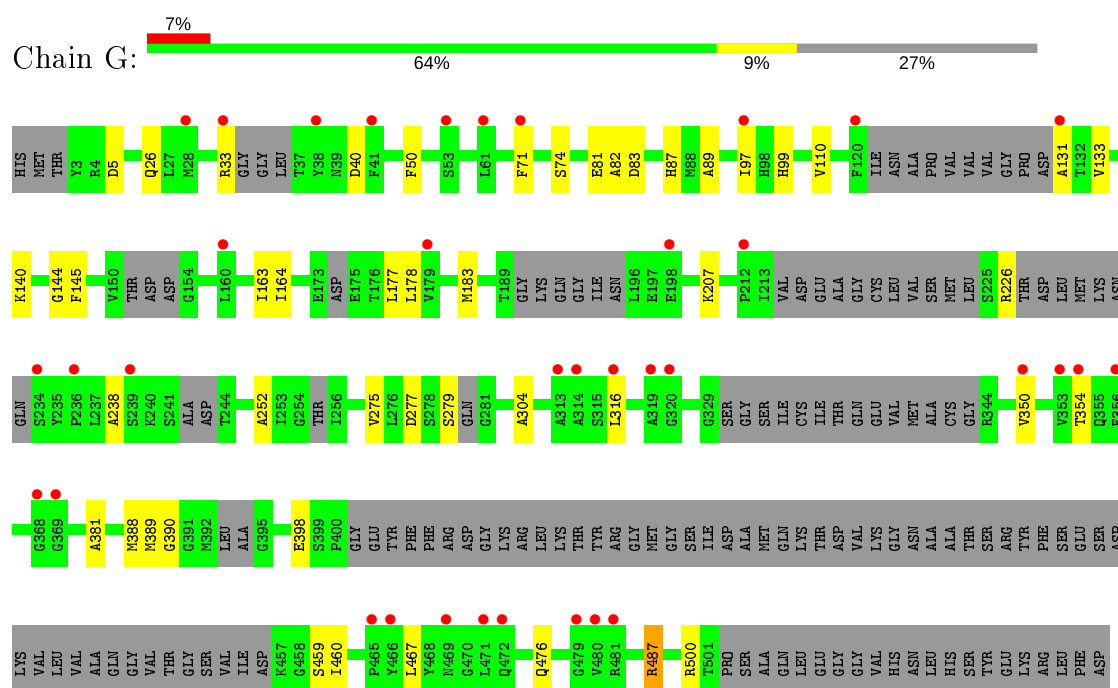


• Molecule 1: Inosine-5'-monophosphate dehydrogenase

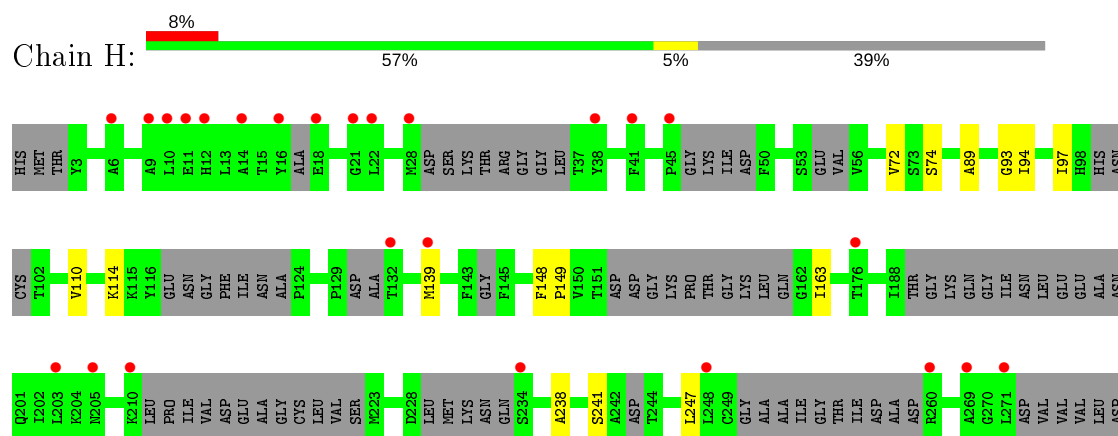


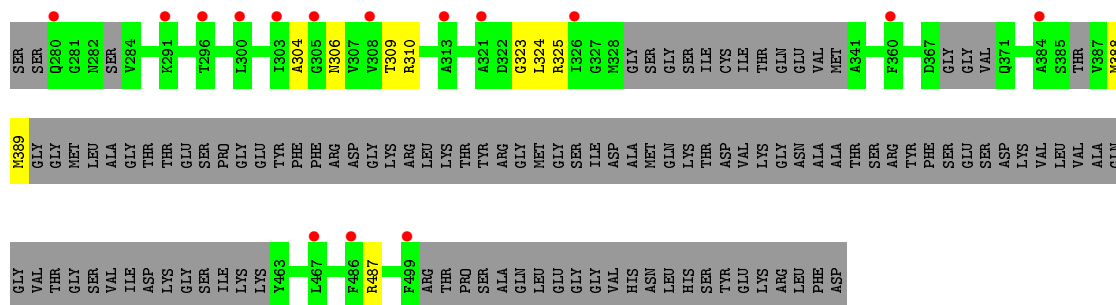


• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.89Å 152.09Å 152.25Å 90.00° 93.03° 90.00°	Depositor
Resolution (Å)	152.04 – 2.40 152.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.04-2.40) 92.3 (152.04-2.40)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.11 _2567: ???)	Depositor
R, $R_{free}$	0.249 , 0.271 0.250 , 0.272	Depositor DCC
$R_{free}$ test set	11359 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	45606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.36	2/3318 (0.1%)	0.48	0/4484
1	B	0.32	0/3300	0.49	0/4469
1	C	0.36	0/3345	0.51	0/4526
1	D	0.30	0/3322	0.48	0/4493
1	E	0.38	0/2678	0.51	0/3629
1	F	0.27	0/2241	0.44	0/3038
1	G	0.36	0/2544	0.50	0/3459
1	H	0.32	0/2004	0.46	0/2716
All	All	0.34	2/22752 (0.0%)	0.49	0/30814

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ARG	CZ-NH2	7.18	1.42	1.33
1	A	33	ARG	CZ-NH1	6.72	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	305	GLY	Peptide

## 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	3275	3293	3286	38	0
1	B	3255	3187	3194	39	0
1	C	3296	3260	3260	25	0
1	D	3274	3267	3262	40	0
1	E	2655	2384	2365	42	0
1	F	2222	1832	1816	21	0
1	G	2514	2066	2057	38	0
1	H	1997	1529	1508	15	0
2	A	93	34	36	6	0
2	B	155	56	60	4	0
2	C	93	34	36	3	0
2	D	93	34	36	4	0
2	E	93	34	36	1	0
2	F	31	12	12	1	0
2	G	93	34	36	4	0
2	H	93	34	36	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	277	0	0	11	0
4	B	283	0	0	7	0
4	C	301	0	0	9	2
4	D	285	0	0	8	2
4	E	51	0	0	5	0
4	F	38	0	0	4	0
4	G	24	0	0	3	0
4	H	17	0	0	0	0
All	All	24516	21090	21036	244	2

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 (244) 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:E:71:PHE:CD1	1:E:389:MET:HE3	1.74	1.22
1:G:133:VAL:HG23	1:G:177:LEU:O	1.38	1.22
1:E:64:LYS:HB2	1:E:301:GLN:NE2	1.54	1.20
1:E:71:PHE:CD1	1:E:389:MET:CE	2.26	1.18
1:E:71:PHE:HD1	1:E:389:MET:CE	1.57	1.14
1:E:71:PHE:HD1	1:E:389:MET:HE3	0.84	0.98
1:G:381:ALA:O	1:G:487:ARG:NH1	1.99	0.95
1:E:64:LYS:HB2	1:E:301:GLN:HE21	1.30	0.95
1:C:231:LYS:NZ	4:C:701:HOH:O	1.91	0.94
1:E:71:PHE:CD1	1:E:389:MET:HE1	2.03	0.94
1:D:225:SER:OG	2:D:602:ATP:O1A	1.87	0.92
1:D:234:SER:O	4:D:701:HOH:O	1.92	0.86
1:D:144:GLY:O	4:D:702:HOH:O	1.95	0.84
1:E:280:GLN:NE2	1:E:312:GLN:OE1	2.11	0.84
1:C:101:CYS:O	1:C:262:ARG:NH2	2.11	0.82
1:E:304:ALA:HB1	1:E:316:LEU:HD13	1.62	0.82
1:E:64:LYS:CB	1:E:301:GLN:NE2	2.41	0.81
1:B:5:ASP:OD1	4:B:701:HOH:O	1.97	0.81
1:E:298:PRO:O	4:E:701:HOH:O	1.98	0.80
1:C:279:SER:OG	2:C:603:ATP:O2B	1.99	0.80
1:F:57:LEU:O	1:F:69:ALA:N	2.16	0.78
1:D:140:LYS:O	1:D:143:PHE:O	2.02	0.77
1:A:33:ARG:HH22	1:D:31:LYS:HA	1.48	0.77
1:A:101:CYS:O	1:A:262:ARG:NH2	2.18	0.76
1:D:101:CYS:O	1:D:262:ARG:NH2	2.19	0.76
1:B:135:ASP:OD2	4:B:702:HOH:O	2.03	0.76
1:A:234:SER:O	4:A:701:HOH:O	2.05	0.75
1:G:133:VAL:CG2	1:G:177:LEU:O	2.30	0.75
1:C:210:LYS:O	2:C:601:ATP:N6	2.19	0.74
1:F:66:THR:OG1	4:F:701:HOH:O	2.04	0.74
1:A:225:SER:OG	2:A:602:ATP:O2A	2.05	0.73
1:E:487:ARG:NH1	1:E:491:ASP:OD1	2.22	0.73
1:B:112:ARG:NH1	4:B:704:HOH:O	2.22	0.72
1:C:152:ASP:OD1	4:C:702:HOH:O	2.08	0.72
1:A:181:GLU:O	4:A:702:HOH:O	2.06	0.72
1:A:466:TYR:OH	4:A:704:HOH:O	2.09	0.71
1:C:182:ILE:O	4:C:703:HOH:O	2.08	0.70
2:A:603:ATP:O1B	4:A:703:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ASP:OD2	4:D:703:HOH:O	2.09	0.70
1:E:478:ILE:O	4:E:702:HOH:O	2.09	0.70
1:B:101:CYS:O	1:B:262:ARG:NH2	2.25	0.70
1:D:203:LEU:HD11	1:D:211:LEU:HB2	1.73	0.69
1:E:71:PHE:CE1	1:E:389:MET:HE1	2.26	0.69
1:F:87:HIS:O	4:F:702:HOH:O	2.10	0.69
1:F:280:GLN:OE1	1:F:312:GLN:NE2	2.26	0.68
1:A:279:SER:OG	2:A:603:ATP:O1B	2.11	0.68
1:F:299:ASP:O	4:F:703:HOH:O	2.11	0.68
1:A:54:GLU:OE1	4:A:705:HOH:O	2.11	0.68
1:E:74:SER:HB3	1:E:390:GLY:HA3	1.77	0.67
1:G:81:GLU:HG3	1:G:82:ALA:H	1.59	0.66
1:E:281:GLY:HA3	1:E:305:GLY:O	1.96	0.66
1:E:64:LYS:HB2	1:E:301:GLN:HE22	1.55	0.66
1:A:168:ASP:OD1	2:A:601:ATP:O3'	2.09	0.65
1:C:371:GLN:O	4:C:704:HOH:O	2.13	0.65
1:E:170:GLN:OE1	4:E:703:HOH:O	2.15	0.64
1:A:31:LYS:HA	1:B:33:ARG:HH22	1.61	0.64
1:A:501:THR:OG1	4:A:706:HOH:O	2.15	0.64
1:G:81:GLU:HG3	1:G:82:ALA:N	2.14	0.63
1:B:226:ARG:HA	1:B:229:LEU:HD23	1.81	0.63
1:E:304:ALA:HB3	1:E:324:LEU:HD23	1.82	0.62
1:E:389:MET:HE1	1:E:467:LEU:HD13	1.80	0.62
1:C:339:VAL:N	4:C:709:HOH:O	2.32	0.61
1:A:33:ARG:NH2	1:D:31:LYS:HA	2.16	0.61
1:E:136:VAL:HG13	1:E:148:PHE:HD2	1.65	0.60
1:E:64:LYS:CG	1:E:301:GLN:HE22	2.14	0.60
1:F:255:THR:O	2:F:601:ATP:N6	2.24	0.60
1:B:279:SER:OG	2:B:603:ATP:O1B	2.20	0.60
1:D:261:GLN:NE2	4:D:710:HOH:O	2.33	0.60
1:G:163:ILE:O	1:G:183:MET:CB	2.50	0.60
1:B:4:ARG:NH1	4:B:715:HOH:O	2.36	0.59
1:B:208:LYS:NZ	4:B:708:HOH:O	2.26	0.59
1:E:71:PHE:CE1	1:E:389:MET:CE	2.84	0.59
1:A:112:ARG:NH2	4:A:710:HOH:O	2.33	0.59
1:A:33:ARG:HG3	1:A:33:ARG:HH11	1.66	0.59
1:A:371:GLN:O	4:A:707:HOH:O	2.16	0.58
1:E:307:VAL:HG11	1:E:316:LEU:HD12	1.85	0.58
1:B:170:GLN:NE2	2:B:605:ATP:O2G	2.32	0.58
1:F:126:VAL:HA	1:F:149:PRO:HD2	1.85	0.57
1:B:152:ASP:OD1	1:B:153:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:LEU:HD11	1:E:211:LEU:HB2	1.86	0.57
1:E:64:LYS:CB	1:E:301:GLN:HE22	2.15	0.57
1:D:152:ASP:OD1	1:D:153:ASP:N	2.38	0.57
1:G:74:SER:CB	1:G:390:GLY:HA3	2.34	0.57
1:H:114:LYS:NZ	1:H:241:SER:OG	2.39	0.56
1:A:359:GLN:OE1	1:B:4:ARG:NH1	2.38	0.56
1:C:150:VAL:HG21	1:C:183:MET:HE1	1.87	0.56
1:B:36:LEU:HD22	1:B:499:PHE:HE1	1.71	0.56
1:C:152:ASP:OD1	1:C:153:ASP:N	2.39	0.56
1:F:20[A]:ASP:OD2	1:H:310:ARG:N	2.39	0.56
1:E:393:LEU:O	1:E:396:THR:HG23	2.06	0.56
1:E:381:ALA:O	1:E:487:ARG:NH2	2.39	0.56
1:A:501:THR:HG21	1:D:40:ASP:OD2	2.06	0.55
1:B:203:LEU:HD11	1:B:211:LEU:HB2	1.88	0.55
1:E:74:SER:CB	1:E:390:GLY:HA3	2.36	0.55
1:B:40:ASP:OD2	1:C:501:THR:HG21	2.07	0.55
1:A:152:ASP:OD1	1:A:153:ASP:N	2.39	0.55
1:H:74:SER:HA	1:H:388:MET:HE2	1.88	0.54
1:E:398:GLU:OE1	1:E:398:GLU:N	2.40	0.54
1:C:203:LEU:HD11	1:C:211:LEU:HB2	1.89	0.54
1:D:139:MET:O	1:D:143:PHE:CD1	2.62	0.53
1:B:120:PHE:CD2	1:B:224:LEU:HD21	2.43	0.53
1:E:191:LYS:O	1:E:194:ILE:HG13	2.08	0.53
1:A:203:LEU:HD11	1:A:211:LEU:HB2	1.91	0.53
1:G:26:GLN:O	1:G:33:ARG:NH2	2.38	0.53
1:G:279:SER:N	2:G:603:ATP:O1B	2.37	0.53
1:G:487:ARG:HA	1:G:487:ARG:HE	1.73	0.53
1:A:499:PHE:O	1:D:35:GLY:HA3	2.09	0.53
1:B:33:ARG:NH2	4:B:703:HOH:O	2.41	0.52
1:G:74:SER:HB3	1:G:390:GLY:HA3	1.91	0.52
1:B:229:LEU:H	1:B:229:LEU:HD22	1.74	0.52
1:F:281:GLY:HA2	1:F:286:GLN:OE1	2.09	0.52
1:F:20[A]:ASP:OD2	1:H:309:THR:CB	2.58	0.52
1:C:33:ARG:HG2	1:C:36:LEU:HD21	1.91	0.51
1:F:143:PHE:HB3	1:F:145:PHE:CE2	2.45	0.51
1:G:398:GLU:CD	1:G:460:ILE:H	2.12	0.51
1:A:140:LYS:NZ	4:A:714:HOH:O	2.36	0.51
1:G:81:GLU:OE2	4:G:701:HOH:O	2.19	0.51
1:A:168:ASP:OD2	2:A:601:ATP:O2'	2.23	0.51
1:E:136:VAL:HG13	1:E:148:PHE:CD2	2.45	0.51
1:D:481:ARG:NH1	4:D:708:HOH:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LYS:NZ	4:C:711:HOH:O	2.34	0.51
1:E:259:ASP:N	1:E:259:ASP:OD1	2.44	0.50
1:G:40:ASP:O	1:G:500:ARG:N	2.41	0.50
1:D:384:ALA:O	4:D:704:HOH:O	2.19	0.49
1:B:229:LEU:N	1:B:229:LEU:HD22	2.26	0.49
1:H:304:ALA:N	1:H:323:GLY:O	2.43	0.49
1:D:227:THR:OG1	2:D:602:ATP:O1A	2.30	0.48
1:H:97:ILE:HD12	1:H:110:VAL:HG22	1.95	0.48
1:C:33:ARG:HD3	1:C:499:PHE:CD1	2.49	0.48
1:E:17:ALA:N	4:E:707:HOH:O	2.42	0.48
1:E:66:THR:OG1	4:E:704:HOH:O	2.20	0.48
1:B:33:ARG:NE	4:B:703:HOH:O	2.08	0.48
1:D:127:VAL:O	1:D:150:VAL:HA	2.14	0.48
1:E:81:GLU:HA	1:E:81:GLU:OE1	2.13	0.47
1:G:164:ILE:HB	1:G:183:MET:CB	2.43	0.47
1:G:5:ASP:OD1	4:G:702:HOH:O	2.20	0.47
1:A:31:LYS:O	1:B:33:ARG:NH2	2.48	0.47
1:D:329:GLY:CA	1:D:340:MET:CE	2.93	0.47
1:A:374:GLY:HA2	1:D:341:ALA:HB2	1.96	0.47
1:C:40:ASP:OD2	1:D:501:THR:HG21	2.14	0.47
1:H:139:MET:SD	1:H:148:PHE:CE2	3.08	0.47
1:D:329:GLY:HA2	1:D:340:MET:CE	2.44	0.47
1:H:304:ALA:O	1:H:324:LEU:HA	2.14	0.47
1:F:494:SER:OG	4:F:704:HOH:O	2.20	0.47
1:A:487:ARG:NH2	1:A:491:ASP:OD1	2.48	0.47
1:B:225:SER:O	1:B:229:LEU:CD2	2.63	0.47
1:B:34:GLY:HA2	4:C:795:HOH:O	2.15	0.47
1:D:487:ARG:NH1	4:D:704:HOH:O	2.47	0.46
1:G:140:LYS:O	1:G:144:GLY:N	2.48	0.46
1:A:487:ARG:NH2	4:A:721:HOH:O	2.46	0.46
1:D:29:ASP:HB3	1:D:32:THR:OG1	2.16	0.46
1:A:373:ILE:HD13	1:A:470:GLY:HA3	1.98	0.46
1:B:131:ALA:O	1:B:179:VAL:HG23	2.16	0.46
1:A:4:ARG:NH1	1:D:359:GLN:OE1	2.49	0.46
1:D:129:PRO:O	1:D:130:ASP:HB2	2.15	0.45
1:D:199:ALA:HB1	1:D:224:LEU:CD1	2.47	0.45
1:A:120:PHE:CD2	1:A:224:LEU:HD21	2.51	0.45
1:C:373:ILE:HD13	1:C:470:GLY:HA3	1.98	0.45
1:A:37:THR:HG21	1:B:504:ALA:HA	1.98	0.45
1:A:33:ARG:NH1	1:A:33:ARG:HG3	2.31	0.45
1:C:120:PHE:CE2	1:C:224:LEU:HD21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:371:GLN:N	1:F:375:HIS:HD1	2.15	0.45
1:C:299:ASP:OD2	4:C:705:HOH:O	2.21	0.45
1:G:350:VAL:O	1:G:354:THR:HG23	2.17	0.45
1:G:81:GLU:CG	1:G:82:ALA:H	2.28	0.45
1:A:127:VAL:O	1:A:150:VAL:HA	2.17	0.45
1:B:42:LEU:HG	1:B:500:ARG:HD2	1.99	0.45
1:F:38:TYR:CE1	1:F:379:ALA:HA	2.51	0.45
1:C:501:THR:HG23	1:C:504:ALA:H	1.82	0.45
1:F:377:THR:HG21	1:F:474:SER:OG	2.17	0.45
1:G:398:GLU:OE2	1:G:459:SER:OG	2.20	0.45
1:E:79:VAL:HG21	1:E:390:GLY:O	2.16	0.45
1:H:72:VAL:O	1:H:389:MET:N	2.38	0.45
1:D:329:GLY:HA2	1:D:340:MET:HE1	1.99	0.45
1:H:149:PRO:HA	1:H:163:ILE:HA	1.98	0.45
1:C:354:THR:OG1	1:C:383:GLY:HA3	2.17	0.44
1:G:389:MET:HE3	1:G:467:LEU:HD13	1.99	0.44
1:B:29:ASP:OD2	1:B:32:THR:HG23	2.18	0.44
1:G:99:HIS:NE2	1:G:277:ASP:OD2	2.42	0.44
1:A:140:LYS:O	1:A:143:PHE:O	2.36	0.44
1:H:114:LYS:HD2	1:H:247:LEU:O	2.18	0.44
1:D:139:MET:O	1:D:143:PHE:CE1	2.71	0.44
1:D:301:GLN:HA	1:D:322:ASP:OD2	2.18	0.44
2:E:601:ATP:O2A	2:E:601:ATP:H8	2.01	0.44
1:B:28:MET:CE	1:B:348:THR:HA	2.48	0.43
1:E:326:ILE:O	1:E:367:ASP:HB3	2.18	0.43
1:G:74:SER:HB2	1:G:390:GLY:HA3	1.99	0.43
1:D:42:LEU:HG	1:D:500:ARG:HD2	2.00	0.43
1:H:306:ASN:HA	1:H:325:ARG:O	2.19	0.43
1:A:120:PHE:CE2	1:A:224:LEU:HD21	2.52	0.43
1:A:40:ASP:OD2	1:B:501:THR:HG21	2.18	0.43
1:F:57:LEU:HA	1:F:483:LEU:HG	2.01	0.43
1:G:83:ASP:OD1	1:G:87:HIS:NE2	2.51	0.43
1:A:199:ALA:O	1:A:203:LEU:HD13	2.19	0.43
1:B:225:SER:OG	2:B:602:ATP:O2A	2.28	0.43
1:G:81:GLU:HG3	4:G:701:HOH:O	2.19	0.43
1:F:327:GLY:HA2	1:F:346:GLN:OE1	2.18	0.43
2:G:603:ATP:O1G	2:G:603:ATP:O2B	2.36	0.43
1:D:199:ALA:HB1	1:D:224:LEU:HD12	2.00	0.43
1:C:37:THR:HG21	1:D:504:ALA:HA	2.00	0.43
1:B:146:ALA:HB3	1:B:166:SER:OG	2.19	0.43
1:G:389:MET:CE	1:G:467:LEU:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ALA:O	1:B:487:ARG:NH1	2.45	0.42
1:G:140:LYS:HA	1:G:145:PHE:O	2.20	0.42
1:H:89:ALA:HA	1:H:93:GLY:O	2.19	0.42
1:B:35:GLY:N	1:C:499:PHE:O	2.49	0.42
1:D:58:SER:O	4:D:705:HOH:O	2.21	0.42
1:E:215:ASP:OD1	1:E:216:GLU:N	2.53	0.42
1:G:81:GLU:CG	1:G:82:ALA:N	2.81	0.42
1:B:120:PHE:CD2	1:B:224:LEU:CD2	3.02	0.42
1:C:340:MET:HE3	4:C:779:HOH:O	2.20	0.42
1:G:97:ILE:HD12	1:G:110:VAL:HG22	2.02	0.42
1:G:89:ALA:O	1:G:238:ALA:HA	2.20	0.42
1:D:279:SER:OG	2:D:603:ATP:O2B	2.35	0.42
1:G:304:ALA:HB1	1:G:316:LEU:HD13	2.02	0.42
1:H:89:ALA:O	1:H:238:ALA:HA	2.20	0.42
1:B:373:ILE:HD13	1:B:470:GLY:HA3	2.02	0.42
1:D:210:LYS:HE3	2:D:602:ATP:O3A	2.20	0.42
1:F:275:VAL:HG22	1:F:303:ILE:HB	2.01	0.41
1:B:37:THR:HG21	1:C:504:ALA:HA	2.01	0.41
1:D:373:ILE:HD13	1:D:470:GLY:HA3	2.02	0.41
1:B:35:GLY:HA3	1:B:345:PRO:HG2	2.02	0.41
1:B:501:THR:HG23	1:B:504:ALA:H	1.85	0.41
1:E:304:ALA:HB3	1:E:324:LEU:CD2	2.49	0.41
1:F:89:ALA:O	1:F:238:ALA:HA	2.21	0.41
2:G:603:ATP:O2B	2:G:603:ATP:O2A	2.39	0.41
1:G:145:PHE:CG	2:G:602:ATP:C8	3.09	0.41
1:D:225:SER:OG	1:D:227:THR:OG1	2.38	0.41
1:G:207:LYS:HA	1:G:226:ARG:HH12	1.86	0.41
1:G:50:PHE:O	1:G:476:GLN:NE2	2.37	0.41
1:D:383:GLY:HA2	1:D:487:ARG:CZ	2.51	0.41
1:A:262:ARG:NH1	4:A:735:HOH:O	2.54	0.40
1:D:329:GLY:CA	1:D:340:MET:HE3	2.51	0.40
1:G:252:ALA:HA	1:G:275:VAL:O	2.21	0.40
1:G:74:SER:HA	1:G:388:MET:SD	2.61	0.40
2:B:605:ATP:HO3'	1:F:168:ASP:CG	2.24	0.40
2:C:601:ATP:O2G	2:C:602:ATP:O2G	2.40	0.40
1:A:228:ASP:OD1	2:A:602:ATP:H3'	2.20	0.40
1:E:304:ALA:N	1:E:323:GLY:O	2.45	0.40
1:H:72:VAL:HA	1:H:94:ILE:O	2.21	0.40
1:E:19:LYS:HG3	1:F:311:GLU:OE2	2.20	0.40
1:B:120:PHE:CE2	1:B:224:LEU:HD21	2.56	0.40
1:G:131:ALA:O	1:G:178:LEU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:PHE:CD1	1:G:389:MET:SD	3.14	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:705:HOH:O	4:D:802:HOH:O[2_554]	2.09	0.11
4:C:975:HOH:O	4:D:873:HOH:O[2_554]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/523 (82%)	421 (98%)	9 (2%)	0	100	100
1	B	436/523 (83%)	430 (99%)	6 (1%)	0	100	100
1	C	441/523 (84%)	432 (98%)	9 (2%)	0	100	100
1	D	436/523 (83%)	426 (98%)	10 (2%)	0	100	100
1	E	356/523 (68%)	343 (96%)	13 (4%)	0	100	100
1	F	306/523 (58%)	295 (96%)	11 (4%)	0	100	100
1	G	354/523 (68%)	346 (98%)	8 (2%)	0	100	100
1	H	279/523 (53%)	272 (98%)	7 (2%)	0	100	100
All	All	3038/4184 (73%)	2965 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	350/430 (81%)	347 (99%)	3 (1%)	78	90
1	B	337/430 (78%)	334 (99%)	3 (1%)	78	90
1	C	345/430 (80%)	342 (99%)	3 (1%)	78	90
1	D	343/430 (80%)	339 (99%)	4 (1%)	71	85
1	E	234/430 (54%)	234 (100%)	0	100	100
1	F	165/430 (38%)	164 (99%)	1 (1%)	86	94
1	G	191/430 (44%)	190 (100%)	1 (0%)	88	95
1	H	128/430 (30%)	127 (99%)	1 (1%)	81	91
All	All	2093/3440 (61%)	2077 (99%)	16 (1%)	81	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	486	PHE
1	A	487	ARG
1	B	280	GLN
1	B	486	PHE
1	B	487	ARG
1	C	280	GLN
1	C	486	PHE
1	C	487	ARG
1	D	143	PHE
1	D	280	GLN
1	D	486	PHE
1	D	487	ARG
1	F	487	ARG
1	G	487	ARG
1	H	487	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	GLN
1	E	286	GLN

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Mol	Chain	Res	Type
1	E	301	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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$
2	ATP	H	601	3	26,33,33	1.85	4 (15%)	31,52,52	2.38	10 (32%)
2	ATP	B	605	3	26,33,33	1.86	4 (15%)	31,52,52	2.37	8 (25%)
2	ATP	G	602	3	26,33,33	1.94	4 (15%)	31,52,52	2.32	8 (25%)
2	ATP	H	603	-	26,33,33	1.84	3 (11%)	31,52,52	2.30	9 (29%)
2	ATP	B	603	-	26,33,33	1.79	3 (11%)	31,52,52	2.32	10 (32%)
2	ATP	C	601	3	26,33,33	1.87	4 (15%)	31,52,52	2.35	10 (32%)
2	ATP	B	606	3	26,33,33	1.86	3 (11%)	31,52,52	2.33	9 (29%)
2	ATP	A	602	3	26,33,33	1.86	2 (7%)	31,52,52	2.31	10 (32%)
2	ATP	B	602	3	26,33,33	1.81	3 (11%)	31,52,52	2.33	8 (25%)
2	ATP	C	603	-	26,33,33	1.83	4 (15%)	31,52,52	2.28	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ATP	A	603	-	26,33,33	1.85	4 (15%)	31,52,52	2.34	9 (29%)
2	ATP	E	601	3	26,33,33	1.98	3 (11%)	31,52,52	2.18	9 (29%)
2	ATP	C	602	3	26,33,33	1.73	2 (7%)	31,52,52	2.36	10 (32%)
2	ATP	D	602	3	26,33,33	1.81	3 (11%)	31,52,52	2.27	10 (32%)
2	ATP	E	603	-	26,33,33	1.91	5 (19%)	31,52,52	2.26	7 (22%)
2	ATP	B	601	3	26,33,33	1.84	4 (15%)	31,52,52	2.35	9 (29%)
2	ATP	H	602	3	26,33,33	1.91	5 (19%)	31,52,52	2.30	10 (32%)
2	ATP	E	602	3	26,33,33	1.84	3 (11%)	31,52,52	2.35	9 (29%)
2	ATP	F	601	-	26,33,33	1.92	3 (11%)	31,52,52	2.28	9 (29%)
2	ATP	G	603	-	26,33,33	1.86	4 (15%)	31,52,52	2.20	9 (29%)
2	ATP	D	601	3	26,33,33	1.73	3 (11%)	31,52,52	2.37	10 (32%)
2	ATP	D	603	-	26,33,33	1.86	4 (15%)	31,52,52	2.36	9 (29%)
2	ATP	G	601	3	26,33,33	1.84	4 (15%)	31,52,52	2.35	9 (29%)
2	ATP	A	601	3	26,33,33	1.77	4 (15%)	31,52,52	2.34	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	H	601	3	-	2/18/38/38	0/3/3/3
2	ATP	B	605	3	-	4/18/38/38	0/3/3/3
2	ATP	G	602	3	-	1/18/38/38	0/3/3/3
2	ATP	H	603	-	-	2/18/38/38	0/3/3/3
2	ATP	B	603	-	-	3/18/38/38	0/3/3/3
2	ATP	C	601	3	-	4/18/38/38	0/3/3/3
2	ATP	B	606	3	-	3/18/38/38	0/3/3/3
2	ATP	A	602	3	-	4/18/38/38	0/3/3/3
2	ATP	B	602	3	-	0/18/38/38	0/3/3/3
2	ATP	C	603	-	-	0/18/38/38	0/3/3/3
2	ATP	A	603	-	-	0/18/38/38	0/3/3/3
2	ATP	E	601	3	-	1/18/38/38	0/3/3/3
2	ATP	C	602	3	-	5/18/38/38	0/3/3/3
2	ATP	D	602	3	-	6/18/38/38	0/3/3/3
2	ATP	E	603	-	-	2/18/38/38	0/3/3/3
2	ATP	B	601	3	-	1/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	H	602	3	-	6/18/38/38	0/3/3/3
2	ATP	E	602	3	-	3/18/38/38	0/3/3/3
2	ATP	F	601	-	-	5/18/38/38	0/3/3/3
2	ATP	G	603	-	-	4/18/38/38	0/3/3/3
2	ATP	D	601	3	-	2/18/38/38	0/3/3/3
2	ATP	D	603	-	-	2/18/38/38	0/3/3/3
2	ATP	G	601	3	-	2/18/38/38	0/3/3/3
2	ATP	A	601	3	-	1/18/38/38	0/3/3/3

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	ATP	PA-O5'	8.38	1.93	1.59
2	F	601	ATP	PA-O5'	7.81	1.90	1.59
2	H	602	ATP	PA-O5'	7.73	1.90	1.59
2	A	602	ATP	PA-O5'	7.70	1.90	1.59
2	G	602	ATP	PA-O5'	7.63	1.90	1.59
2	G	603	ATP	PA-O5'	7.53	1.89	1.59
2	E	603	ATP	PA-O5'	7.51	1.89	1.59
2	A	603	ATP	PA-O5'	7.49	1.89	1.59
2	B	606	ATP	PA-O5'	7.49	1.89	1.59
2	D	603	ATP	PA-O5'	7.42	1.89	1.59
2	H	603	ATP	PA-O5'	7.40	1.89	1.59
2	D	602	ATP	PA-O5'	7.36	1.89	1.59
2	B	602	ATP	PA-O5'	7.36	1.89	1.59
2	B	605	ATP	PA-O5'	7.33	1.89	1.59
2	C	603	ATP	PA-O5'	7.28	1.88	1.59
2	E	602	ATP	PA-O5'	7.25	1.88	1.59
2	C	601	ATP	PA-O5'	7.18	1.88	1.59
2	H	601	ATP	PA-O5'	7.13	1.88	1.59
2	B	603	ATP	PA-O5'	7.12	1.88	1.59
2	B	601	ATP	PA-O5'	7.10	1.88	1.59
2	C	602	ATP	PA-O5'	7.02	1.87	1.59
2	G	601	ATP	PA-O5'	6.97	1.87	1.59
2	A	601	ATP	PA-O5'	6.87	1.87	1.59
2	D	601	ATP	PA-O5'	6.77	1.86	1.59
2	H	601	ATP	O5'-C5'	-2.79	1.34	1.44
2	G	601	ATP	C2'-C1'	2.79	1.58	1.53
2	G	601	ATP	O5'-C5'	-2.78	1.34	1.44
2	A	602	ATP	O5'-C5'	-2.72	1.34	1.44
2	H	601	ATP	C2'-C1'	2.72	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	602	ATP	C2'-C1'	2.72	1.57	1.53
2	C	601	ATP	C2'-C1'	2.71	1.57	1.53
2	B	602	ATP	O5'-C5'	-2.70	1.34	1.44
2	E	602	ATP	O5'-C5'	-2.69	1.34	1.44
2	C	602	ATP	O5'-C5'	-2.65	1.34	1.44
2	C	601	ATP	O5'-C5'	-2.65	1.34	1.44
2	B	601	ATP	O5'-C5'	-2.64	1.34	1.44
2	A	601	ATP	O5'-C5'	-2.63	1.34	1.44
2	D	601	ATP	O5'-C5'	-2.61	1.34	1.44
2	B	605	ATP	O5'-C5'	-2.60	1.34	1.44
2	B	603	ATP	O5'-C5'	-2.60	1.34	1.44
2	D	603	ATP	O5'-C5'	-2.57	1.34	1.44
2	B	601	ATP	C2'-C1'	2.56	1.57	1.53
2	G	602	ATP	O5'-C5'	-2.54	1.35	1.44
2	F	601	ATP	O5'-C5'	-2.52	1.35	1.44
2	B	606	ATP	O5'-C5'	-2.52	1.35	1.44
2	E	603	ATP	O5'-C5'	-2.51	1.35	1.44
2	A	603	ATP	O5'-C5'	-2.50	1.35	1.44
2	C	603	ATP	O5'-C5'	-2.50	1.35	1.44
2	H	603	ATP	O5'-C5'	-2.47	1.35	1.44
2	H	602	ATP	O5'-C5'	-2.45	1.35	1.44
2	G	603	ATP	O5'-C5'	-2.45	1.35	1.44
2	D	602	ATP	O5'-C5'	-2.42	1.35	1.44
2	B	605	ATP	C2'-C1'	2.41	1.57	1.53
2	F	601	ATP	C2-N1	2.40	1.38	1.33
2	E	602	ATP	C2-N1	2.39	1.38	1.33
2	E	601	ATP	O5'-C5'	-2.38	1.35	1.44
2	C	601	ATP	C2-N1	2.36	1.38	1.33
2	B	606	ATP	C2-N1	2.35	1.38	1.33
2	G	602	ATP	C2-N1	2.34	1.38	1.33
2	B	605	ATP	C2-N1	2.34	1.38	1.33
2	E	601	ATP	C2-N1	2.33	1.38	1.33
2	H	601	ATP	C2-N1	2.33	1.38	1.33
2	G	603	ATP	C2-N1	2.31	1.38	1.33
2	H	602	ATP	C2-N1	2.30	1.38	1.33
2	E	603	ATP	C2-N1	2.29	1.38	1.33
2	B	601	ATP	C2-N1	2.28	1.38	1.33
2	H	603	ATP	C2-N1	2.28	1.38	1.33
2	G	601	ATP	C2-N1	2.25	1.38	1.33
2	D	603	ATP	C2-N1	2.25	1.38	1.33
2	H	602	ATP	C2'-C1'	2.25	1.57	1.53
2	C	603	ATP	C2-N1	2.25	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	603	ATP	C2'-C1'	2.23	1.57	1.53
2	A	603	ATP	C2-N1	2.22	1.38	1.33
2	B	603	ATP	C2-N1	2.20	1.38	1.33
2	B	602	ATP	C2-N1	2.18	1.38	1.33
2	C	603	ATP	C2'-C1'	2.17	1.57	1.53
2	A	601	ATP	C2-N1	2.16	1.37	1.33
2	E	603	ATP	C4-N3	2.15	1.38	1.35
2	D	601	ATP	C2-N1	2.10	1.37	1.33
2	A	601	ATP	C2'-C1'	2.09	1.56	1.53
2	D	603	ATP	C2'-C1'	2.08	1.56	1.53
2	D	602	ATP	C2-N1	2.03	1.37	1.33
2	H	602	ATP	C4-N3	2.00	1.38	1.35
2	A	603	ATP	C2'-C1'	2.00	1.56	1.53
2	G	603	ATP	C4-N3	2.00	1.38	1.35

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	603	ATP	PA-O3A-PB	-7.02	108.74	132.83
2	B	606	ATP	PA-O3A-PB	-6.91	109.12	132.83
2	H	601	ATP	PA-O3A-PB	-6.85	109.31	132.83
2	G	601	ATP	PA-O3A-PB	-6.82	109.41	132.83
2	A	601	ATP	PA-O3A-PB	-6.81	109.47	132.83
2	H	602	ATP	PA-O3A-PB	-6.80	109.48	132.83
2	B	605	ATP	PA-O3A-PB	-6.78	109.58	132.83
2	A	603	ATP	PA-O3A-PB	-6.72	109.76	132.83
2	A	602	ATP	PA-O3A-PB	-6.72	109.77	132.83
2	C	603	ATP	PA-O3A-PB	-6.69	109.88	132.83
2	F	601	ATP	PA-O3A-PB	-6.69	109.88	132.83
2	E	602	ATP	PA-O3A-PB	-6.68	109.90	132.83
2	B	601	ATP	PA-O3A-PB	-6.67	109.93	132.83
2	E	603	ATP	PA-O3A-PB	-6.65	110.02	132.83
2	G	602	ATP	PA-O3A-PB	-6.55	110.36	132.83
2	C	602	ATP	PA-O3A-PB	-6.54	110.38	132.83
2	B	602	ATP	PA-O3A-PB	-6.50	110.54	132.83
2	D	602	ATP	PA-O3A-PB	-6.48	110.58	132.83
2	C	601	ATP	PA-O3A-PB	-6.48	110.58	132.83
2	D	601	ATP	PA-O3A-PB	-6.47	110.63	132.83
2	B	603	ATP	PA-O3A-PB	-6.45	110.68	132.83
2	H	603	ATP	PA-O3A-PB	-6.20	111.55	132.83
2	B	605	ATP	PB-O3B-PG	-5.86	112.71	132.83
2	D	601	ATP	PB-O3B-PG	-5.76	113.05	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	PB-O3B-PG	-5.75	113.08	132.83
2	C	603	ATP	PB-O3B-PG	-5.73	113.18	132.83
2	G	602	ATP	PB-O3B-PG	-5.73	113.18	132.83
2	B	601	ATP	PB-O3B-PG	-5.72	113.20	132.83
2	H	602	ATP	PB-O3B-PG	-5.72	113.20	132.83
2	D	603	ATP	PB-O3B-PG	-5.71	113.25	132.83
2	E	602	ATP	PB-O3B-PG	-5.70	113.28	132.83
2	B	602	ATP	PB-O3B-PG	-5.69	113.31	132.83
2	G	603	ATP	PA-O3A-PB	-5.69	113.31	132.83
2	H	601	ATP	PB-O3B-PG	-5.69	113.31	132.83
2	A	602	ATP	PB-O3B-PG	-5.67	113.37	132.83
2	A	603	ATP	PB-O3B-PG	-5.66	113.42	132.83
2	B	603	ATP	PB-O3B-PG	-5.65	113.44	132.83
2	D	602	ATP	PB-O3B-PG	-5.64	113.46	132.83
2	F	601	ATP	PB-O3B-PG	-5.61	113.58	132.83
2	E	601	ATP	PB-O3B-PG	-5.58	113.69	132.83
2	G	601	ATP	PB-O3B-PG	-5.57	113.70	132.83
2	B	606	ATP	PB-O3B-PG	-5.56	113.76	132.83
2	C	601	ATP	PB-O3B-PG	-5.56	113.76	132.83
2	E	603	ATP	PB-O3B-PG	-5.55	113.79	132.83
2	H	603	ATP	PB-O3B-PG	-5.53	113.84	132.83
2	C	602	ATP	PB-O3B-PG	-5.49	113.97	132.83
2	E	601	ATP	PA-O3A-PB	-5.33	114.53	132.83
2	G	603	ATP	PB-O3B-PG	-5.02	115.59	132.83
2	C	602	ATP	O5'-PA-O1A	-5.02	89.44	109.07
2	G	602	ATP	O5'-PA-O1A	-4.98	89.61	109.07
2	A	602	ATP	O5'-PA-O1A	-4.95	89.73	109.07
2	A	601	ATP	O5'-PA-O1A	-4.82	90.22	109.07
2	E	601	ATP	O5'-PA-O1A	-4.81	90.28	109.07
2	H	602	ATP	O5'-PA-O1A	-4.80	90.31	109.07
2	B	605	ATP	O5'-PA-O1A	-4.77	90.42	109.07
2	C	601	ATP	O5'-PA-O1A	-4.77	90.44	109.07
2	H	603	ATP	O5'-PA-O1A	-4.71	90.67	109.07
2	G	601	ATP	O5'-PA-O1A	-4.71	90.67	109.07
2	D	601	ATP	O5'-PA-O1A	-4.68	90.78	109.07
2	E	603	ATP	O5'-PA-O1A	-4.68	90.80	109.07
2	B	603	ATP	O5'-PA-O1A	-4.68	90.80	109.07
2	H	601	ATP	O5'-PA-O1A	-4.66	90.84	109.07
2	B	602	ATP	O5'-PA-O1A	-4.65	90.89	109.07
2	B	601	ATP	O5'-PA-O1A	-4.65	90.91	109.07
2	G	603	ATP	O5'-PA-O1A	-4.64	90.92	109.07
2	D	602	ATP	O5'-PA-O1A	-4.64	90.92	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	ATP	O5'-PA-O1A	-4.60	91.08	109.07
2	D	603	ATP	O5'-PA-O1A	-4.59	91.13	109.07
2	B	606	ATP	O5'-PA-O1A	-4.55	91.28	109.07
2	C	603	ATP	O5'-PA-O1A	-4.54	91.33	109.07
2	E	602	ATP	O5'-PA-O1A	-4.53	91.35	109.07
2	F	601	ATP	O5'-PA-O1A	-4.19	92.71	109.07
2	E	602	ATP	O2A-PA-O5'	-3.95	89.42	107.75
2	D	601	ATP	O2A-PA-O5'	-3.90	89.62	107.75
2	G	601	ATP	O2A-PA-O5'	-3.82	90.01	107.75
2	G	603	ATP	O2A-PA-O5'	-3.81	90.04	107.75
2	B	602	ATP	O2A-PA-O5'	-3.81	90.05	107.75
2	B	606	ATP	O2A-PA-O5'	-3.78	90.17	107.75
2	H	603	ATP	O2A-PA-O5'	-3.78	90.21	107.75
2	C	602	ATP	O2A-PA-O5'	-3.76	90.26	107.75
2	D	602	ATP	O2A-PA-O5'	-3.76	90.29	107.75
2	C	603	ATP	O2A-PA-O5'	-3.71	90.50	107.75
2	B	601	ATP	O2A-PA-O5'	-3.70	90.55	107.75
2	C	601	ATP	O2A-PA-O5'	-3.70	90.55	107.75
2	H	601	ATP	O2A-PA-O5'	-3.69	90.60	107.75
2	B	605	ATP	O2A-PA-O5'	-3.67	90.72	107.75
2	E	603	ATP	O2A-PA-O5'	-3.65	90.78	107.75
2	B	603	ATP	O2A-PA-O5'	-3.63	90.88	107.75
2	A	603	ATP	O2A-PA-O5'	-3.62	90.92	107.75
2	F	601	ATP	O2A-PA-O5'	-3.61	90.99	107.75
2	D	603	ATP	O2A-PA-O5'	-3.57	91.16	107.75
2	A	601	ATP	O2A-PA-O5'	-3.48	91.59	107.75
2	G	602	ATP	O2A-PA-O5'	-3.45	91.74	107.75
2	E	601	ATP	O2A-PA-O5'	-3.38	92.04	107.75
2	H	602	ATP	O2A-PA-O5'	-3.32	92.34	107.75
2	G	602	ATP	O3G-PG-O3B	-2.96	94.70	104.64
2	G	601	ATP	O3B-PG-O1G	-2.95	94.84	111.19
2	B	603	ATP	O3B-PG-O1G	-2.93	94.92	111.19
2	B	602	ATP	O3B-PG-O1G	-2.92	94.97	111.19
2	C	601	ATP	O3G-PG-O3B	-2.92	94.85	104.64
2	C	602	ATP	O3G-PG-O3B	-2.91	94.86	104.64
2	D	603	ATP	C5'-C4'-C3'	-2.90	104.30	115.18
2	A	603	ATP	O3G-PG-O2G	2.90	118.73	107.64
2	A	602	ATP	O3B-PG-O1G	-2.90	95.12	111.19
2	D	603	ATP	O3G-PG-O2G	2.89	118.70	107.64
2	D	601	ATP	O3G-PG-O3B	-2.89	94.94	104.64
2	B	606	ATP	O3G-PG-O3B	-2.87	95.01	104.64
2	D	601	ATP	O3G-PG-O2G	2.87	118.59	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	O3B-PG-O1G	-2.87	95.30	111.19
2	D	602	ATP	O3G-PG-O3B	-2.85	95.06	104.64
2	B	601	ATP	O3G-PG-O3B	-2.85	95.08	104.64
2	A	603	ATP	O3G-PG-O3B	-2.85	95.09	104.64
2	B	601	ATP	O3G-PG-O2G	2.84	118.47	107.64
2	E	602	ATP	O3G-PG-O2G	2.83	118.46	107.64
2	E	601	ATP	O3G-PG-O3B	-2.83	95.15	104.64
2	G	603	ATP	O3G-PG-O2G	2.82	118.42	107.64
2	E	601	ATP	O3G-PG-O2G	2.82	118.41	107.64
2	H	603	ATP	O3G-PG-O2G	2.81	118.39	107.64
2	D	603	ATP	O3G-PG-O3B	-2.81	95.20	104.64
2	H	601	ATP	O3G-PG-O2G	2.81	118.38	107.64
2	E	602	ATP	O3G-PG-O3B	-2.81	95.21	104.64
2	C	602	ATP	O3G-PG-O2G	2.81	118.36	107.64
2	H	602	ATP	O3B-PG-O1G	-2.81	95.63	111.19
2	B	606	ATP	O3G-PG-O2G	2.80	118.35	107.64
2	F	601	ATP	O3B-PG-O1G	-2.79	95.72	111.19
2	H	603	ATP	PA-O5'-C5'	-2.78	105.35	121.68
2	B	605	ATP	C5'-C4'-C3'	-2.78	104.75	115.18
2	C	601	ATP	O3G-PG-O2G	2.77	118.22	107.64
2	C	603	ATP	C5'-C4'-C3'	-2.76	104.82	115.18
2	G	602	ATP	C5'-C4'-C3'	-2.76	104.83	115.18
2	A	603	ATP	C5'-C4'-C3'	-2.76	104.84	115.18
2	C	603	ATP	O3G-PG-O3B	-2.74	95.43	104.64
2	C	602	ATP	PA-O5'-C5'	-2.73	105.64	121.68
2	A	602	ATP	O2A-PA-O5'	-2.72	95.11	107.75
2	D	601	ATP	PA-O5'-C5'	-2.72	105.75	121.68
2	E	603	ATP	PA-O5'-C5'	-2.71	105.81	121.68
2	B	603	ATP	PA-O5'-C5'	-2.70	105.83	121.68
2	G	603	ATP	C5'-C4'-C3'	-2.70	105.07	115.18
2	B	602	ATP	PA-O5'-C5'	-2.69	105.90	121.68
2	F	601	ATP	O3G-PG-O2G	2.68	117.87	107.64
2	G	601	ATP	PA-O5'-C5'	-2.67	106.00	121.68
2	H	601	ATP	O3B-PG-O1G	-2.67	96.35	111.19
2	G	603	ATP	O3G-PG-O3B	-2.66	95.70	104.64
2	B	603	ATP	C5'-C4'-C3'	-2.66	105.20	115.18
2	B	603	ATP	O3G-PG-O2G	2.66	117.80	107.64
2	G	603	ATP	PA-O5'-C5'	-2.66	106.11	121.68
2	H	603	ATP	O3G-PG-O3B	-2.66	95.73	104.64
2	H	602	ATP	O3G-PG-O2G	2.65	117.75	107.64
2	C	601	ATP	O3B-PG-O1G	-2.64	96.53	111.19
2	C	602	ATP	C5'-C4'-C3'	-2.64	105.29	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ATP	PA-O5'-C5'	-2.64	106.20	121.68
2	B	601	ATP	PA-O5'-C5'	-2.63	106.23	121.68
2	B	602	ATP	O3G-PG-O2G	2.62	117.65	107.64
2	B	606	ATP	C5'-C4'-C3'	-2.62	105.37	115.18
2	H	601	ATP	PA-O5'-C5'	-2.62	106.34	121.68
2	B	605	ATP	PA-O5'-C5'	-2.61	106.36	121.68
2	A	602	ATP	C5'-C4'-C3'	-2.61	105.41	115.18
2	E	603	ATP	C5'-C4'-C3'	-2.60	105.46	115.18
2	A	602	ATP	O3G-PG-O2G	2.59	117.55	107.64
2	C	601	ATP	PA-O5'-C5'	-2.59	106.50	121.68
2	A	603	ATP	PA-O5'-C5'	-2.59	106.50	121.68
2	F	601	ATP	C5'-C4'-C3'	-2.59	105.49	115.18
2	D	601	ATP	O3B-PG-O1G	-2.58	96.88	111.19
2	E	602	ATP	C5'-C4'-C3'	-2.58	105.52	115.18
2	B	605	ATP	O3G-PG-O3B	-2.58	96.00	104.64
2	A	601	ATP	O3G-PG-O2G	2.57	117.46	107.64
2	G	601	ATP	O3G-PG-O2G	2.55	117.38	107.64
2	B	605	ATP	O2G-PG-O3B	-2.54	96.13	104.64
2	H	601	ATP	O3G-PG-O3B	-2.54	96.13	104.64
2	D	603	ATP	PA-O5'-C5'	-2.53	106.83	121.68
2	E	603	ATP	O3G-PG-O3B	-2.50	96.24	104.64
2	G	601	ATP	C5'-C4'-C3'	-2.50	105.83	115.18
2	E	602	ATP	PA-O5'-C5'	-2.49	107.11	121.68
2	C	603	ATP	PA-O5'-C5'	-2.47	107.19	121.68
2	H	602	ATP	C5'-C4'-C3'	-2.46	105.95	115.18
2	B	601	ATP	C5'-C4'-C3'	-2.46	105.97	115.18
2	F	601	ATP	PA-O5'-C5'	-2.46	107.28	121.68
2	H	601	ATP	C5'-C4'-C3'	-2.45	106.00	115.18
2	C	601	ATP	C5'-C4'-C3'	-2.45	106.00	115.18
2	B	602	ATP	C5'-C4'-C3'	-2.44	106.04	115.18
2	E	602	ATP	O3B-PG-O1G	-2.43	97.74	111.19
2	D	601	ATP	C5'-C4'-C3'	-2.42	106.11	115.18
2	A	601	ATP	C5'-C4'-C3'	-2.38	106.28	115.18
2	C	602	ATP	O3B-PG-O1G	-2.37	98.07	111.19
2	A	602	ATP	C1'-N9-C4	-2.35	122.52	126.64
2	E	601	ATP	O3B-PG-O1G	-2.34	98.18	111.19
2	H	603	ATP	C5'-C4'-C3'	-2.34	106.40	115.18
2	B	606	ATP	O3B-PG-O1G	-2.34	98.20	111.19
2	B	601	ATP	O3B-PG-O1G	-2.34	98.22	111.19
2	G	602	ATP	PA-O5'-C5'	-2.33	108.03	121.68
2	A	603	ATP	O3B-PG-O1G	-2.32	98.33	111.19
2	D	603	ATP	O3B-PG-O1G	-2.30	98.43	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	ATP	PA-O5'-C5'	-2.28	108.30	121.68
2	H	603	ATP	O3B-PG-O1G	-2.25	98.69	111.19
2	G	602	ATP	O2G-PG-O3B	-2.23	97.17	104.64
2	D	602	ATP	C5'-C4'-C3'	-2.22	106.87	115.18
2	B	606	ATP	PA-O5'-C5'	-2.20	108.77	121.68
2	D	601	ATP	C1'-N9-C4	-2.19	122.78	126.64
2	E	601	ATP	C5'-C4'-C3'	-2.18	107.01	115.18
2	C	601	ATP	O2G-PG-O3B	2.18	111.94	104.64
2	B	603	ATP	O3G-PG-O3B	-2.16	97.38	104.64
2	G	603	ATP	O3B-PG-O1G	-2.13	99.40	111.19
2	A	601	ATP	C1'-N9-C4	-2.10	122.96	126.64
2	A	602	ATP	PA-O5'-C5'	-2.06	109.61	121.68
2	G	601	ATP	C1'-N9-C4	-2.05	123.04	126.64
2	D	602	ATP	O3G-PG-O1G	2.04	118.67	110.68
2	H	602	ATP	O3G-PG-O3B	-2.04	97.79	104.64
2	E	601	ATP	PA-O5'-C5'	-2.03	109.76	121.68
2	D	602	ATP	O2G-PG-O3B	-2.03	97.84	104.64
2	H	602	ATP	O2G-PG-O1G	2.02	118.61	110.68
2	A	601	ATP	O2G-PG-O1G	2.02	118.58	110.68
2	D	602	ATP	C1'-N9-C4	-2.02	123.10	126.64
2	C	603	ATP	O3G-PG-O1G	2.01	118.56	110.68
2	F	601	ATP	O2G-PG-O1G	2.01	118.56	110.68
2	B	603	ATP	O2G-PG-O1G	2.01	118.53	110.68
2	C	602	ATP	O2G-PG-O3B	2.01	111.36	104.64
2	H	601	ATP	C1'-N9-C4	-2.00	123.13	126.64
2	A	602	ATP	O3G-PG-O3B	-2.00	97.93	104.64
2	H	602	ATP	PA-O5'-C5'	-2.00	109.95	121.68

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	605	ATP	C5'-O5'-PA-O3A
2	G	602	ATP	PB-O3B-PG-O2G
2	A	602	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O2A
2	E	601	ATP	PB-O3B-PG-O2G
2	C	602	ATP	PB-O3B-PG-O2G
2	D	602	ATP	PB-O3B-PG-O3G
2	D	602	ATP	C5'-O5'-PA-O1A
2	D	602	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	H	602	ATP	C5'-O5'-PA-O1A
2	H	602	ATP	C5'-O5'-PA-O3A
2	F	601	ATP	PB-O3B-PG-O2G
2	F	601	ATP	PB-O3B-PG-O3G
2	G	601	ATP	PB-O3B-PG-O3G
2	D	602	ATP	O4'-C4'-C5'-O5'
2	D	602	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	PB-O3B-PG-O1G
2	E	603	ATP	PA-O3A-PB-O1B
2	A	601	ATP	O4'-C4'-C5'-O5'
2	B	603	ATP	PB-O3B-PG-O1G
2	C	602	ATP	PB-O3B-PG-O3G
2	E	602	ATP	C5'-O5'-PA-O3A
2	F	601	ATP	C5'-O5'-PA-O3A
2	B	605	ATP	PA-O3A-PB-O1B
2	B	605	ATP	C5'-O5'-PA-O2A
2	E	602	ATP	C5'-O5'-PA-O2A
2	F	601	ATP	C5'-O5'-PA-O2A
2	H	602	ATP	O4'-C4'-C5'-O5'
2	C	601	ATP	PG-O3B-PB-O2B
2	C	601	ATP	PA-O3A-PB-O2B
2	C	602	ATP	PA-O3A-PB-O1B
2	G	603	ATP	PG-O3B-PB-O1B
2	G	603	ATP	PG-O3B-PB-O2B
2	D	603	ATP	PB-O3A-PA-O1A
2	C	601	ATP	PG-O3B-PB-O1B
2	H	602	ATP	PB-O3A-PA-O1A
2	G	603	ATP	PA-O3A-PB-O2B
2	G	603	ATP	PB-O3A-PA-O1A
2	B	606	ATP	O4'-C4'-C5'-O5'
2	H	602	ATP	PB-O3B-PG-O1G
2	B	603	ATP	O4'-C4'-C5'-O5'
2	H	603	ATP	PB-O3B-PG-O2G
2	H	603	ATP	PB-O3B-PG-O3G
2	G	601	ATP	PB-O3B-PG-O2G
2	B	606	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C5'-O5'-PA-O3A
2	H	601	ATP	PG-O3B-PB-O2B
2	H	601	ATP	PA-O3A-PB-O2B
2	B	605	ATP	PG-O3B-PB-O2B
2	B	603	ATP	PG-O3B-PB-O1B
2	C	601	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	B	606	ATP	PB-O3A-PA-O1A
2	C	602	ATP	PG-O3B-PB-O1B
2	D	602	ATP	PB-O3A-PA-O2A
2	H	602	ATP	PB-O3A-PA-O2A
2	E	602	ATP	PG-O3B-PB-O1B
2	F	601	ATP	PB-O3A-PA-O2A
2	D	601	ATP	PB-O3A-PA-O2A
2	D	603	ATP	PG-O3B-PB-O1B
2	E	603	ATP	C5'-O5'-PA-O1A
2	D	601	ATP	C5'-O5'-PA-O1A
2	C	602	ATP	PB-O3B-PG-O1G

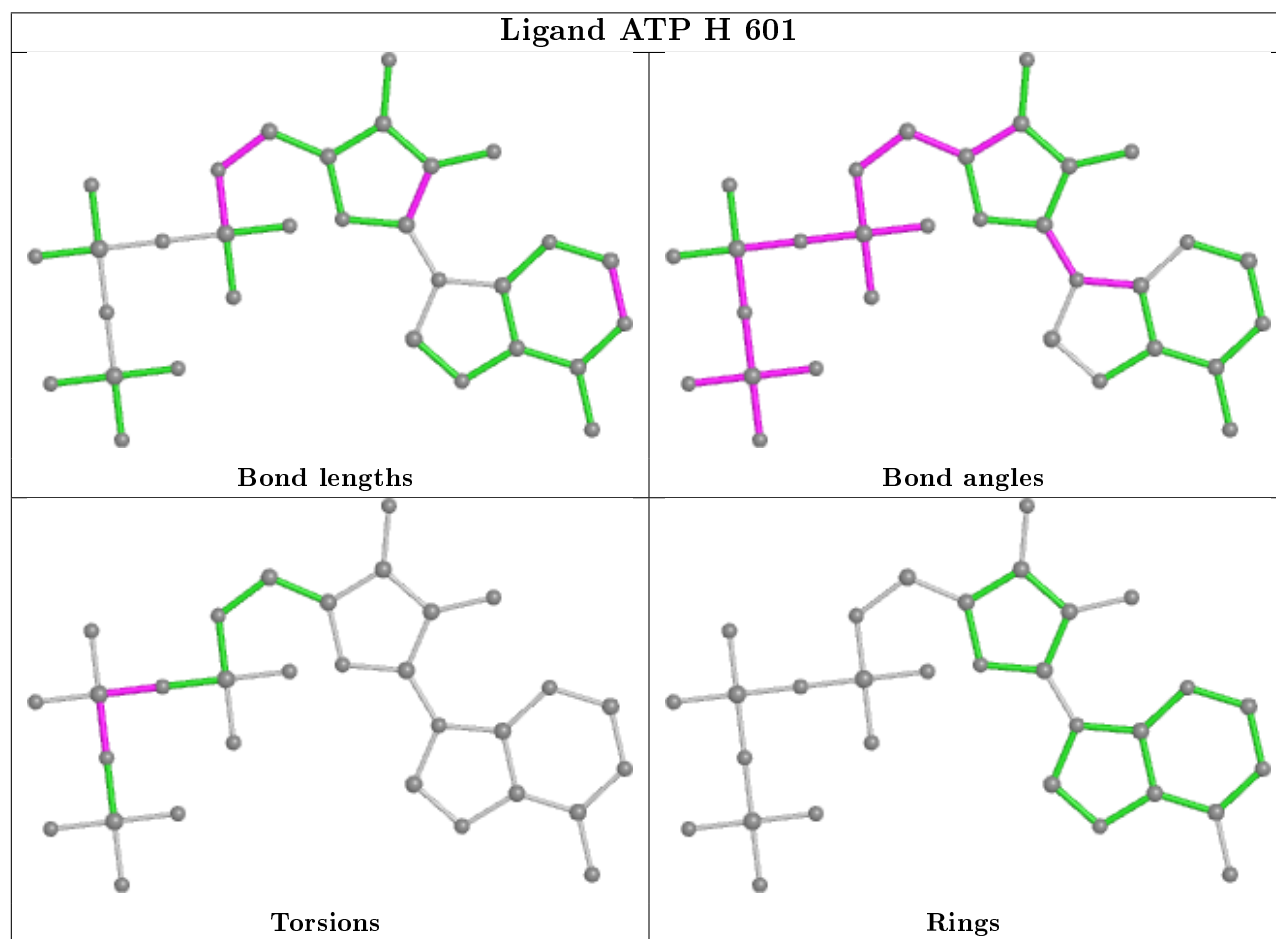
There are no ring outliers.

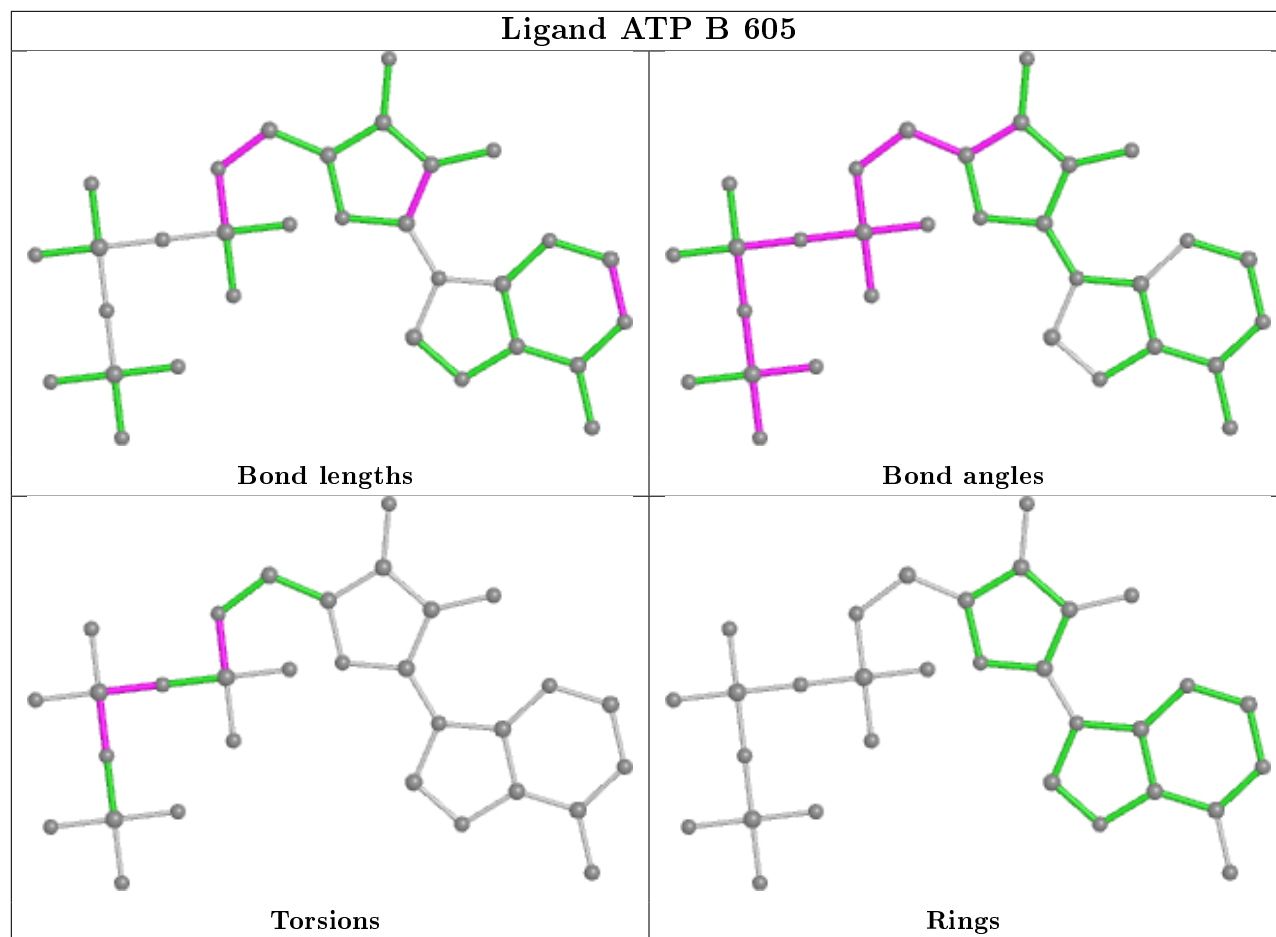
15 monomers are involved in 23 short contacts:

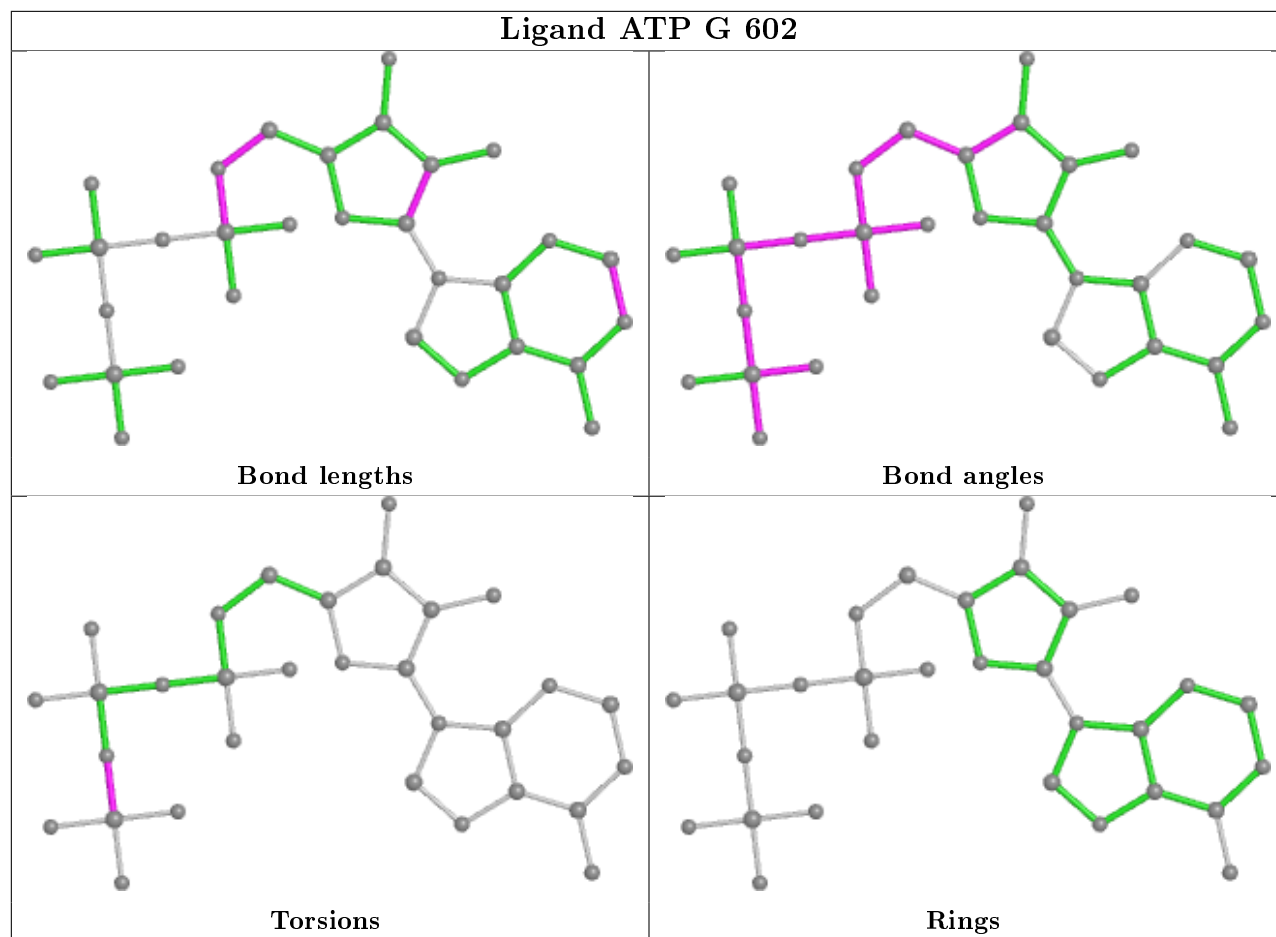
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	605	ATP	2	0
2	G	602	ATP	1	0
2	B	603	ATP	1	0
2	C	601	ATP	2	0
2	A	602	ATP	2	0
2	B	602	ATP	1	0
2	C	603	ATP	1	0
2	A	603	ATP	2	0
2	E	601	ATP	1	0
2	C	602	ATP	1	0
2	D	602	ATP	3	0
2	F	601	ATP	1	0
2	G	603	ATP	3	0
2	D	603	ATP	1	0
2	A	601	ATP	2	0

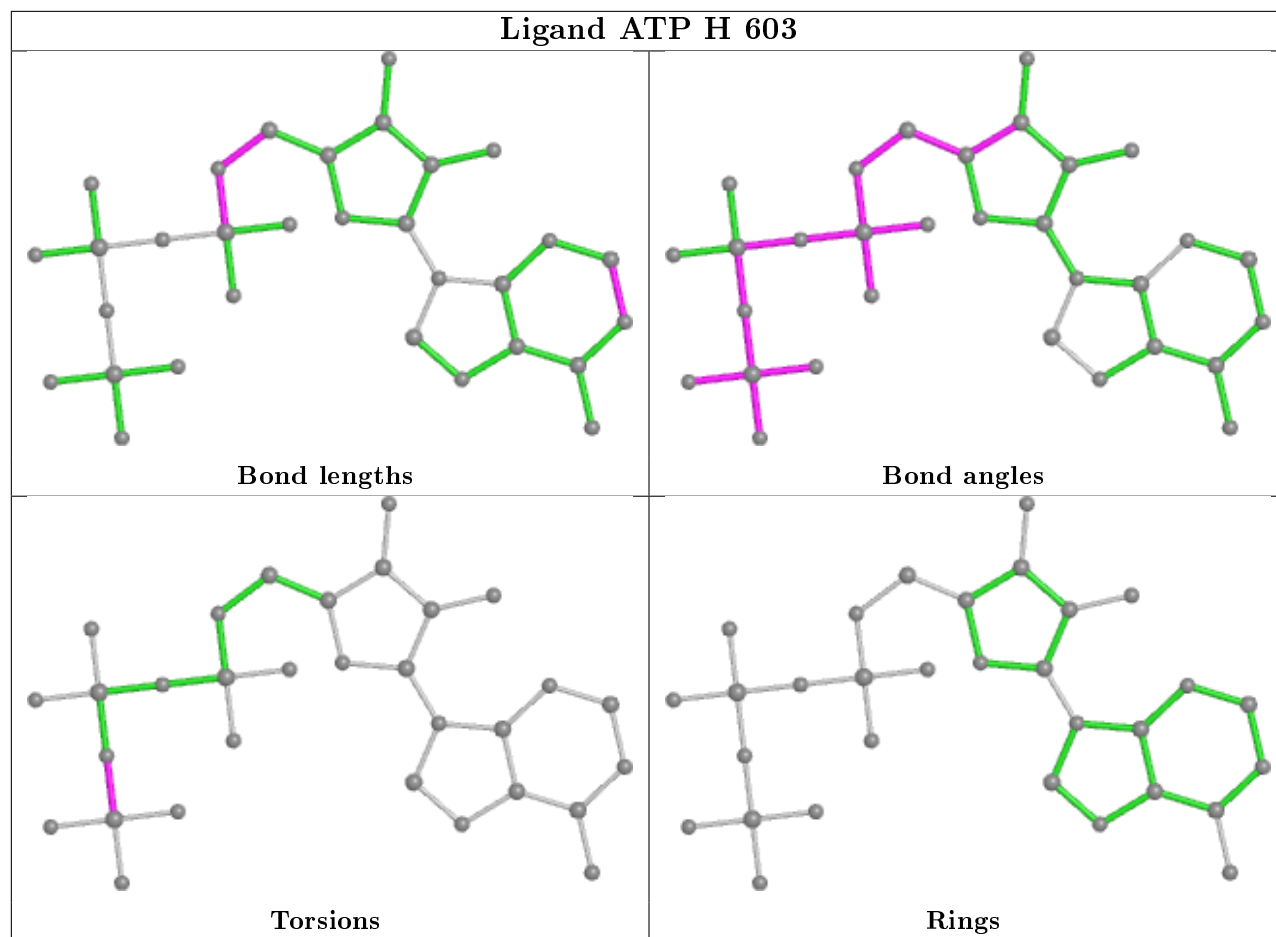
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

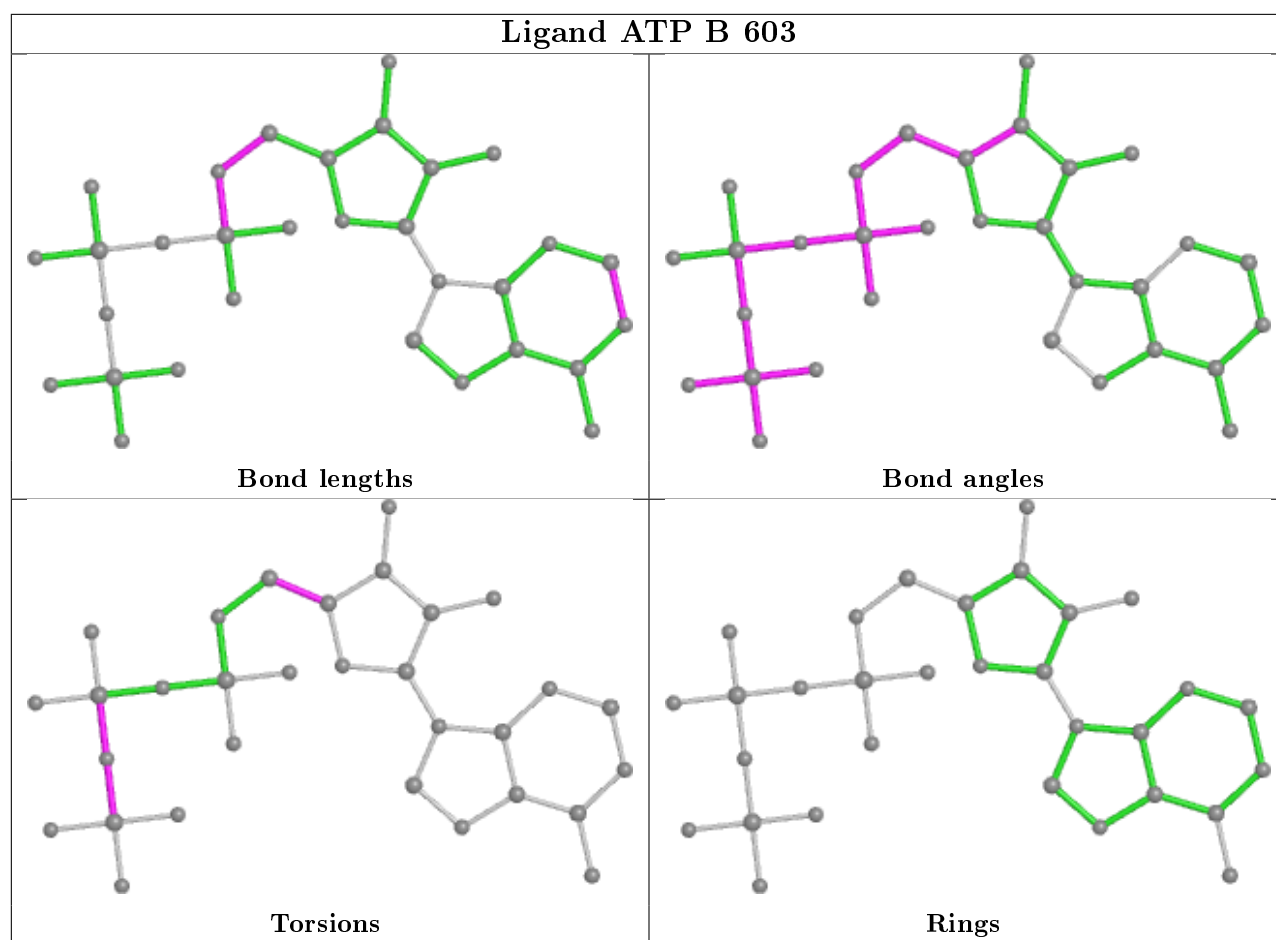
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

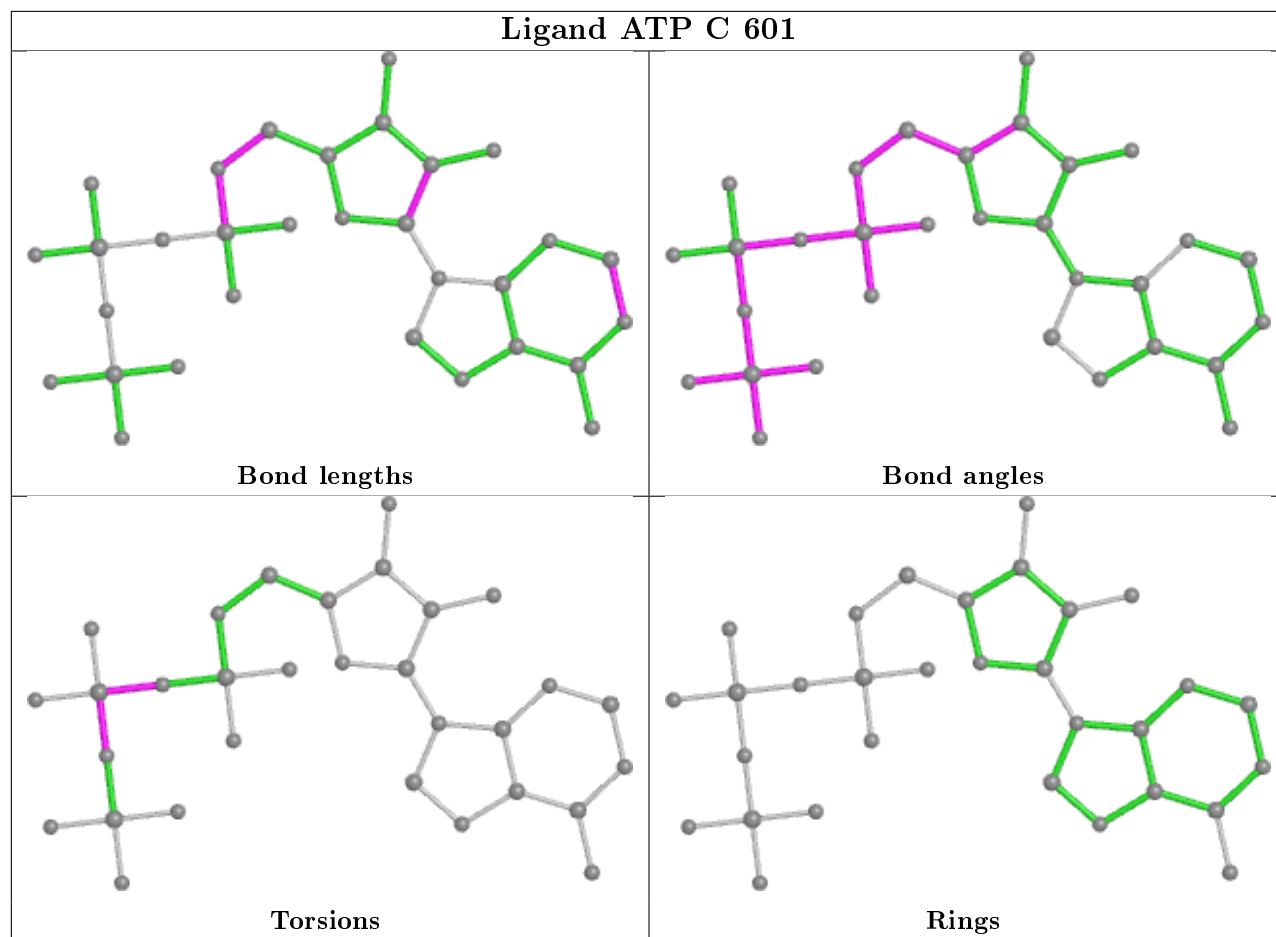




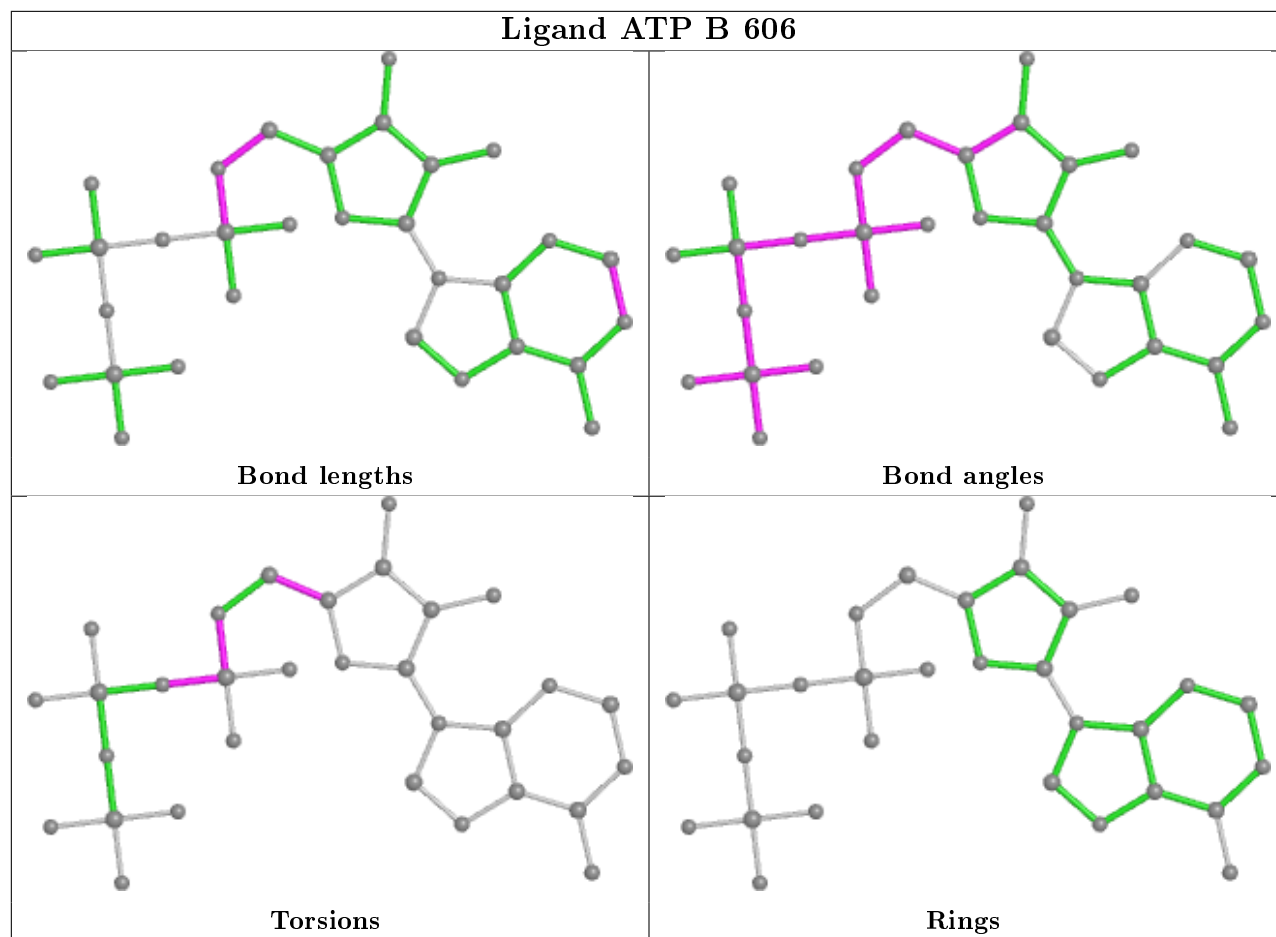


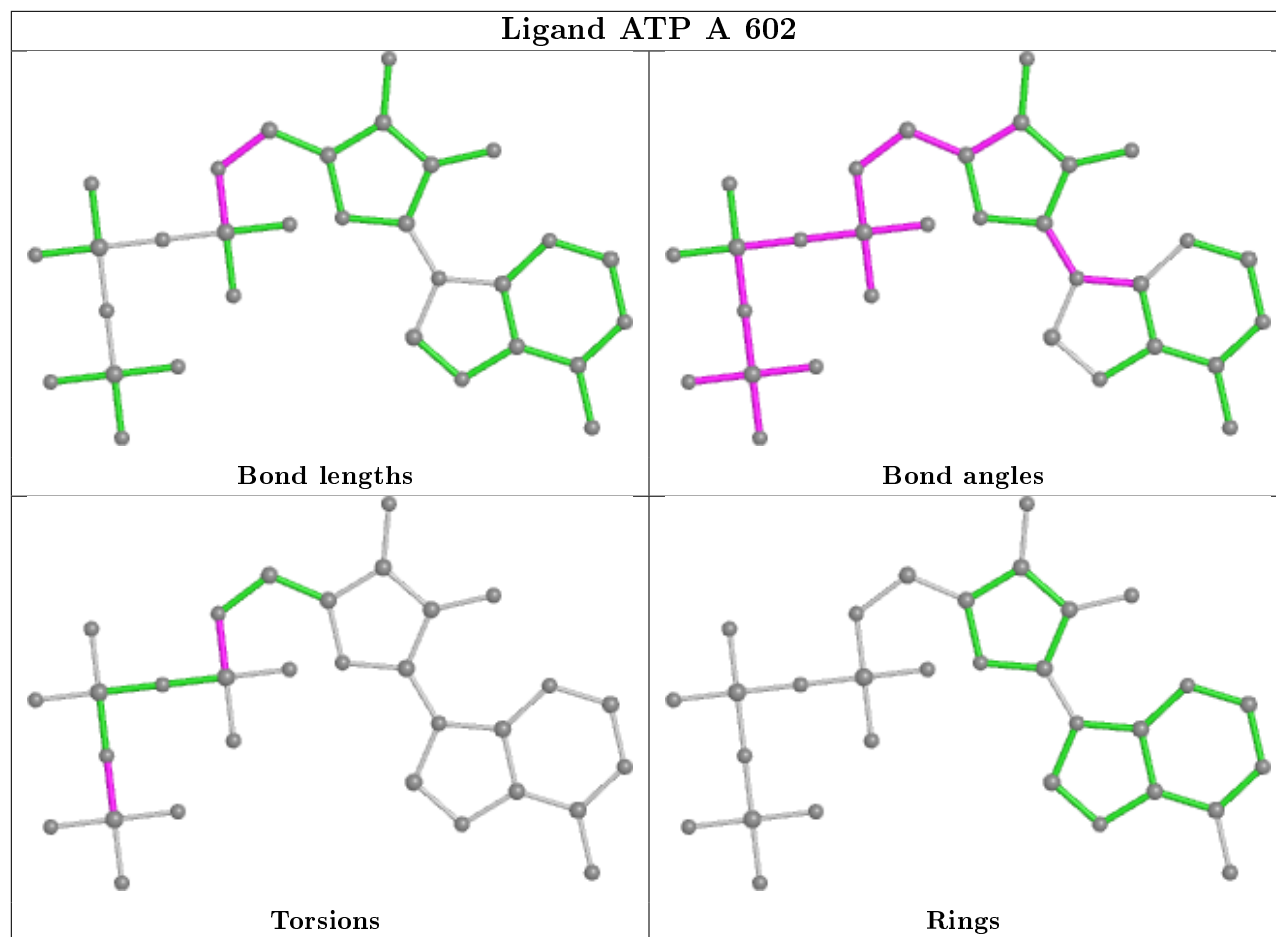


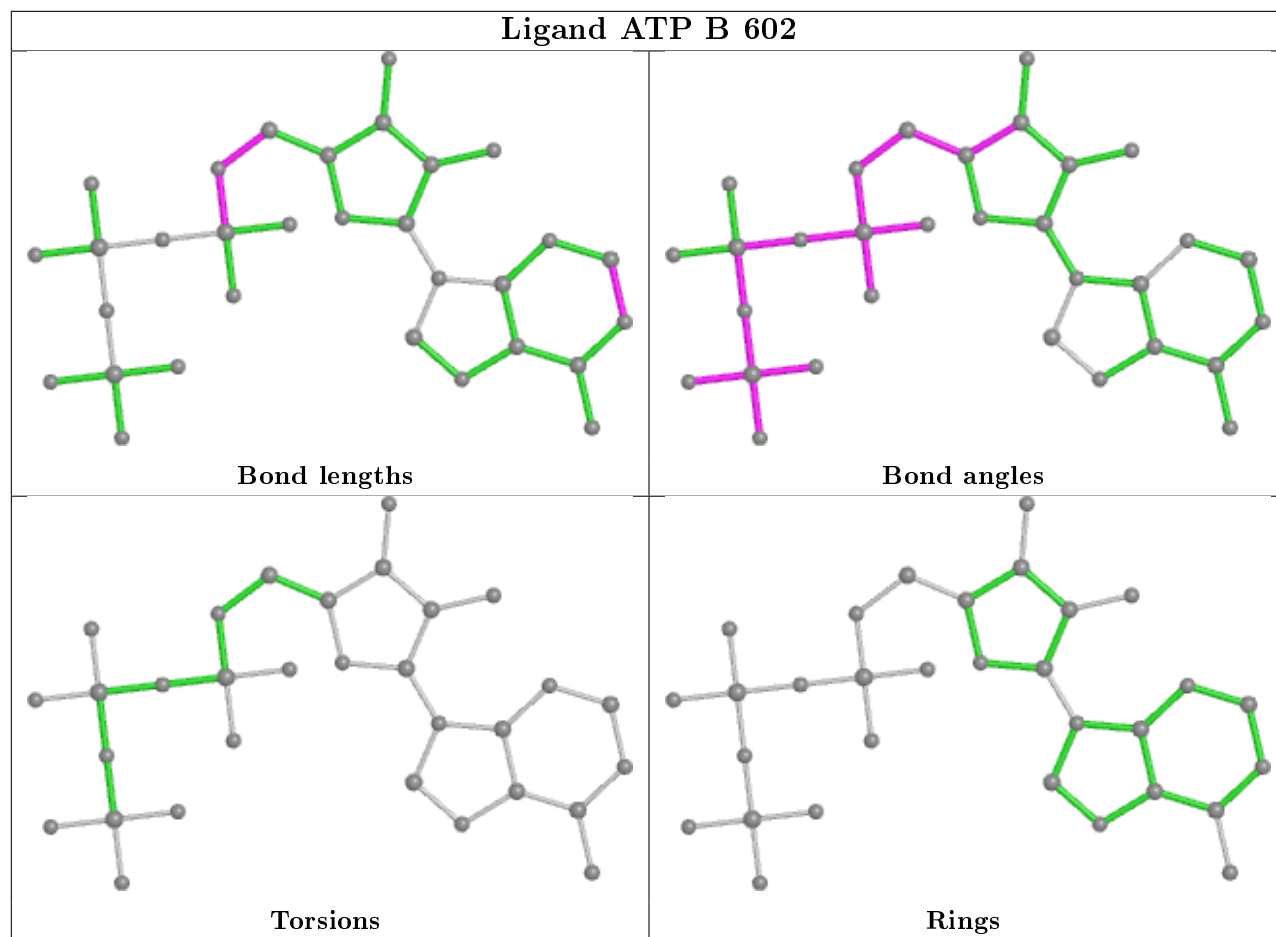


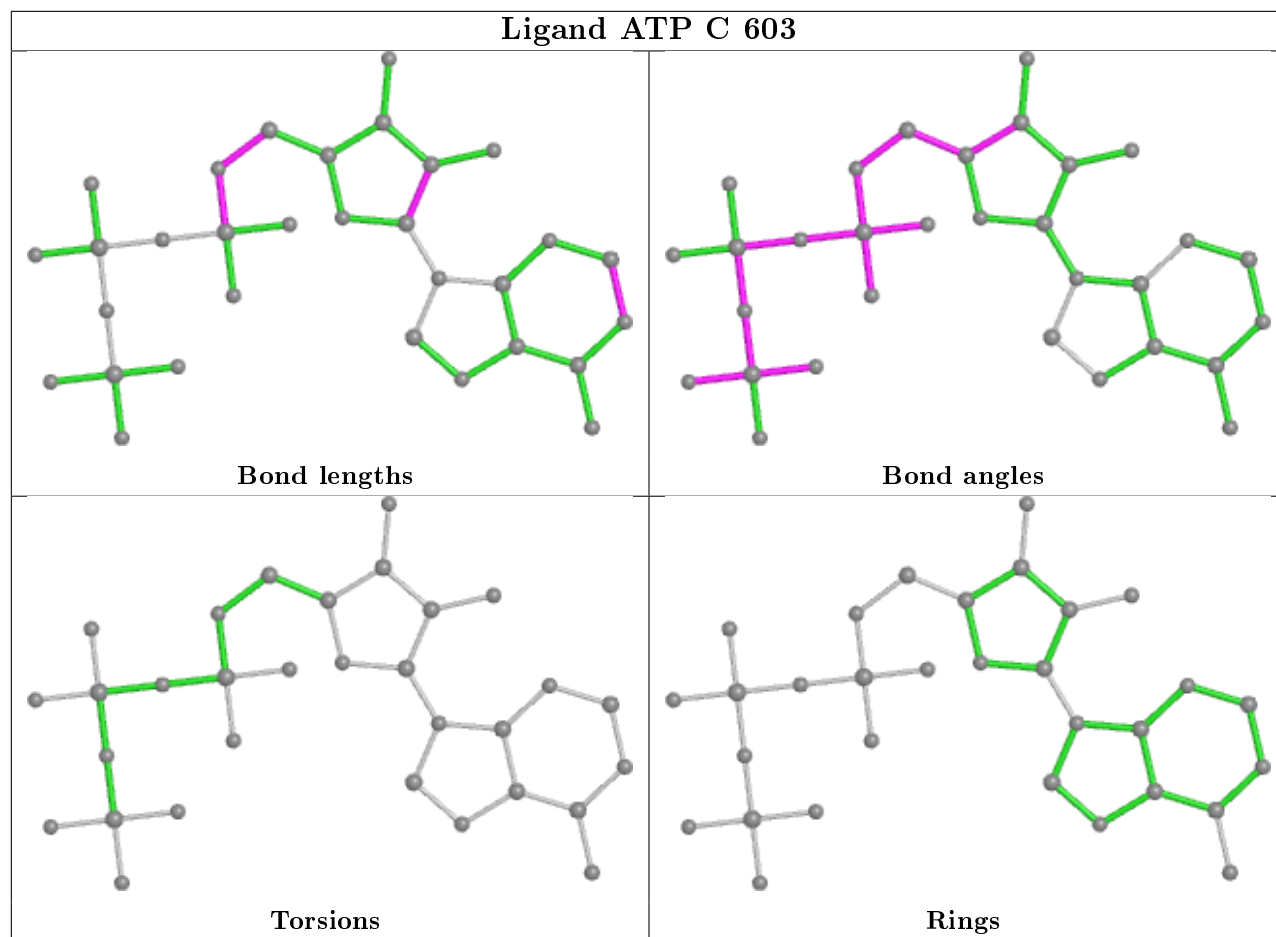


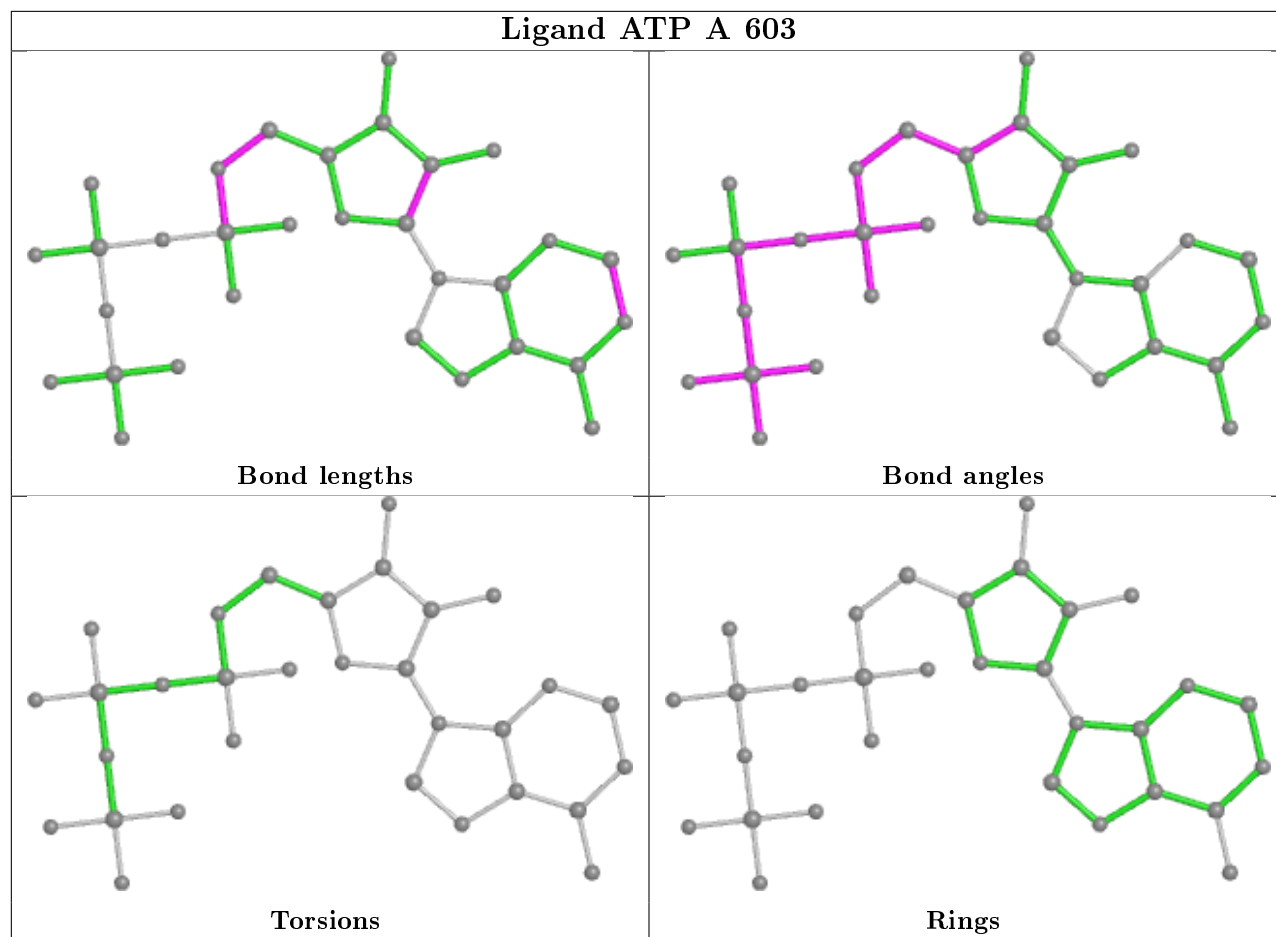


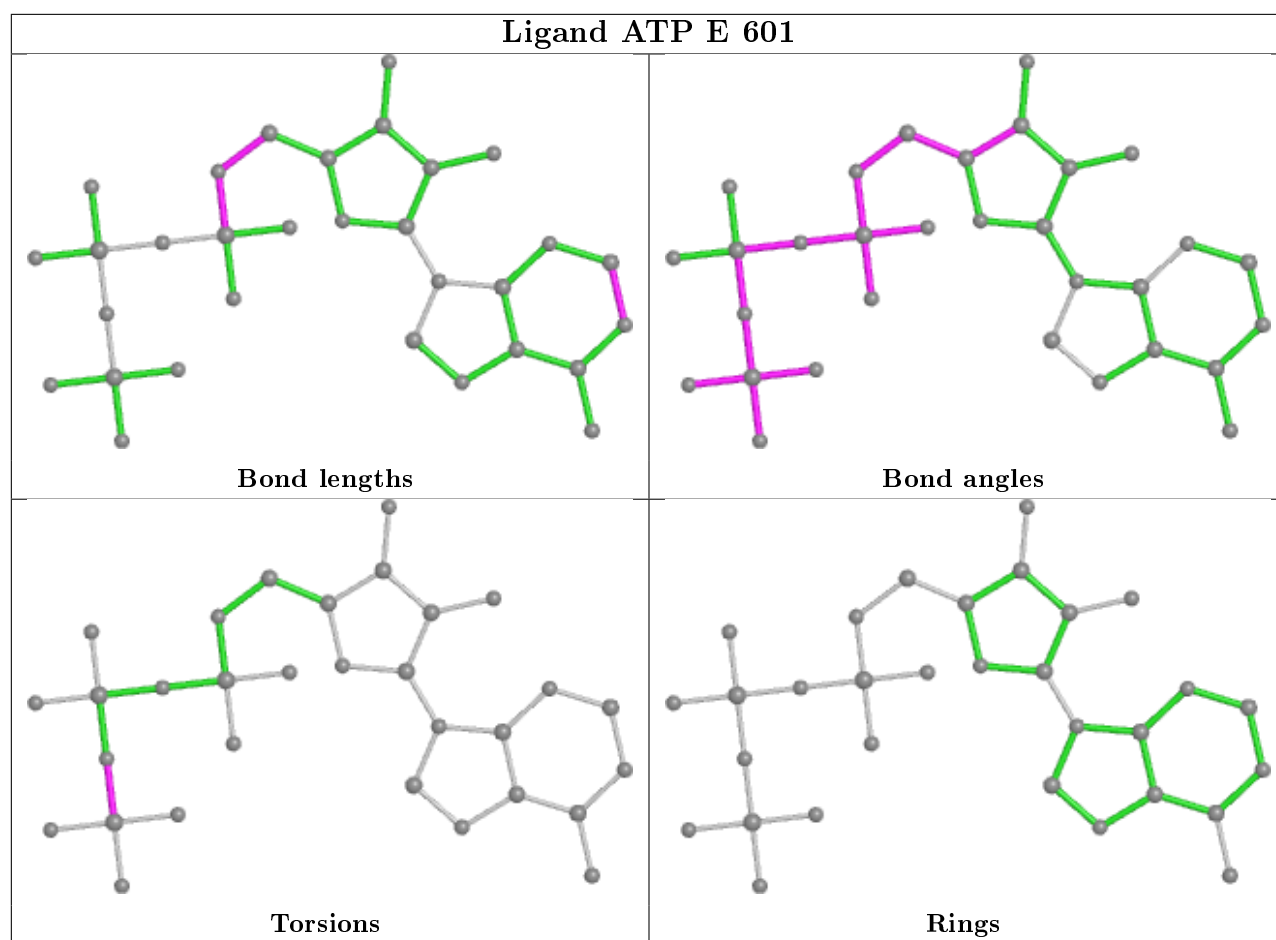


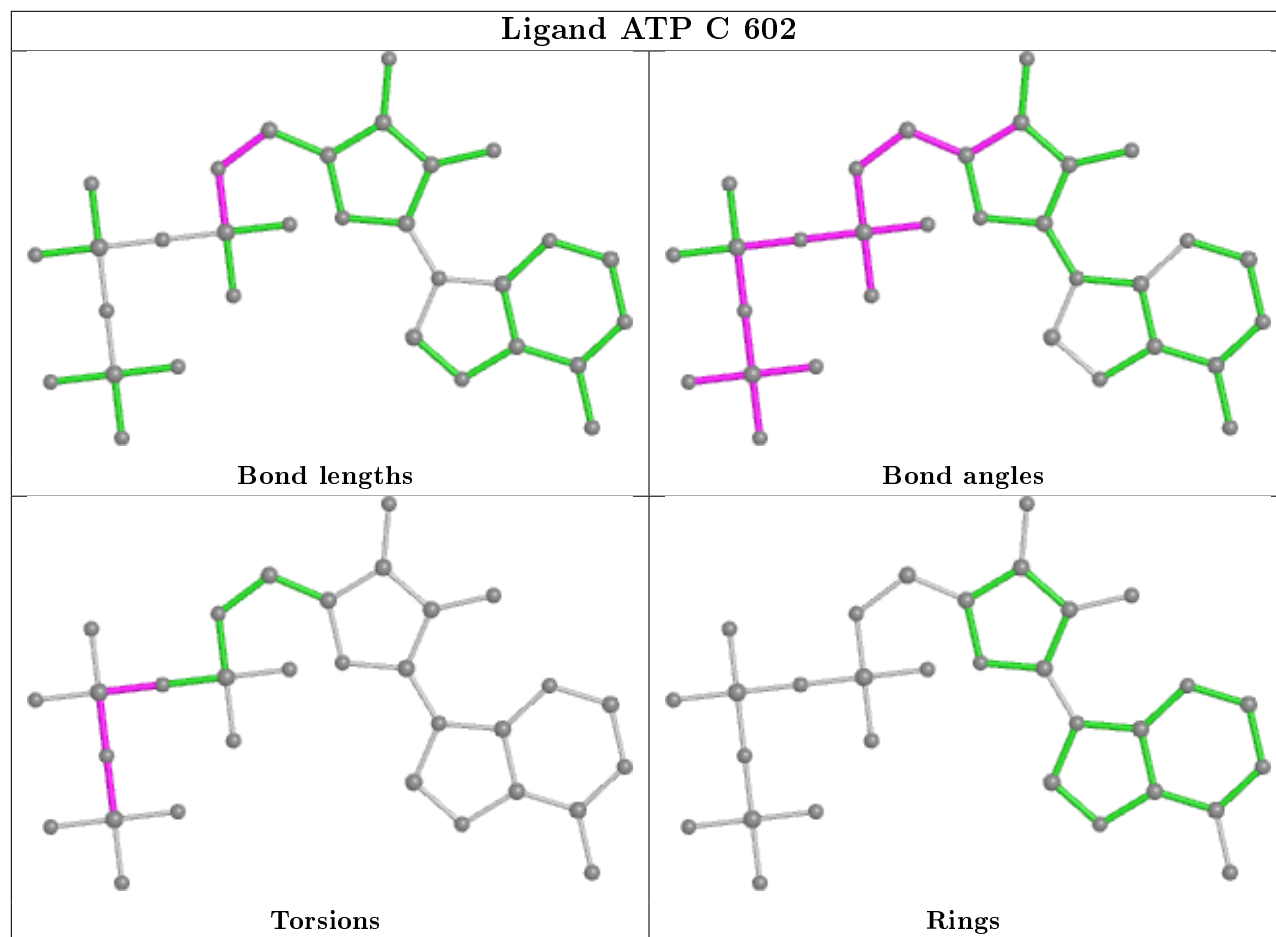


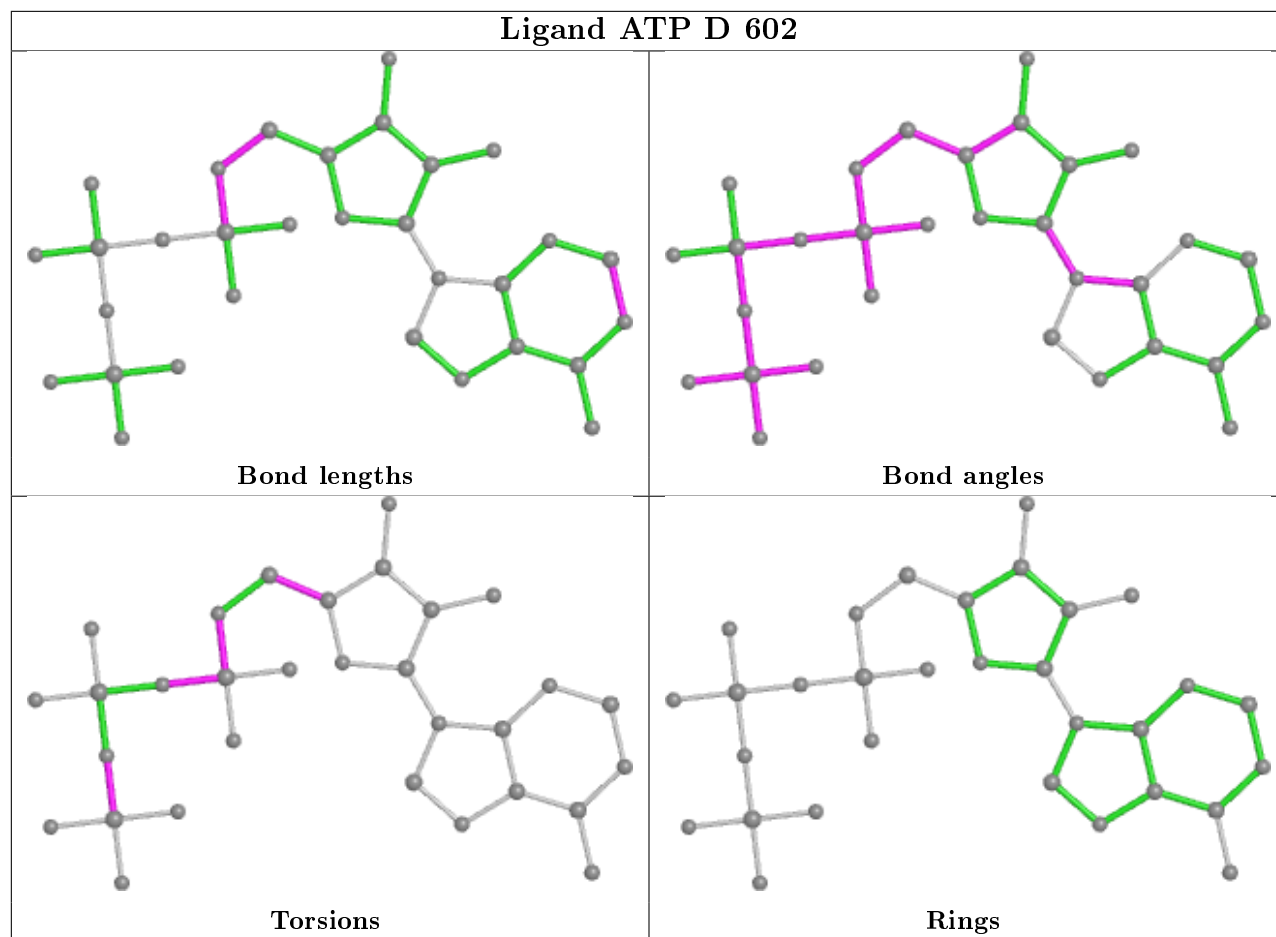




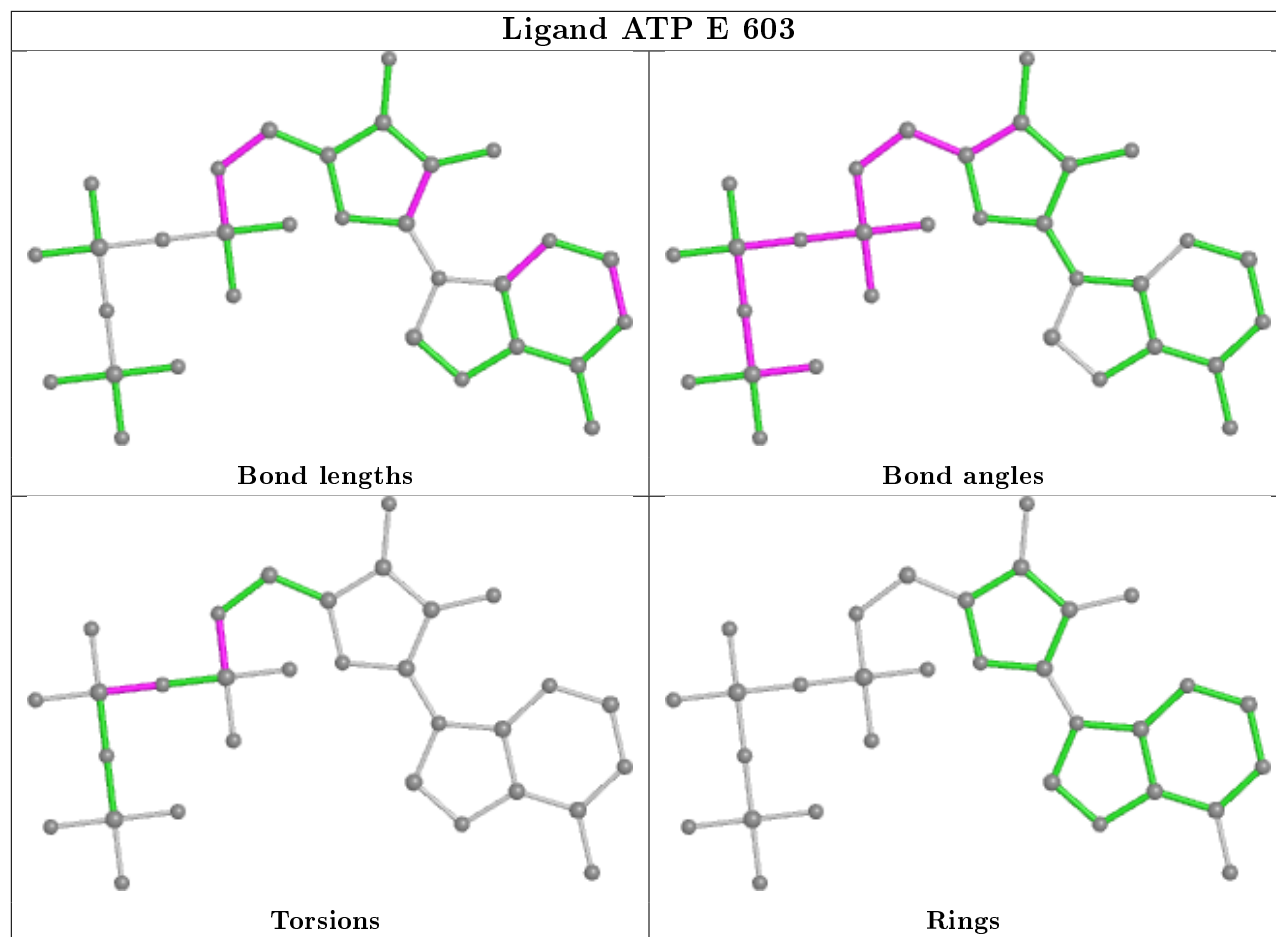


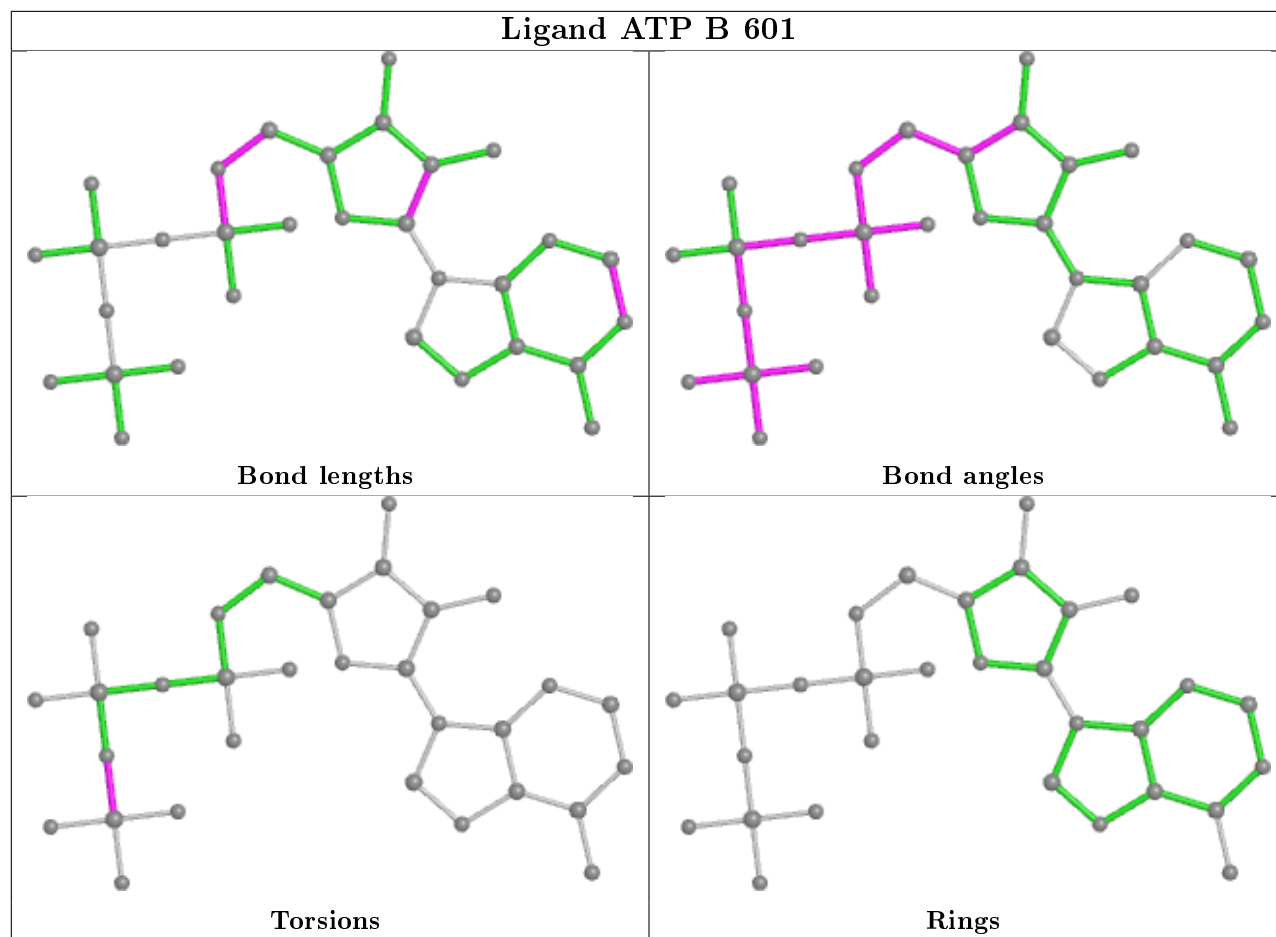


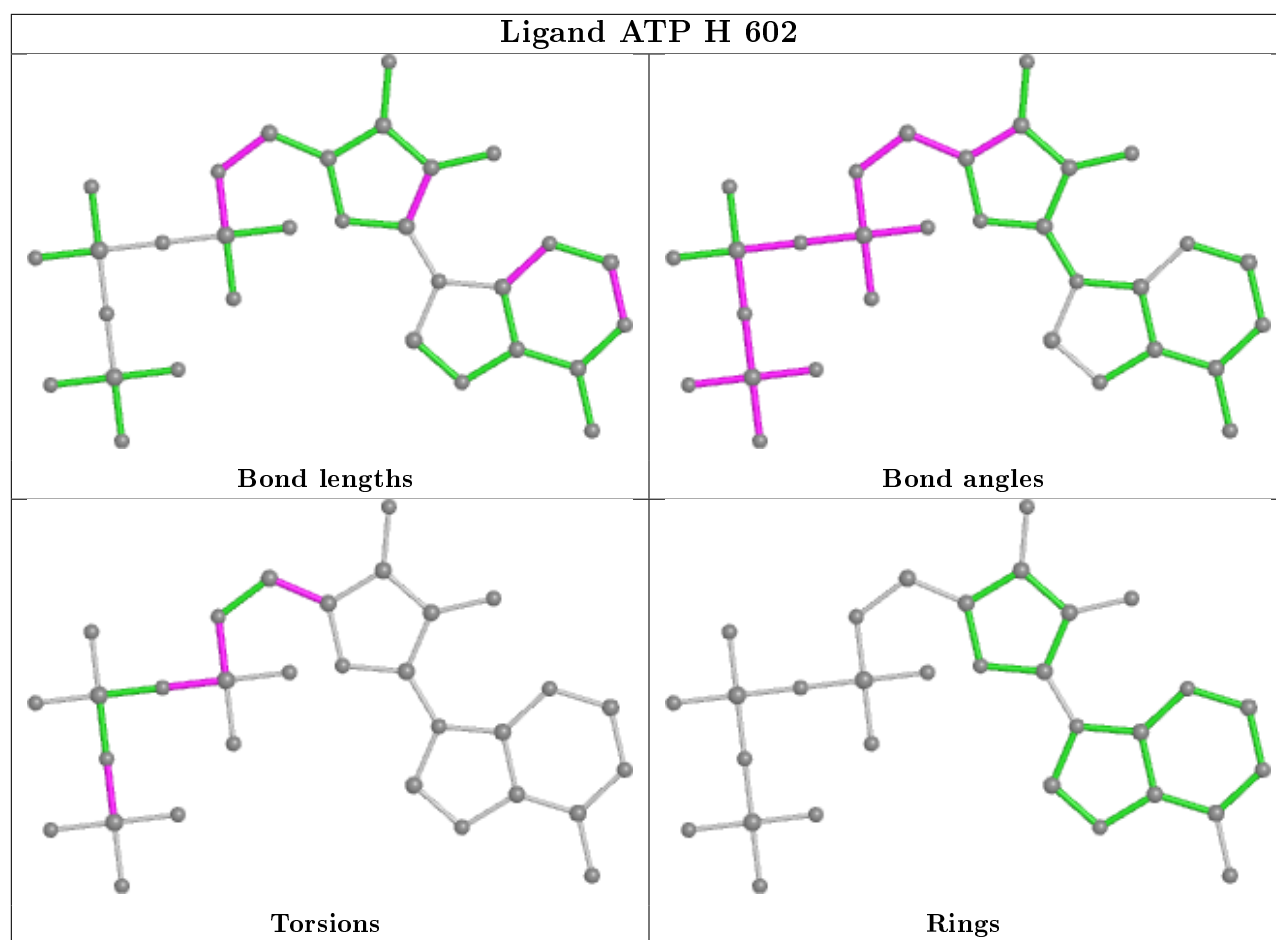


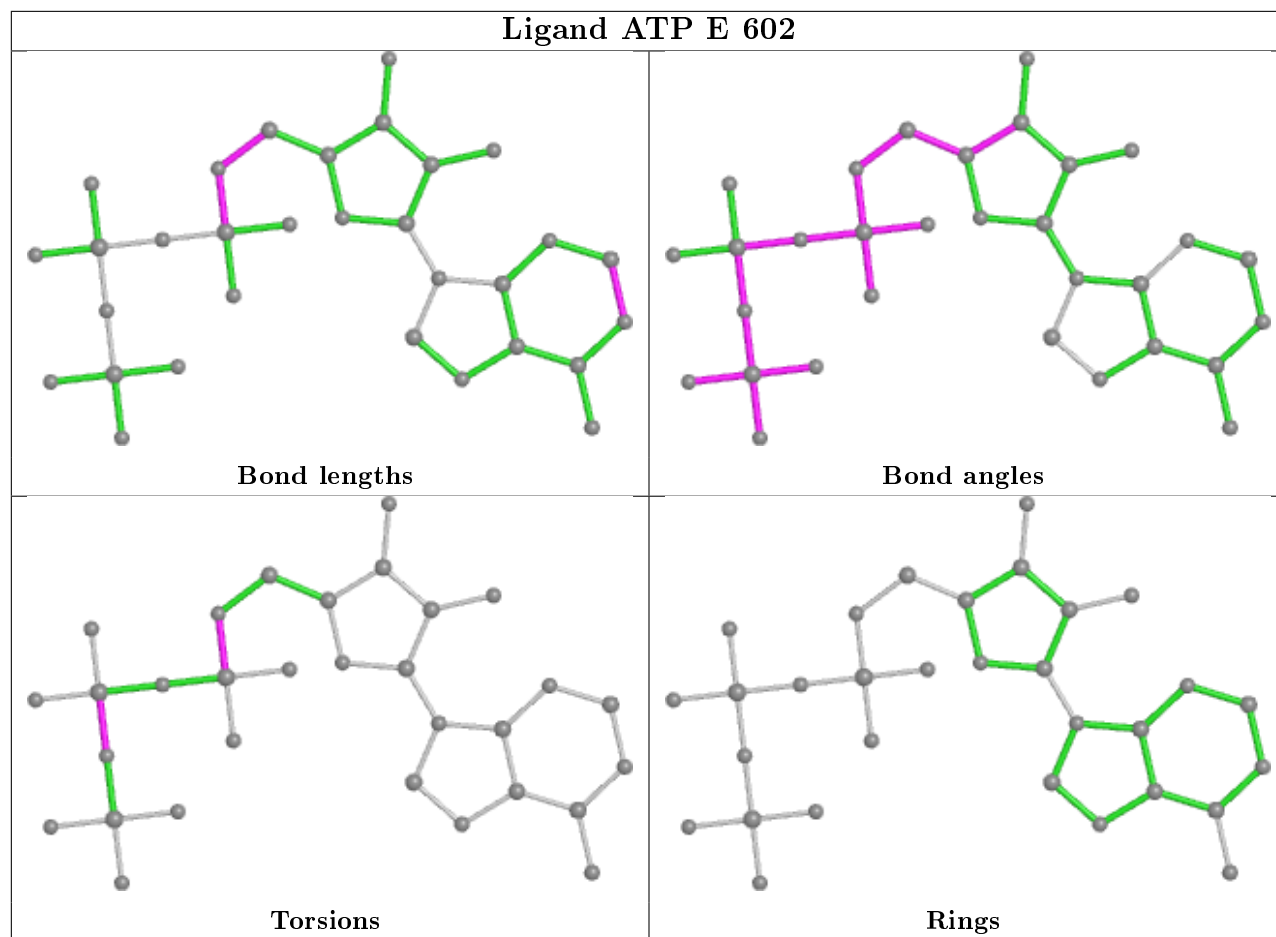


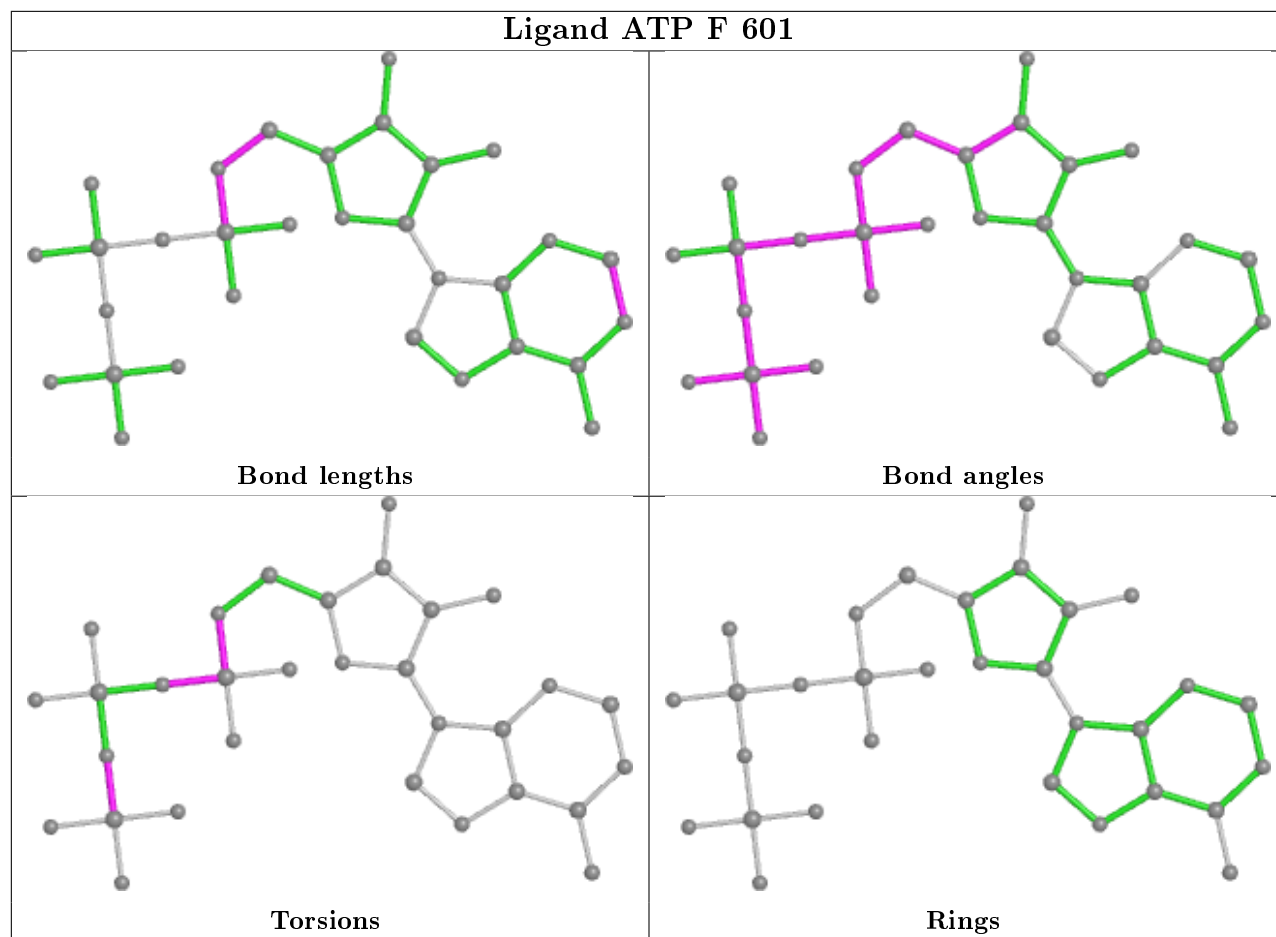


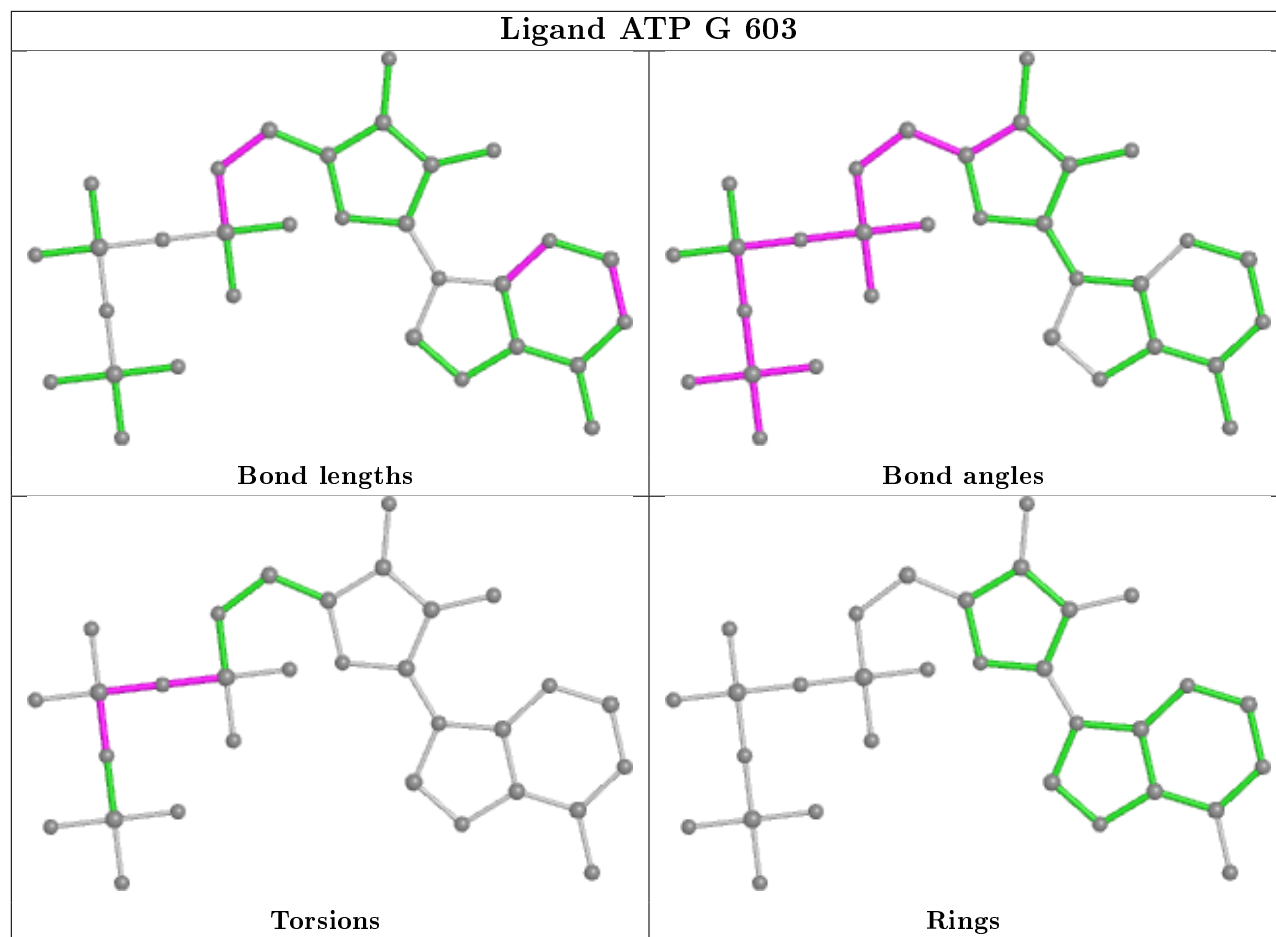


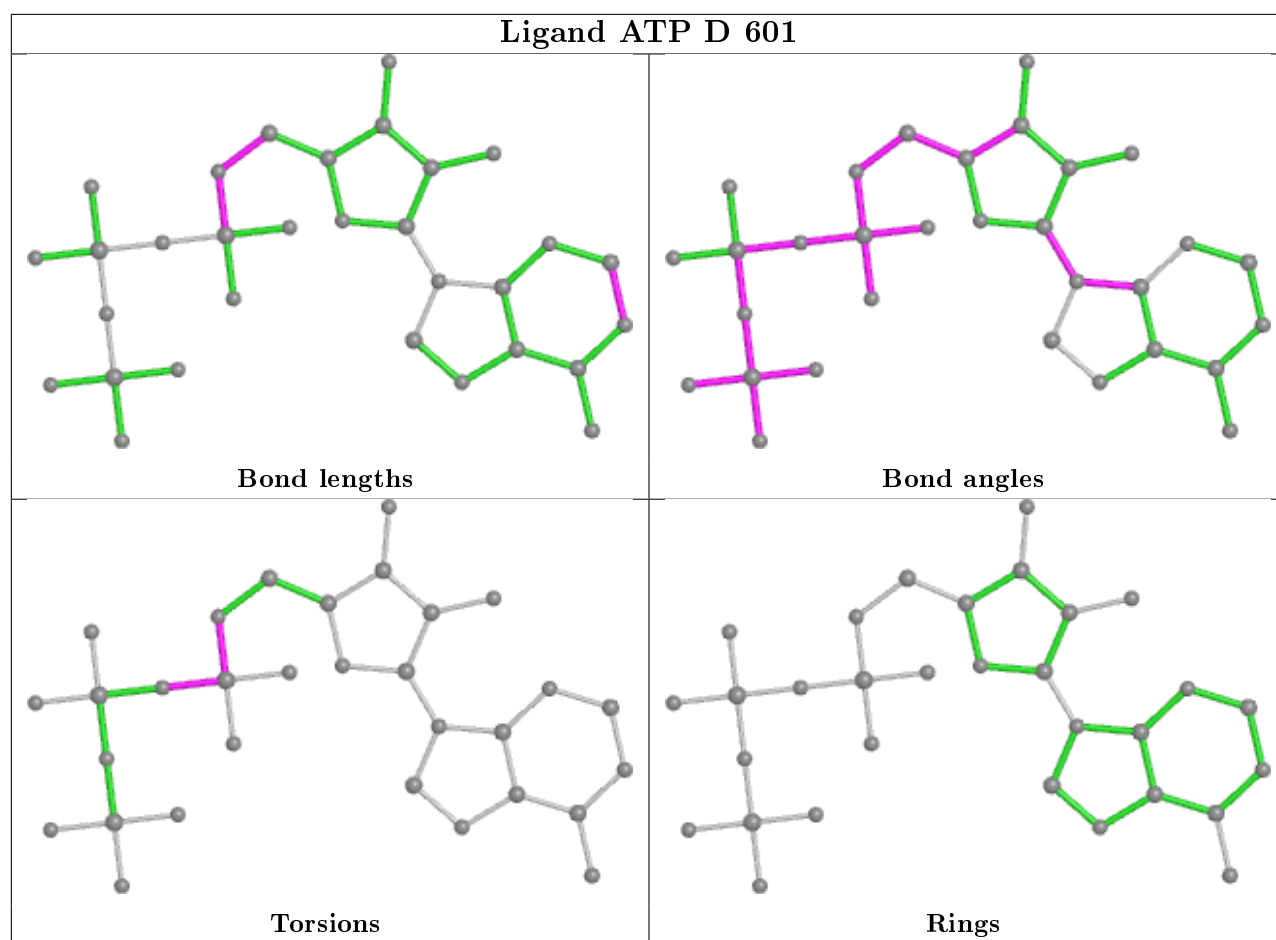


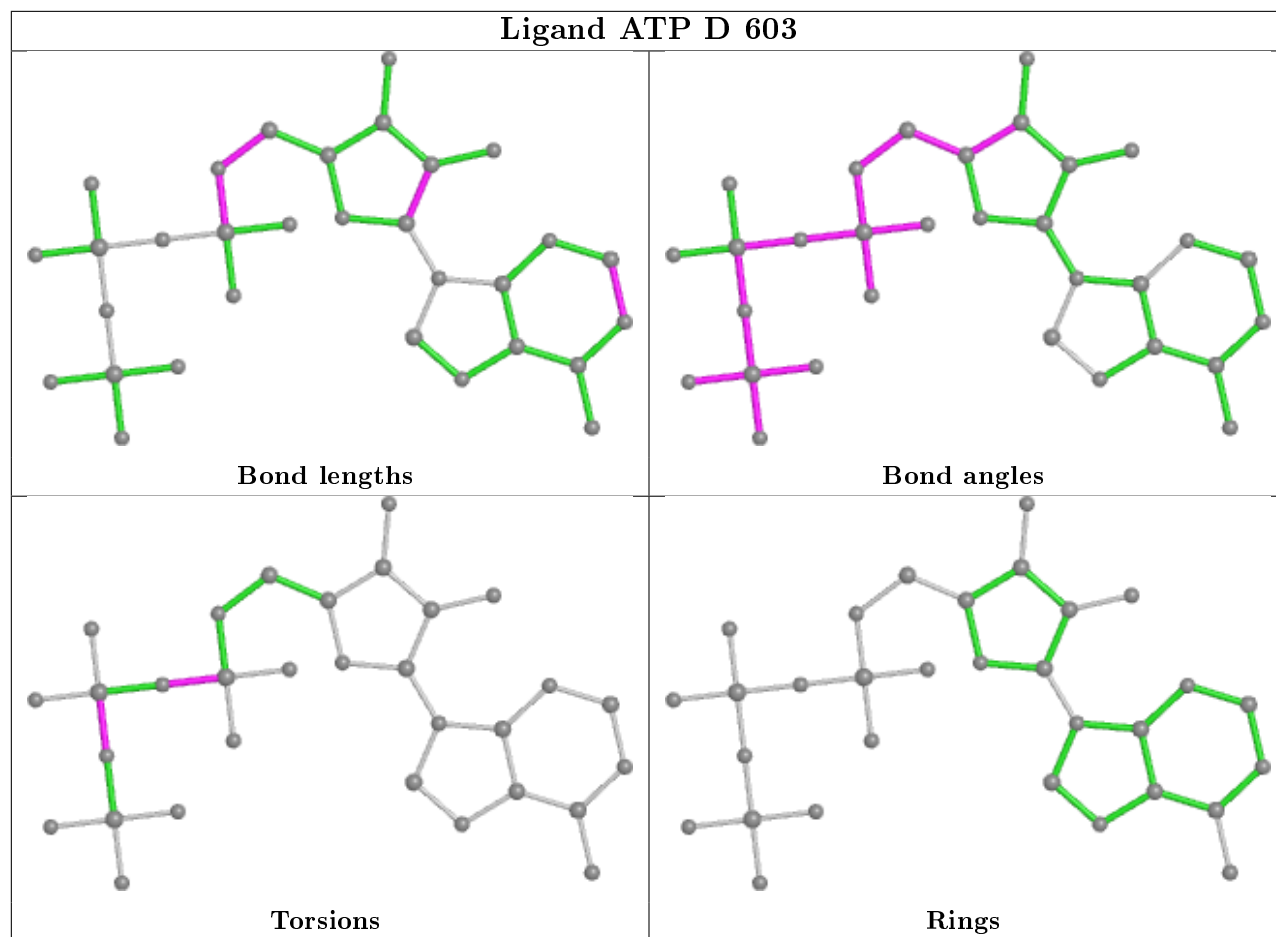




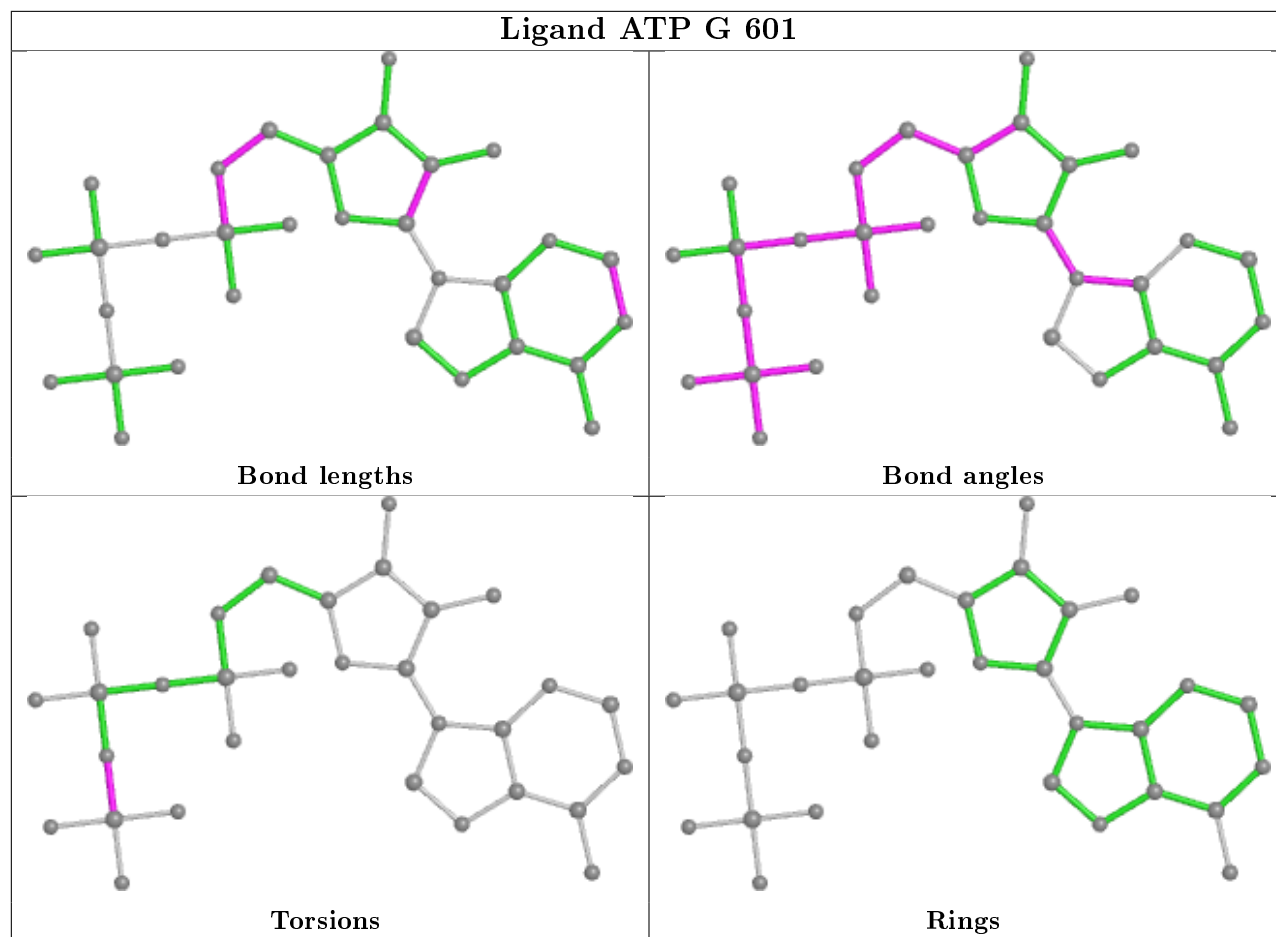


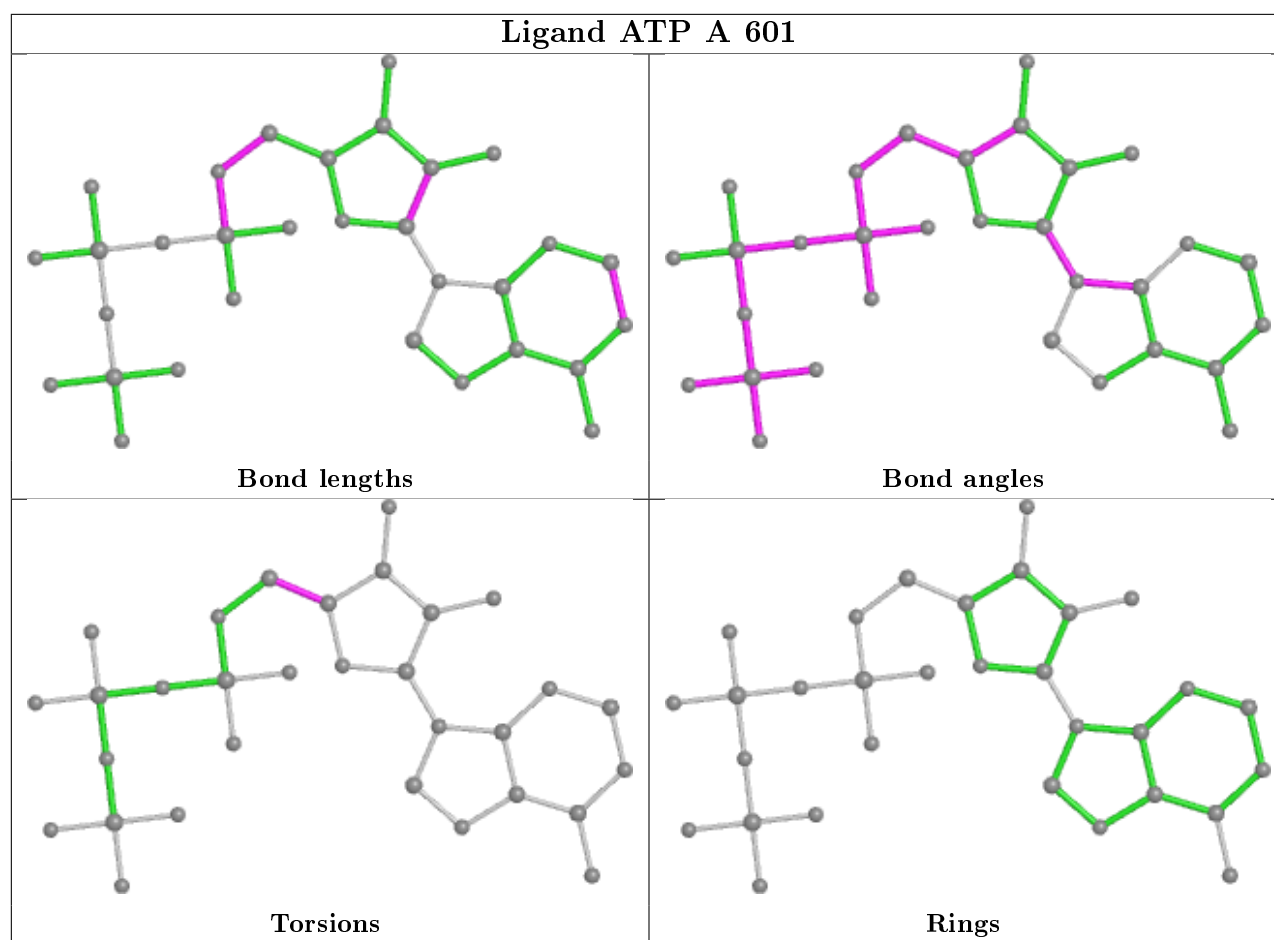












## 5.7 Other polymers [i](#)

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	440/523 (84%)	-0.10	3 (0%) 87 86	19, 36, 92, 167	0
1	B	444/523 (84%)	-0.09	11 (2%) 57 55	22, 37, 100, 144	0
1	C	446/523 (85%)	-0.11	0 100 100	20, 36, 95, 159	0
1	D	443/523 (84%)	-0.07	7 (1%) 72 70	20, 35, 91, 124	0
1	E	387/523 (73%)	0.23	18 (4%) 31 30	23, 99, 141, 182	0
1	F	342/523 (65%)	0.42	26 (7%) 13 12	71, 110, 146, 183	0
1	G	382/523 (73%)	0.52	36 (9%) 8 7	30, 106, 152, 182	0
1	H	321/523 (61%)	0.62	40 (12%) 3 3	80, 114, 153, 183	0
All	All	3205/4184 (76%)	0.15	141 (4%) 34 33	19, 77, 137, 183	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	320	GLY	5.6
1	G	38	TYR	5.4
1	H	9	ALA	4.8
1	H	326	ILE	4.8
1	F	38	TYR	4.5
1	H	486	PHE	4.5
1	H	176	THR	4.5
1	G	120	PHE	4.4
1	G	131	ALA	4.2
1	H	11	GLU	4.2
1	H	45	PRO	4.1
1	D	503	SER	4.1
1	G	472	GLN	4.0
1	H	203	LEU	3.9
1	G	313	ALA	3.9
1	B	330	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	41	PHE	3.9
1	H	360	PHE	3.8
1	E	304	ALA	3.8
1	F	196	LEU	3.7
1	E	139	MET	3.7
1	G	314	ALA	3.6
1	D	330	SER	3.6
1	B	2	THR	3.6
1	H	6	ALA	3.6
1	F	18	GLU	3.5
1	E	22	LEU	3.5
1	G	234	SER	3.5
1	H	12	HIS	3.5
1	E	305	GLY	3.5
1	H	269	ALA	3.4
1	B	232	ASN	3.4
1	F	248	LEU	3.4
1	H	210	LYS	3.4
1	G	481	ARG	3.3
1	H	300	LEU	3.3
1	H	16	TYR	3.3
1	B	226	ARG	3.3
1	H	41	PHE	3.3
1	F	17	ALA	3.2
1	F	499	PHE	3.2
1	F	16	TYR	3.1
1	F	480	VAL	3.1
1	G	479	GLY	3.0
1	H	499	PHE	3.0
1	G	319	ALA	3.0
1	G	353	VAL	3.0
1	E	144	GLY	3.0
1	H	18	GLU	2.9
1	E	300	LEU	2.9
1	E	28	MET	2.9
1	F	382	LEU	2.9
1	H	291	LYS	2.9
1	G	480	VAL	2.8
1	G	33	ARG	2.8
1	B	230	MET	2.8
1	F	61	LEU	2.8
1	E	126	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	170	GLN	2.8
1	H	38	TYR	2.8
1	A	134	ALA	2.8
1	F	320	GLY	2.7
1	E	297	PHE	2.7
1	H	321	ALA	2.7
1	G	212	PRO	2.7
1	F	14	ALA	2.7
1	F	486	PHE	2.7
1	H	384	ALA	2.7
1	F	171	PHE	2.7
1	G	316	LEU	2.7
1	H	234	SER	2.7
1	H	132	THR	2.7
1	G	469	ASN	2.7
1	D	506	LEU	2.6
1	H	10	LEU	2.6
1	G	53	SER	2.6
1	E	303	ILE	2.6
1	B	504	ALA	2.6
1	H	313	ALA	2.6
1	E	212	PRO	2.6
1	F	207	LYS	2.6
1	D	505	GLN	2.6
1	E	209	GLY	2.6
1	A	499	PHE	2.6
1	H	303	ILE	2.6
1	E	308	VAL	2.6
1	H	305	GLY	2.6
1	F	33	ARG	2.5
1	F	346	GLN	2.5
1	H	280	GLN	2.5
1	F	341	ALA	2.5
1	D	178	LEU	2.5
1	G	28	MET	2.4
1	H	139	MET	2.4
1	H	260	ARG	2.4
1	E	309	THR	2.4
1	F	9	ALA	2.3
1	B	329	GLY	2.3
1	G	356	PHE	2.3
1	F	349	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	354	THR	2.3
1	H	467	LEU	2.3
1	H	308	VAL	2.3
1	H	271	LEU	2.3
1	D	156	PRO	2.3
1	G	350	VAL	2.3
1	H	28	MET	2.3
1	E	348	THR	2.3
1	B	139	MET	2.2
1	B	131	ALA	2.2
1	A	500	ARG	2.2
1	F	30	SER	2.2
1	H	296	THR	2.2
1	F	127	VAL	2.2
1	G	71	PHE	2.2
1	G	41	PHE	2.2
1	F	149	PRO	2.2
1	G	369	GLY	2.1
1	E	36	LEU	2.1
1	H	22	LEU	2.1
1	F	351	TYR	2.1
1	G	179	VAL	2.1
1	G	368	GLY	2.1
1	G	466	TYR	2.1
1	E	61	LEU	2.1
1	G	61	LEU	2.1
1	G	198	GLU	2.1
1	G	236	PRO	2.1
1	B	506	LEU	2.1
1	H	248	LEU	2.1
1	F	239	SER	2.1
1	G	471	LEU	2.1
1	H	21	GLY	2.1
1	H	14	ALA	2.0
1	B	339	VAL	2.0
1	H	205	ASN	2.0
1	E	251	ALA	2.0
1	G	239	SER	2.0
1	G	97	ILE	2.0
1	G	160	LEU	2.0
1	G	465	PRO	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 carbohydrates 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.

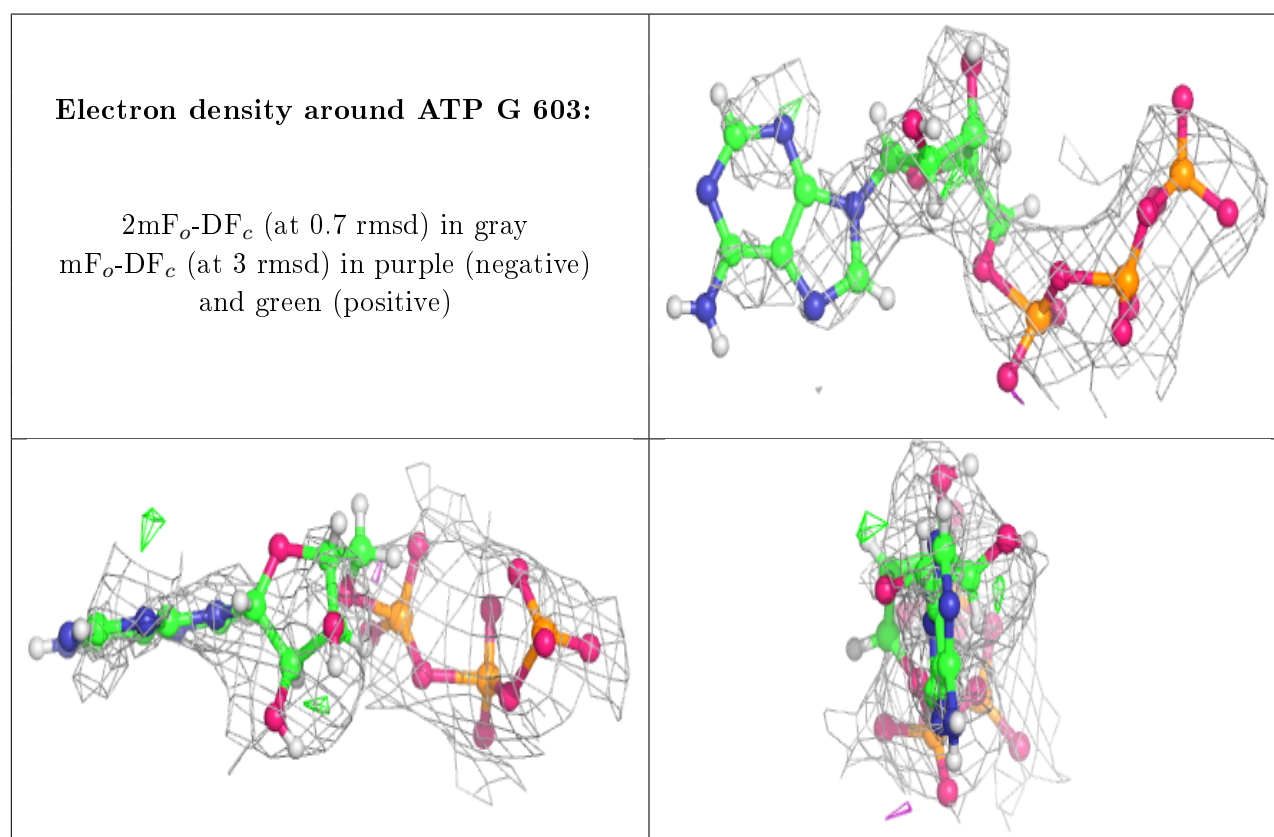
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	605	1/1	0.54	0.17	113,113,113,113	0
3	MG	B	604	1/1	0.60	0.13	79,79,79,79	0
3	MG	C	604	1/1	0.69	0.37	89,89,89,89	0
2	ATP	G	603	31/31	0.74	0.26	100,106,122,125	43
3	MG	E	605	1/1	0.76	0.17	93,93,93,93	0
2	ATP	B	606	31/31	0.77	0.19	97,103,121,123	0
2	ATP	H	603	31/31	0.80	0.19	101,111,126,129	43
2	ATP	E	603	31/31	0.80	0.20	133,141,164,166	0
2	ATP	F	601	31/31	0.84	0.13	118,133,146,153	0
2	ATP	E	602	31/31	0.84	0.17	100,102,121,124	0
2	ATP	G	602	31/31	0.86	0.15	98,105,122,123	0
2	ATP	H	602	31/31	0.86	0.14	92,97,112,117	0
3	MG	G	604	1/1	0.87	0.28	64,64,64,64	0
2	ATP	E	601	31/31	0.87	0.13	83,90,105,109	0
2	ATP	H	601	31/31	0.88	0.13	89,97,114,119	0
2	ATP	C	601	31/31	0.89	0.16	64,69,81,82	0
2	ATP	C	602	31/31	0.89	0.16	46,54,70,93	0
2	ATP	B	603	31/31	0.90	0.13	54,62,72,72	0
2	ATP	A	603	31/31	0.91	0.13	47,57,71,71	0
2	ATP	B	605	31/31	0.91	0.12	92,100,118,127	0
2	ATP	D	603	31/31	0.91	0.14	53,59,73,74	0
2	ATP	G	601	31/31	0.91	0.12	81,89,103,108	0
3	MG	F	602	1/1	0.92	0.24	95,95,95,95	0
2	ATP	C	603	31/31	0.92	0.14	50,59,70,73	0
2	ATP	D	602	31/31	0.93	0.13	45,49,63,68	0
2	ATP	A	601	31/31	0.93	0.16	50,58,67,70	0
2	ATP	B	601	31/31	0.94	0.14	63,67,80,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ATP	B	602	31/31	0.94	0.12	49,59,67,68	0
2	ATP	A	602	31/31	0.94	0.15	49,55,64,68	0
3	MG	D	604	1/1	0.95	0.18	87,87,87,87	0
3	MG	E	604	1/1	0.95	0.34	86,86,86,86	0
2	ATP	D	601	31/31	0.95	0.13	49,51,61,75	0

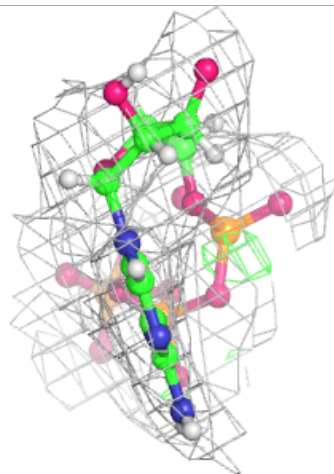
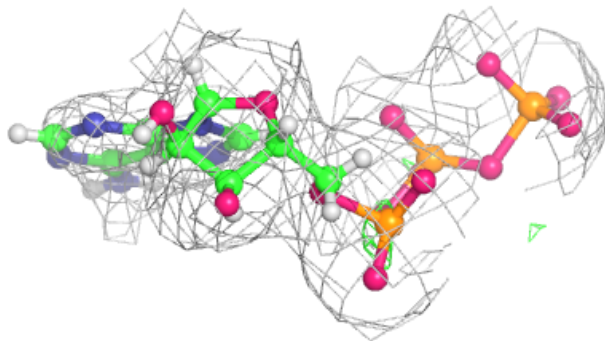
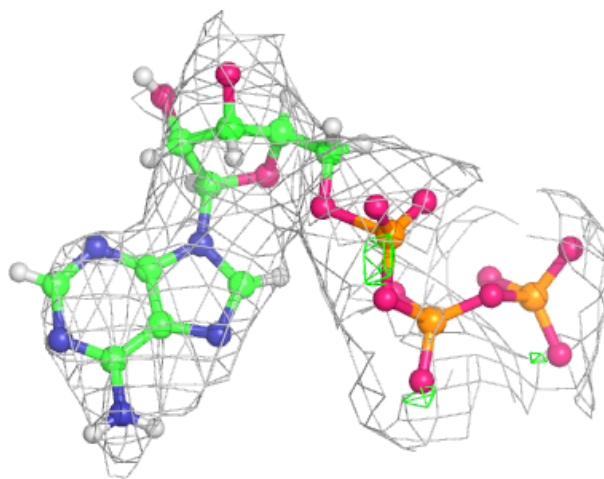
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





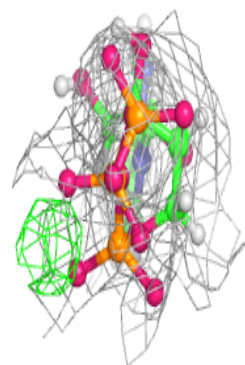
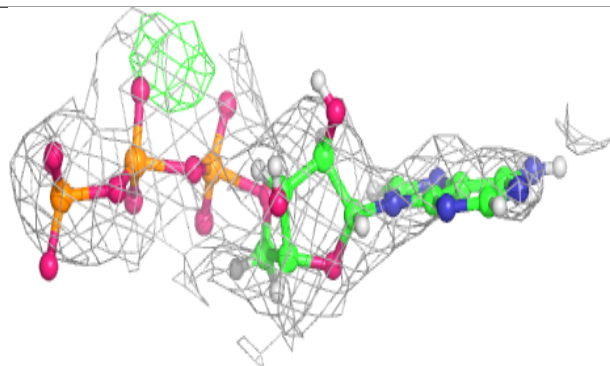
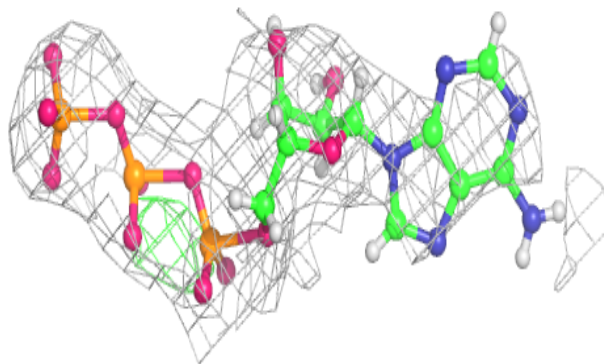
**Electron density around ATP B 606:**

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

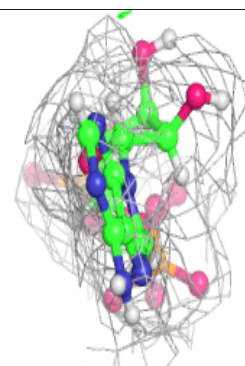
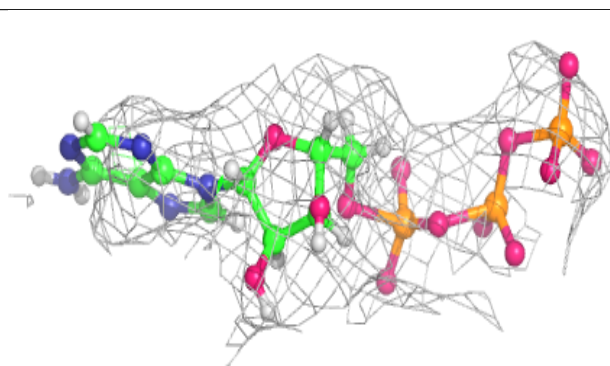
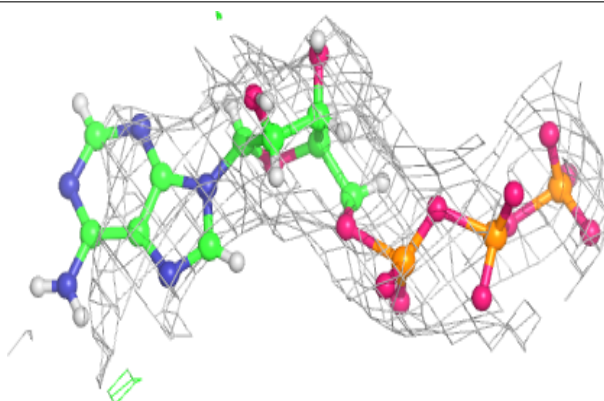


**Electron density around ATP H 603:**

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and green (positive)

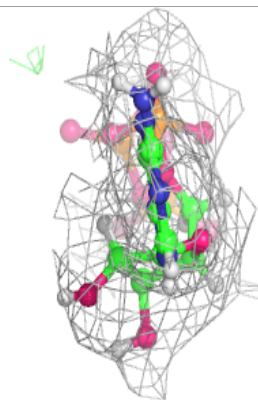
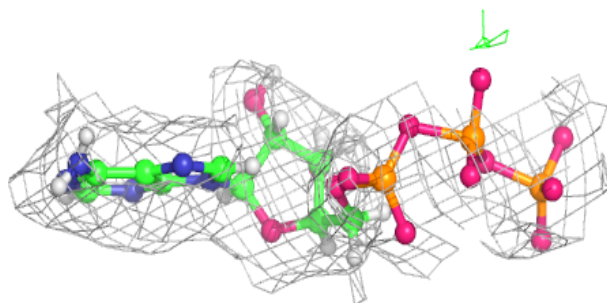
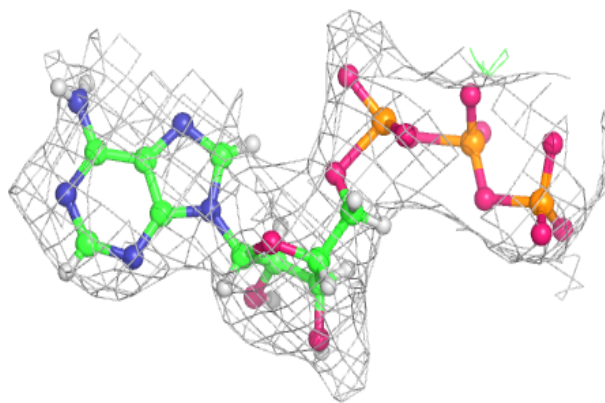
**Electron density around ATP E 603:**

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and green (positive)

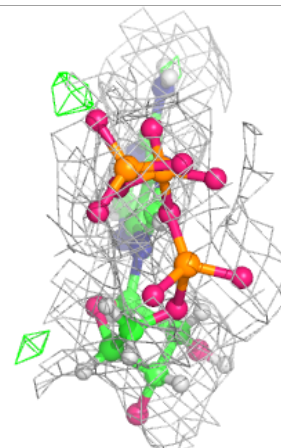
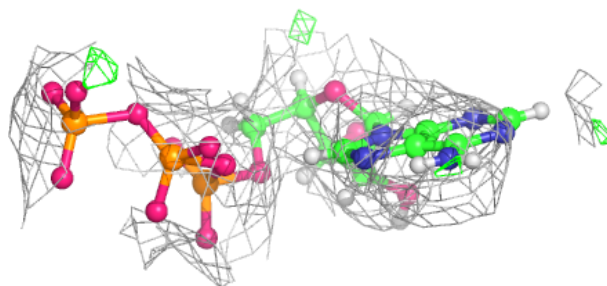
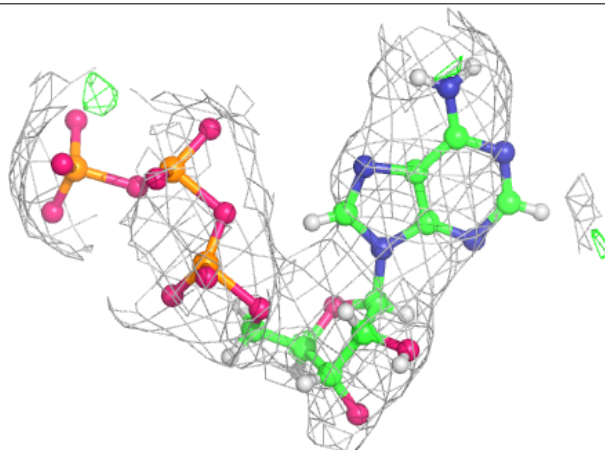


**Electron density around ATP F 601:**

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and green (positive)

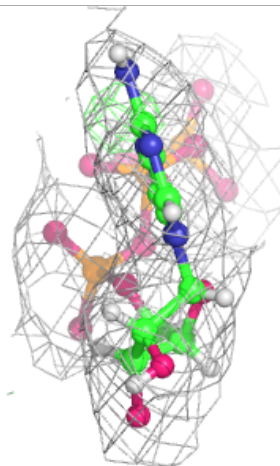
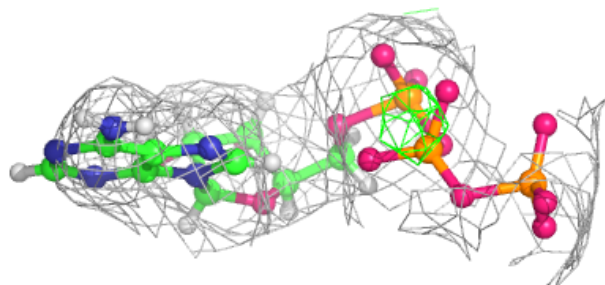
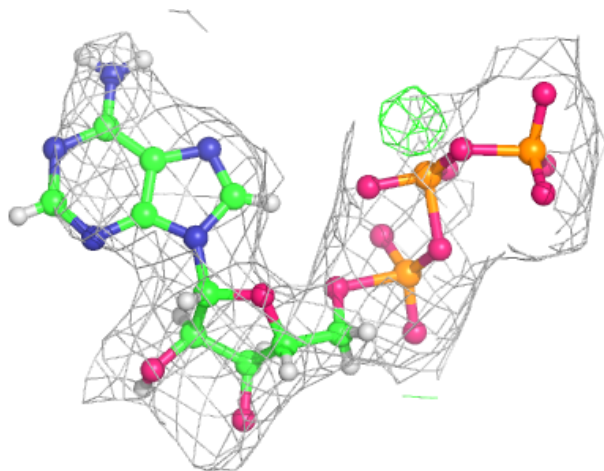
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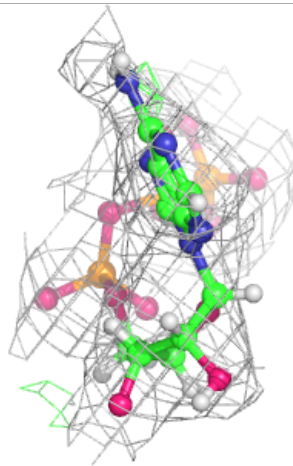
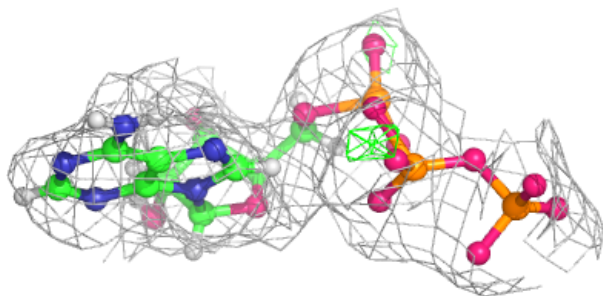
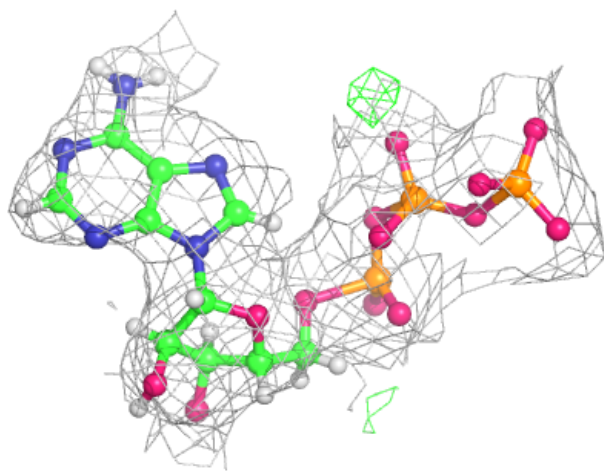
**Electron density around ATP G 602:**

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and green (positive)



**Electron density around ATP H 602:**

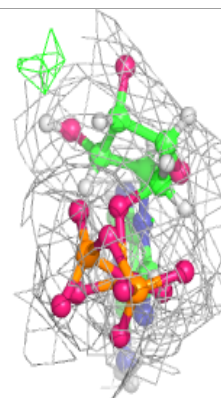
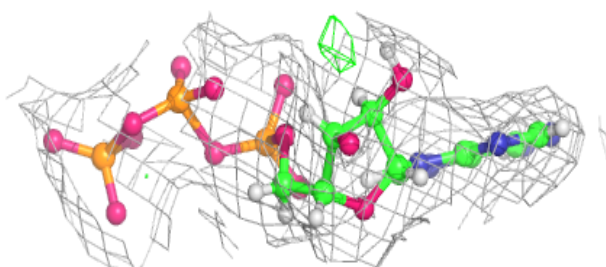
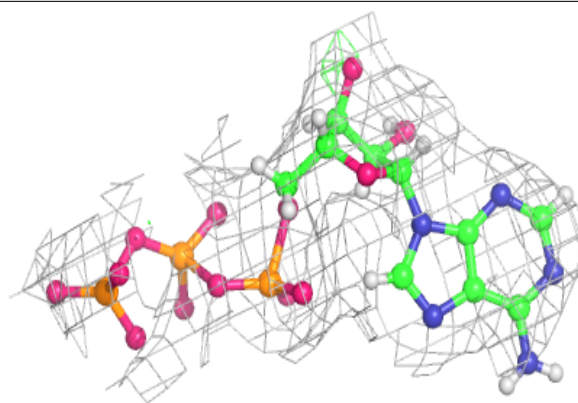
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and green (positive)



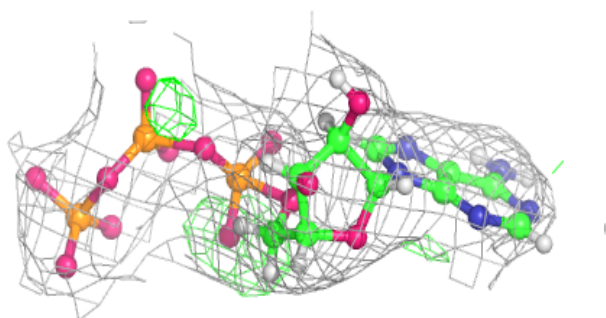
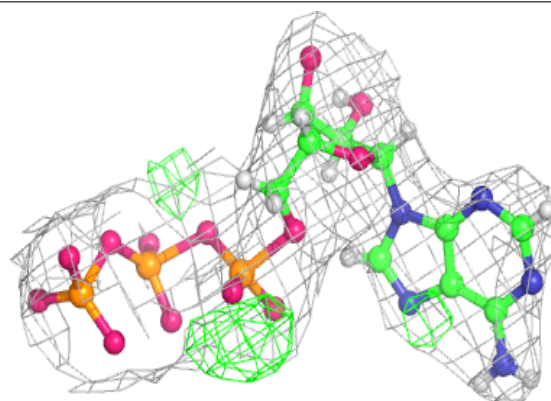


**Electron density around ATP E 601:**

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and green (positive)

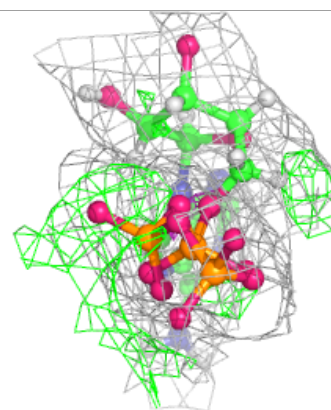
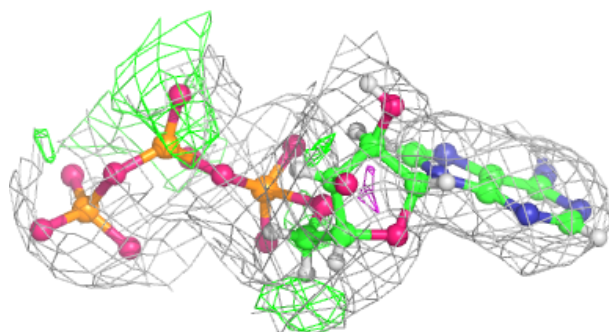
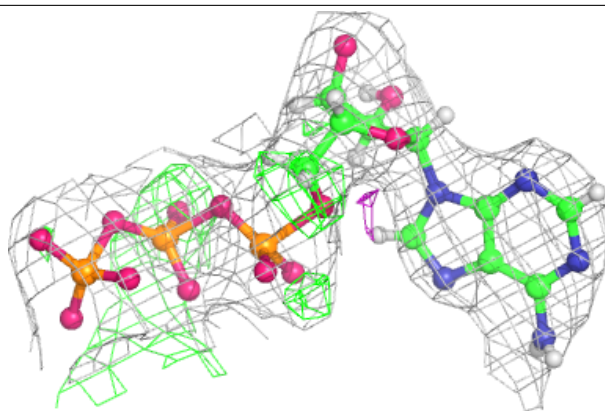
**Electron density around ATP H 601:**

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and green (positive)



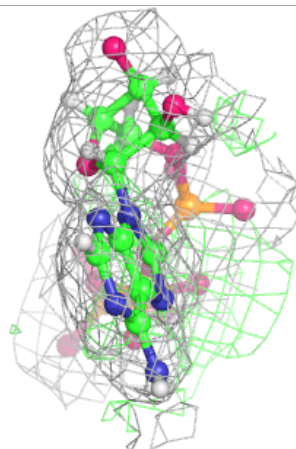
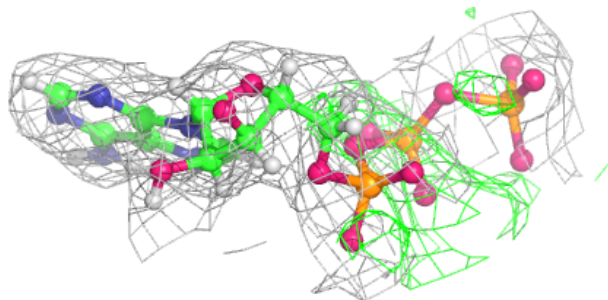
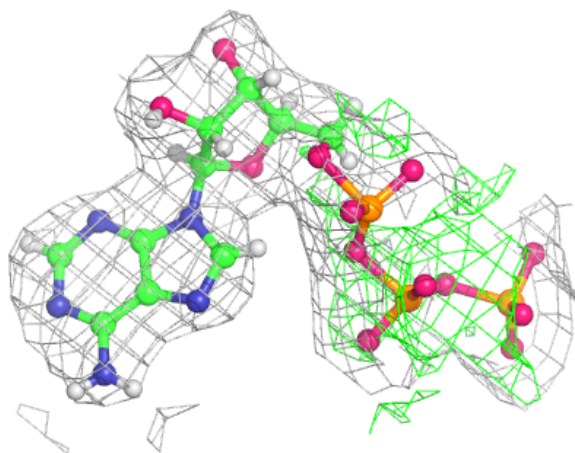
**Electron density around ATP C 601:**

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and green (positive)



**Electron density around ATP C 602:**

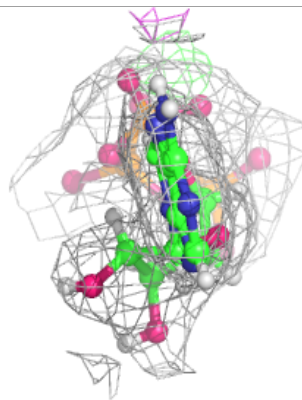
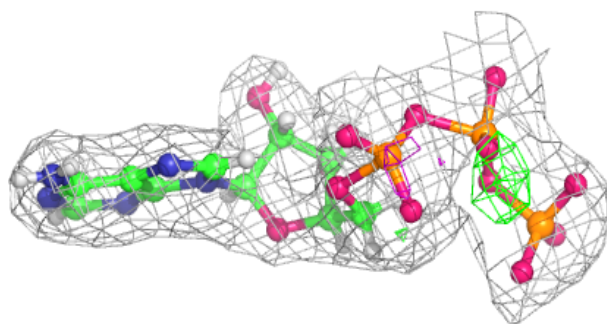
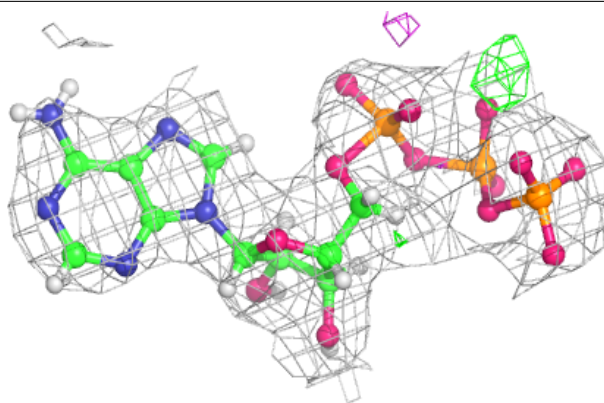
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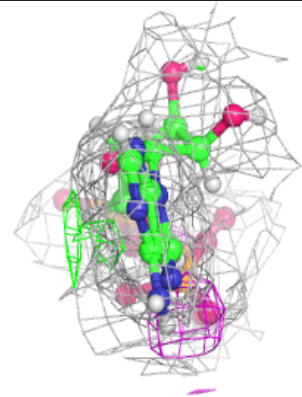
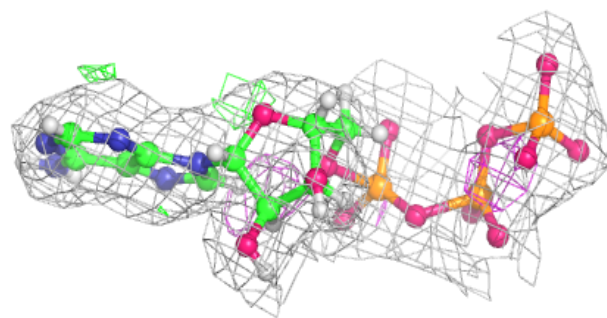
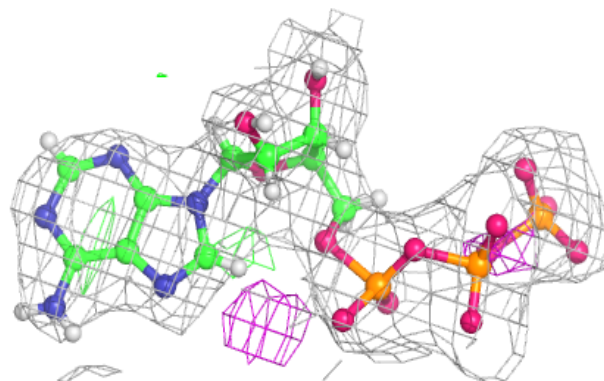


**Electron density around ATP B 603:**

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and green (positive)

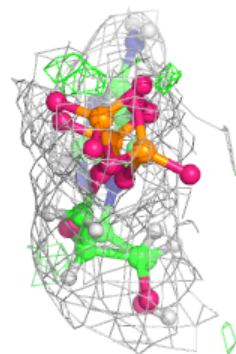
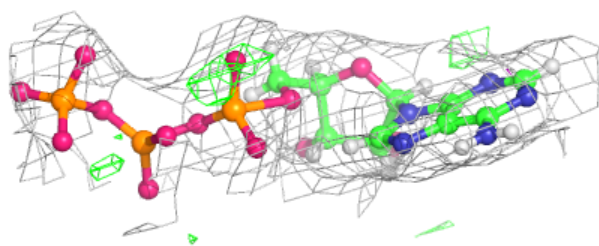
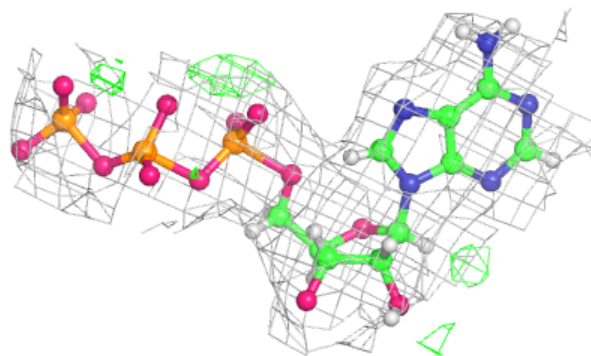
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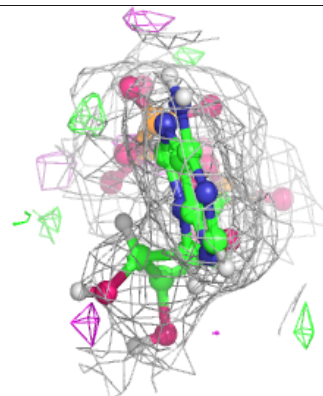
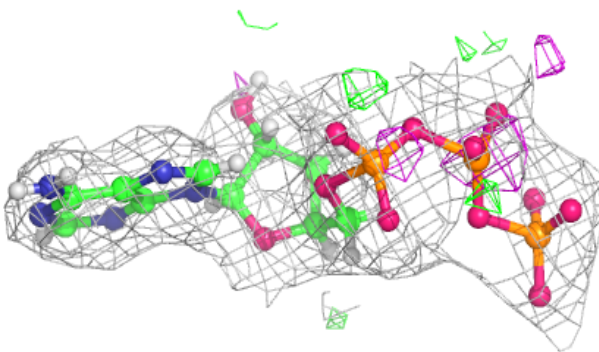
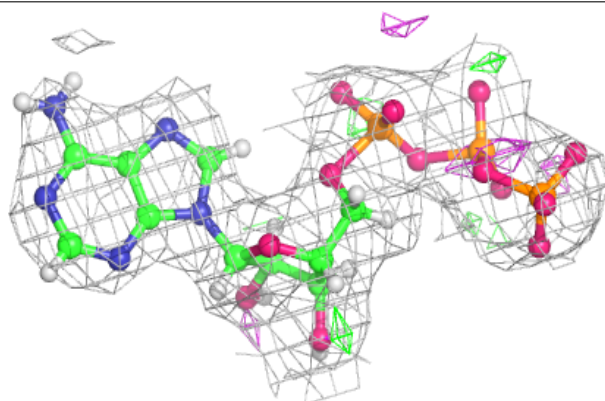


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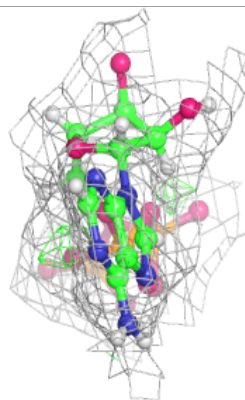
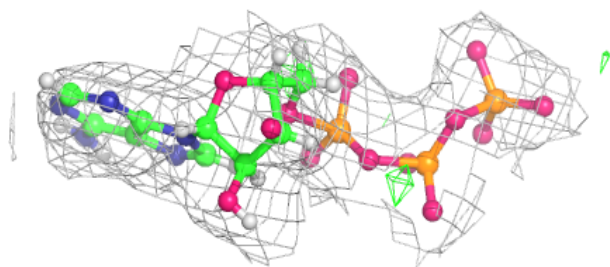
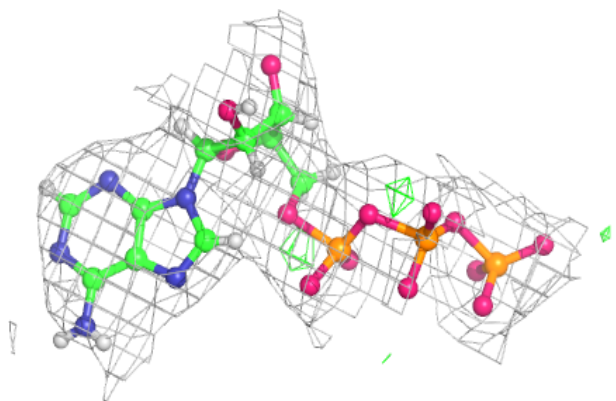
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and green (positive)

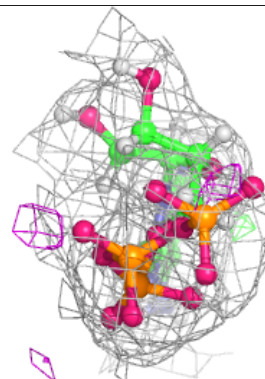
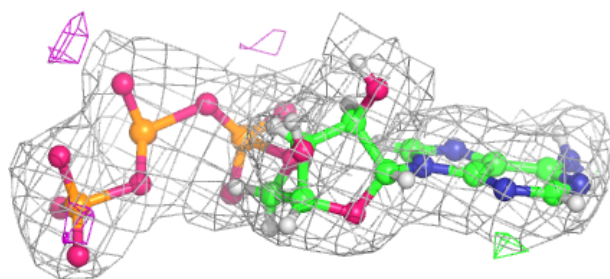
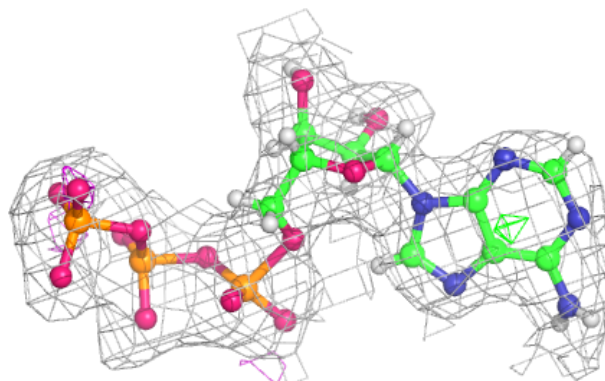


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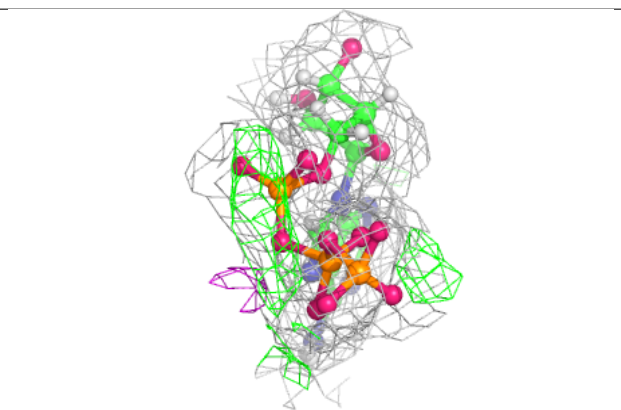
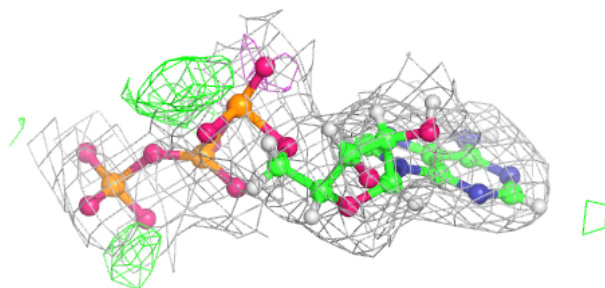
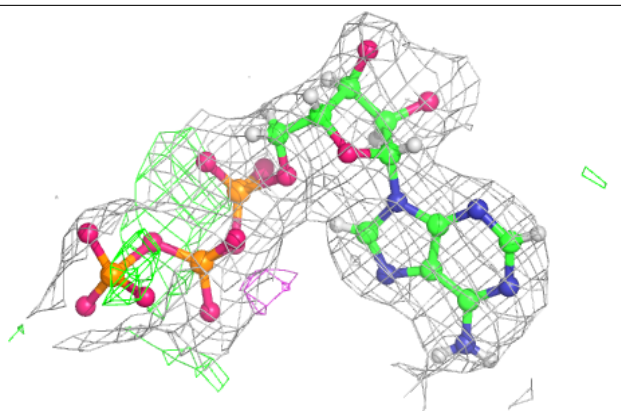
**Electron density around ATP C 603:**

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

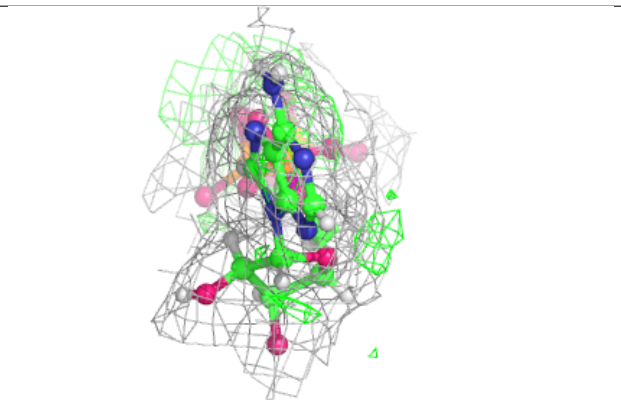
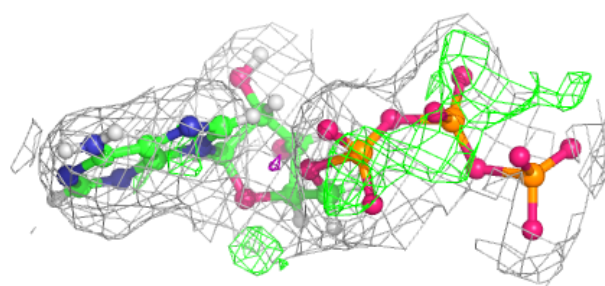
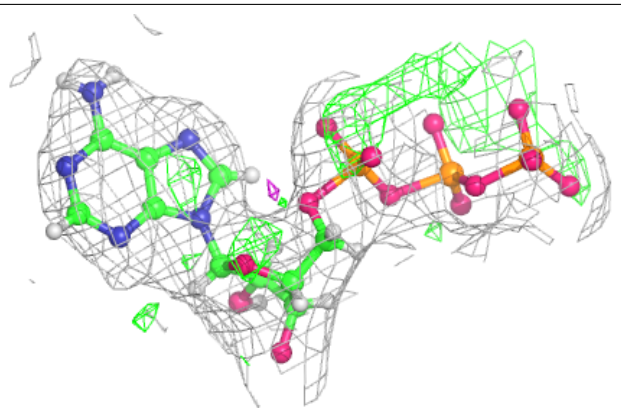


**Electron density around ATP D 602:**

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

**Electron density around ATP A 601:**

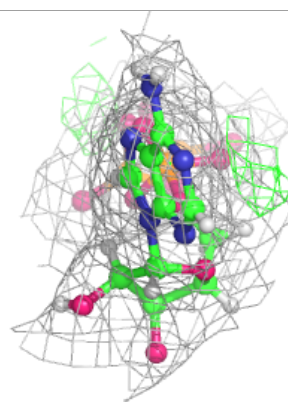
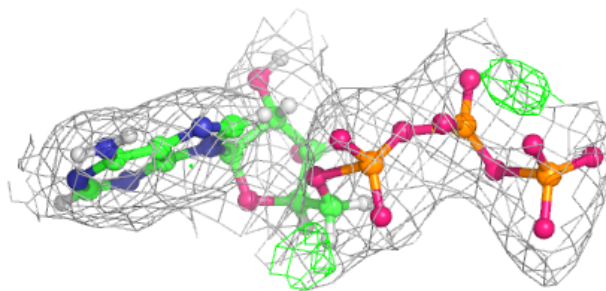
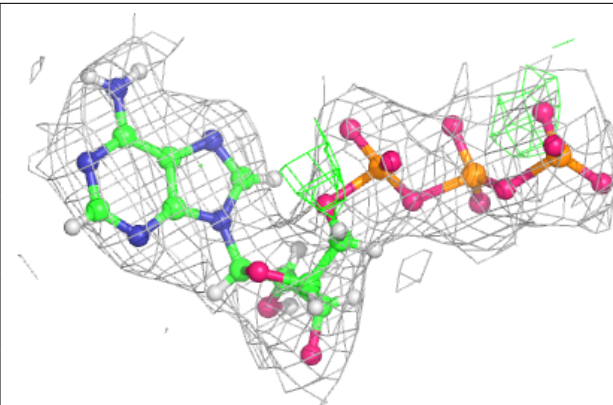
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





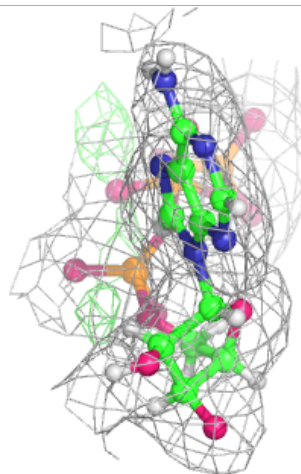
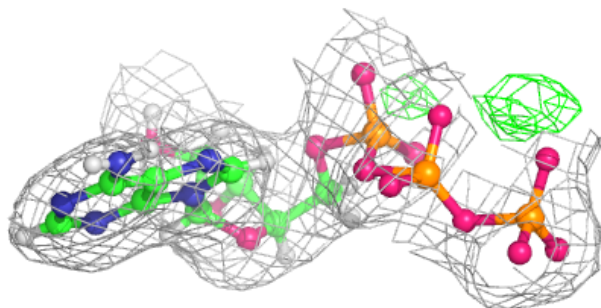
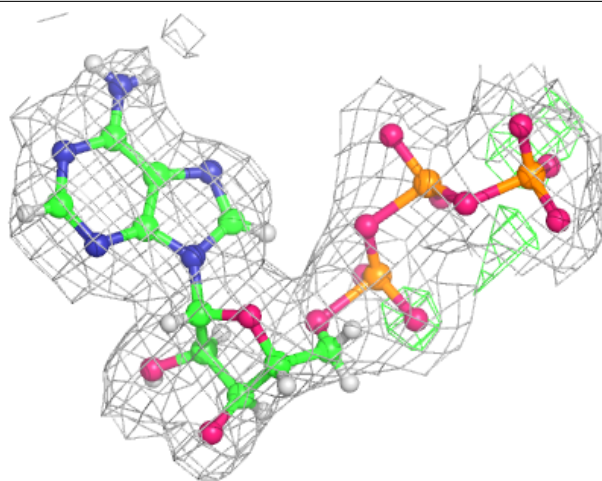
**Electron density around ATP B 601:**

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



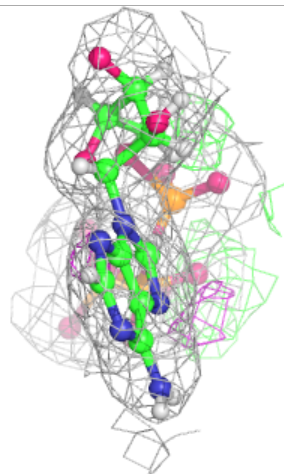
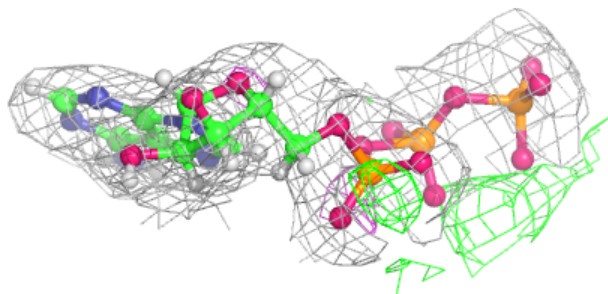
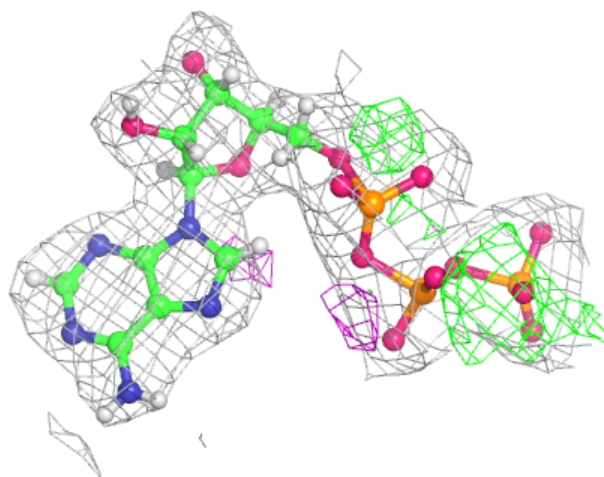
**Electron density around ATP B 602:**

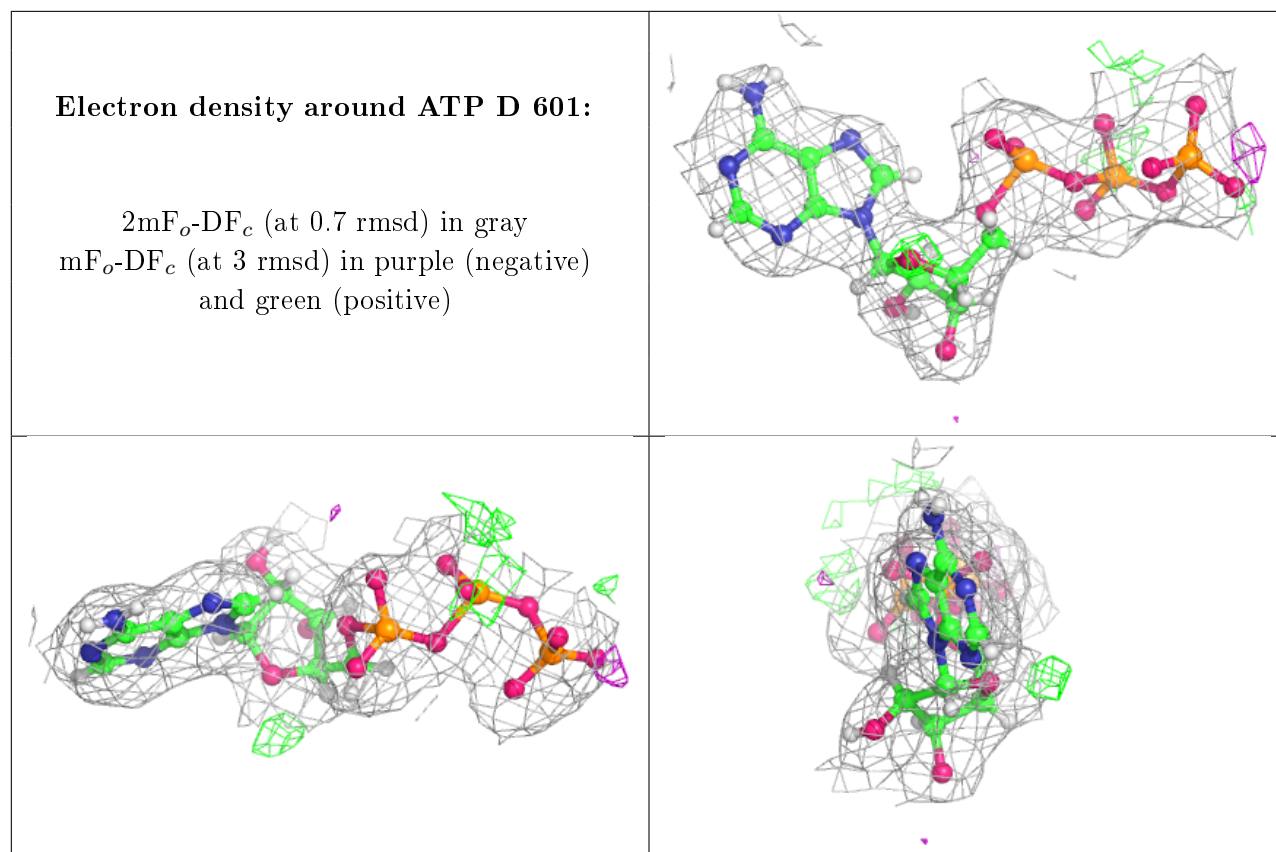
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 602:**

$2mF_o-DF_c$  (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.