



# Full wwPDB X-ray Structure Validation Report ⓘ

May 10, 2022 – 12:14 AM JST

PDB ID : 7DY1  
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC  
Authors : Furuike, Y.; Akiyama, S.  
Deposited on : 2021-01-20  
Resolution : 2.20 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 : 2.28.1  
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) : 2.28.1

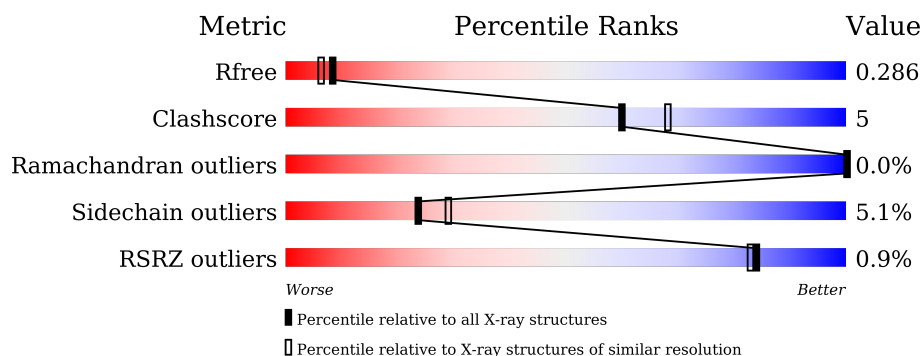
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	518	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 11%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>76%</span> <span>11%</span> <span>•</span> <span>12%</span> </div> </div>
2	B	518	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 77%, yellow 10%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>77%</span> <span>10%</span> <span>•</span> <span>13%</span> </div> </div>
2	C	518	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 75%, yellow 12%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span></span> <span>75%</span> <span>12%</span> <span>•</span> <span>12%</span> </div> </div>
2	D	518	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 11%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>76%</span> <span>11%</span> <span>•</span> <span>12%</span> </div> </div>
2	E	518	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 75%, yellow 12%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>75%</span> <span>12%</span> <span>•</span> <span>12%</span> </div> </div>
2	F	518	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 11%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>76%</span> <span>11%</span> <span></span> <span>12%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21975 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	P	S	0	1	0
			3462	2197	596	658	1	10			

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	452	Total	C	N	O	P	S	0	1	0
			3413	2163	586	652	2	10			
2	C	456	Total	C	N	O	P	S	0	0	0
			3459	2187	600	660	2	10			
2	D	458	Total	C	N	O	P	S	0	2	0
			3491	2213	600	666	2	10			
2	E	455	Total	C	N	O	P	S	0	1	0
			3481	2205	598	666	2	10			
2	F	456	Total	C	N	O	P	S	0	0	0
			3448	2188	596	652	2	10			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

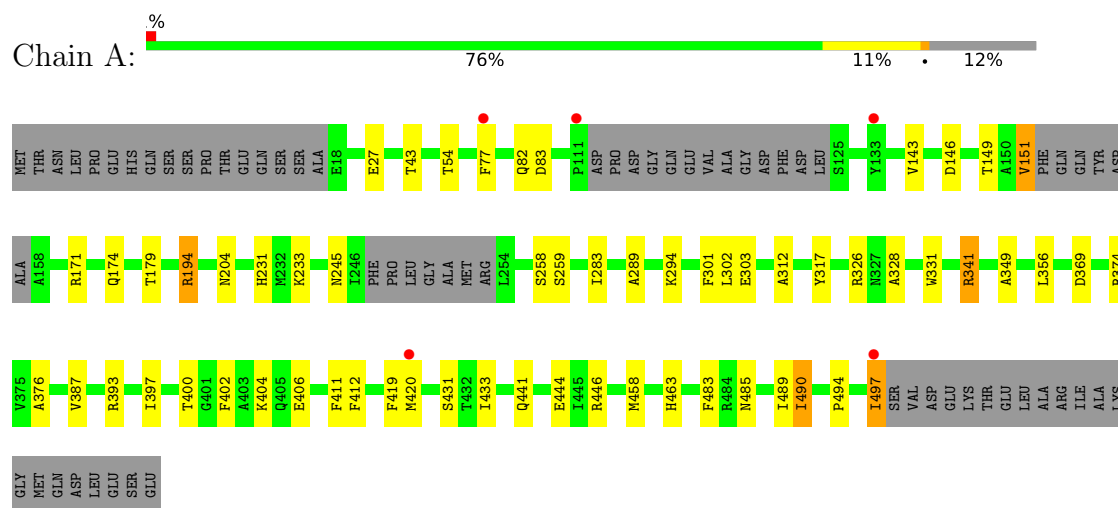
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	137	Total O 137 137	0	0
5	B	137	Total O 137 137	0	0
5	C	142	Total O 142 142	0	0
5	D	161	Total O 161 161	0	0
5	E	127	Total O 127 127	0	0
5	F	133	Total O 133 133	0	0

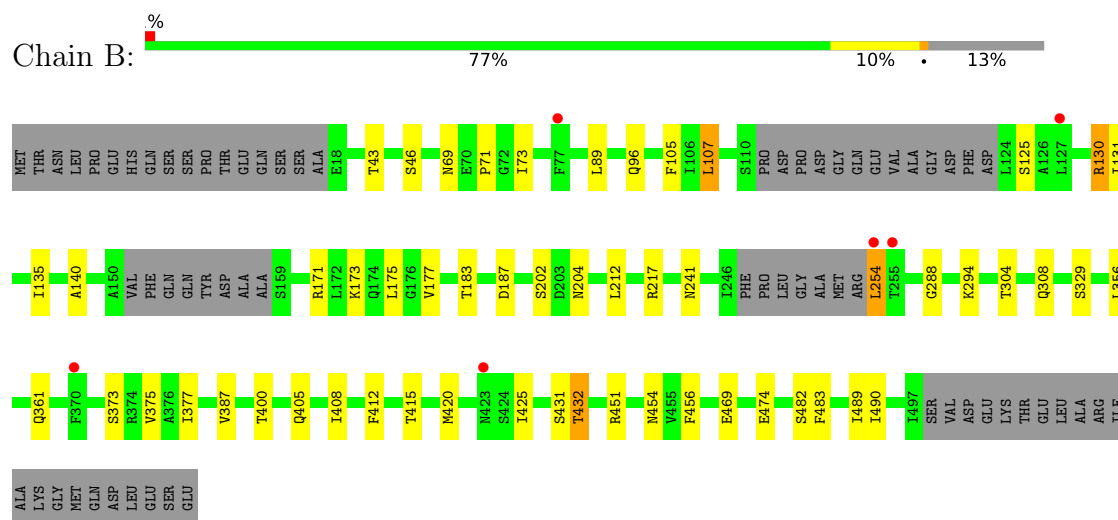
### 3 Residue-property plots [i](#)

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: Circadian clock protein kinase KaiC

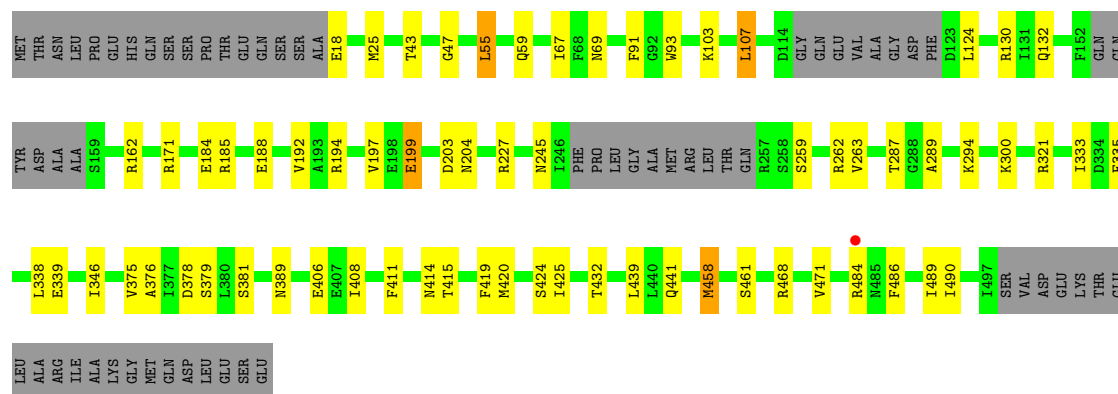


#### • Molecule 2: Circadian clock protein kinase KaiC

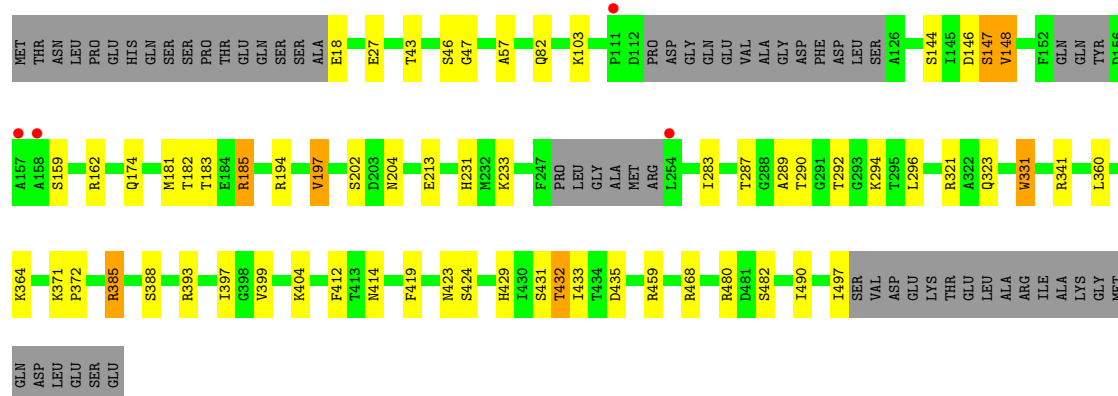
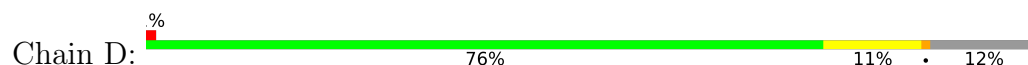


#### • Molecule 2: Circadian clock protein kinase KaiC

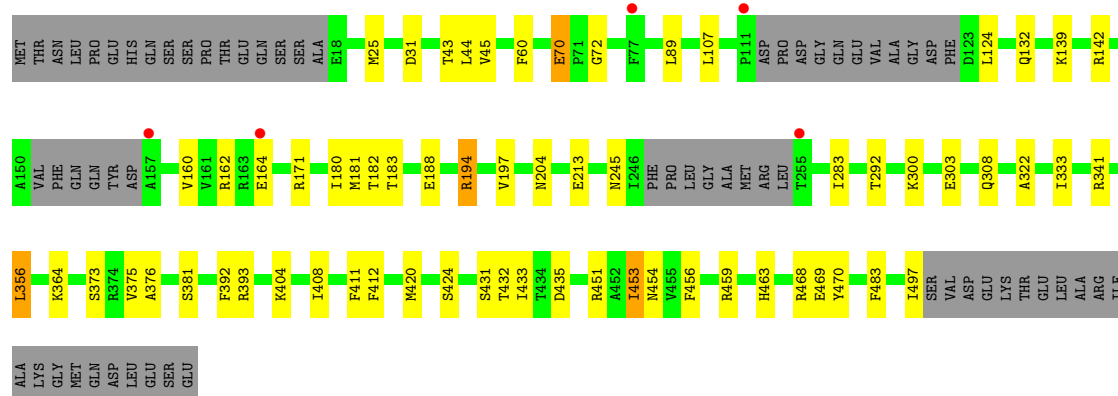
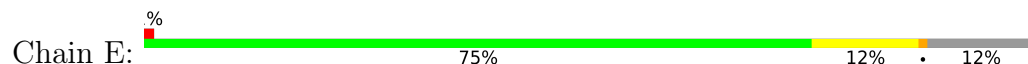




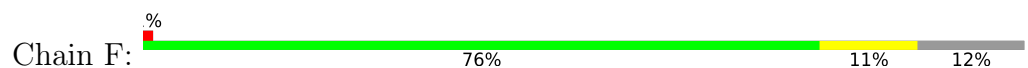
• Molecule 2: Circadian clock protein kinase KaiC

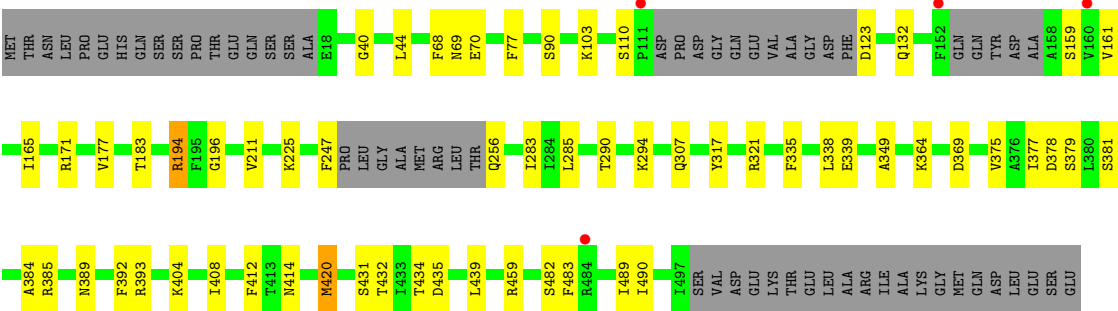


• Molecule 2: Circadian clock protein kinase KaiC



• Molecule 2: Circadian clock protein kinase KaiC







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.10Å 136.49Å 190.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 2.20 47.28 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.28-2.20) 99.7 (47.28-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.233 , 0.284 0.238 , 0.286	Depositor DCC
$R_{free}$ test set	8569 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5310e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, SEP, TPO

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	0.75	0/3508	0.85	0/4738
2	B	0.74	0/3446	0.82	0/4659
2	C	0.74	0/3492	0.84	0/4716
2	D	0.76	0/3529	0.84	0/4769
2	E	0.73	0/3516	0.84	1/4747 (0.0%)
2	F	0.74	0/3480	0.83	0/4703
All	All	0.74	0/20971	0.84	1/28332 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	70	GLU	CB-CA-C	5.26	120.92	110.40

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	3462	0	3409	35	0
2	B	3413	0	3333	30	0
2	C	3459	0	3361	37	0
2	D	3491	0	3428	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3481	0	3424	31	0
2	F	3448	0	3367	36	0
3	A	62	0	24	0	0
3	B	62	0	24	0	0
3	C	62	0	24	1	0
3	D	62	0	24	2	0
3	E	62	0	24	1	0
3	F	62	0	24	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	137	0	0	1	0
5	B	137	0	0	3	0
5	C	142	0	0	4	0
5	D	161	0	0	4	0
5	E	127	0	0	0	0
5	F	133	0	0	3	0
All	All	21975	0	20466	191	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 5.

All (191) 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)
2:D:432:TPO:O3P	5:D:701:HOH:O	1.86	0.92
2:C:192:VAL:CB	2:C:199:GLU:HG2	2.11	0.80
2:D:162:ARG:HG3	2:D:197:VAL:HG22	1.65	0.79
2:C:335:PHE:O	2:C:339:GLU:HG3	1.88	0.73
2:E:160:VAL:O	2:E:164:GLU:HG2	1.89	0.73
2:F:90:SER:HG	3:F:601:ATP:HN61	1.39	0.70
2:B:432:TPO:O3P	5:B:701:HOH:O	2.10	0.70
2:C:59:GLN:HG3	2:C:93:TRP:CH2	2.28	0.68
2:D:162:ARG:HG3	2:D:197:VAL:CG2	2.25	0.67
2:C:375:VAL:HG23	2:C:408:ILE:HG21	1.78	0.66
2:D:435:ASP:HA	2:D:459:ARG:HD2	1.77	0.65
2:D:393:ARG:NH2	2:D:429:HIS:O	2.28	0.65
2:F:90:SER:OG	3:F:601:ATP:N6	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:LEU:HD21	2:C:91:PHE:CE2	2.32	0.65
2:D:432:TPO:P	5:D:701:HOH:O	2.54	0.64
2:F:335:PHE:O	2:F:339:GLU:HG3	1.97	0.63
2:B:131:ILE:O	2:B:135:ILE:HG13	1.98	0.63
2:C:300:LYS:HD3	2:C:333:ILE:HD11	1.79	0.63
2:C:441:GLN:HE22	2:C:490:ILE:HA	1.62	0.63
2:F:123:ASP:N	5:F:701:HOH:O	2.31	0.62
2:B:420:MET:SD	2:C:490:ILE:HG21	2.38	0.62
2:D:296:LEU:HD13	2:D:331:TRP:CE2	2.36	0.61
1:A:483:PHE:HB2	1:A:489:ILE:HD11	1.81	0.60
2:D:46:SER:CB	2:D:183:THR:HG23	2.33	0.58
2:D:283:ILE:HG12	2:D:404:LYS:HD3	1.85	0.58
2:E:283:ILE:HG23	2:E:412:PHE:CE2	2.38	0.58
2:E:44:LEU:HD11	2:E:183:THR:HG23	1.85	0.58
2:D:385:ARG:HD3	2:E:393:ARG:NH1	2.18	0.58
2:B:425:ILE:HG12	5:B:735:HOH:O	2.04	0.57
2:E:375:VAL:HG23	2:E:408:ILE:HG21	1.86	0.57
2:E:162:ARG:HB2	2:E:197:VAL:HG11	1.85	0.56
2:B:304:THR:O	2:B:308:GLN:HG2	2.05	0.56
3:E:601:ATP:O3G	2:F:225:LYS:NZ	2.35	0.56
2:F:375:VAL:HG23	2:F:408:ILE:HG21	1.87	0.55
2:E:44:LEU:HD11	2:E:183:THR:CG2	2.36	0.55
2:F:68:PHE:HB2	2:F:70:GLU:HG3	1.90	0.54
2:C:162:ARG:HB2	2:C:197:VAL:HG11	1.90	0.54
2:E:322:ALA:HB3	2:F:256:GLN:O	2.07	0.54
1:A:483:PHE:HB2	1:A:489:ILE:CD1	2.37	0.54
2:F:375:VAL:HG23	2:F:408:ILE:CG2	2.38	0.53
2:F:377:ILE:HB	2:F:412:PHE:HD2	1.73	0.53
2:C:406:GLU:HB2	2:C:408:ILE:HG13	1.90	0.53
2:E:132:GLN:OE1	2:E:171:ARG:NE	2.37	0.53
2:C:486:PHE:CB	2:C:489:ILE:HD11	2.39	0.53
2:F:283:ILE:HG23	2:F:412:PHE:CE1	2.44	0.53
2:D:148:VAL:HG21	2:D:181:MET:HE3	1.92	0.53
2:C:132:GLN:OE1	2:C:171:ARG:NH2	2.34	0.52
2:B:73:ILE:HD12	2:B:105:PHE:HB3	1.91	0.52
2:B:454:ASN:ND2	2:B:456:PHE:HA	2.25	0.52
2:D:289:ALA:HB2	2:D:419:PHE:HA	1.92	0.52
2:C:59:GLN:HG3	2:C:93:TRP:HH2	1.71	0.52
2:E:454:ASN:ND2	2:E:456:PHE:HA	2.24	0.52
1:A:369:ASP:OD1	1:A:369:ASP:C	2.48	0.52
2:D:290:THR:HA	3:D:602:ATP:O1G	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:LEU:HD13	2:D:399[B]:VAL:HG13	1.93	0.51
2:B:241:ASN:ND2	2:B:361:GLN:HG2	2.26	0.51
2:C:25:MET:HG3	2:C:67:ILE:HD13	1.93	0.51
2:B:212:LEU:HD13	2:B:217:ARG:NE	2.26	0.51
1:A:400:THR:HG22	1:A:412:PHE:HE1	1.76	0.50
1:A:43:THR:HA	1:A:204:ASN:HB2	1.93	0.50
1:A:420:MET:SD	2:B:490:ILE:HG21	2.52	0.50
1:A:289:ALA:HB2	1:A:419:PHE:HA	1.93	0.50
1:A:393:ARG:CZ	2:F:385:ARG:HD2	2.42	0.50
2:D:385:ARG:HD3	2:E:393:ARG:CZ	2.40	0.50
2:F:389:ASN:O	2:F:393:ARG:HG3	2.11	0.50
2:C:376:ALA:HA	2:C:411:PHE:O	2.11	0.50
2:C:55:LEU:HD21	2:C:91:PHE:HE2	1.75	0.49
2:F:194:ARG:CG	2:F:194:ARG:HH21	2.25	0.49
1:A:404:LYS:HE3	5:A:708:HOH:O	2.12	0.49
3:C:601:ATP:O2'	2:D:231:HIS:CE1	2.65	0.49
2:D:287:THR:HA	2:D:414:ASN:O	2.13	0.49
2:F:369:ASP:C	2:F:369:ASP:OD1	2.51	0.49
2:D:46:SER:HB3	2:D:183:THR:CG2	2.43	0.48
2:C:486:PHE:HB2	2:C:489:ILE:HD11	1.95	0.48
1:A:317:TYR:HA	1:A:349:ALA:O	2.14	0.48
2:B:356:LEU:HD11	2:B:387:VAL:HG21	1.96	0.48
2:C:381:SER:HB3	2:C:414:ASN:ND2	2.29	0.48
2:D:147:SER:HB2	2:D:182:THR:OG1	2.14	0.48
2:E:72:GLY:HA2	2:E:142:ARG:O	2.13	0.48
2:D:388:SER:HB2	5:D:837:HOH:O	2.13	0.48
2:D:47:GLY:HA2	2:D:185:ARG:HD2	1.96	0.47
2:B:400:THR:HG22	2:B:412:PHE:HE2	1.79	0.47
2:C:25:MET:CE	5:C:771:HOH:O	2.62	0.47
2:C:107:LEU:C	2:C:107:LEU:HD12	2.34	0.47
1:A:490:ILE:HG21	2:F:420:MET:SD	2.55	0.47
2:F:247:PHE:C	5:F:759:HOH:O	2.52	0.47
1:A:301:PHE:O	1:A:374:ARG:NH1	2.47	0.47
2:B:483:PHE:HB2	2:B:489:ILE:HD11	1.96	0.47
1:A:171:ARG:O	1:A:174:GLN:HB2	2.14	0.47
2:C:184:GLU:OE1	2:C:194:ARG:NH1	2.47	0.47
2:E:60:PHE:CD2	2:E:180:ILE:HG13	2.50	0.47
1:A:356:LEU:HD11	1:A:387:VAL:HG21	1.97	0.47
2:B:135:ILE:HD13	2:B:177:VAL:HG11	1.97	0.46
1:A:83:ASP:OD2	2:B:173:LYS:HE2	2.15	0.46
1:A:328:ALA:HA	1:A:331:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:LEU:CD1	2:C:130:ARG:NH2	2.79	0.46
2:F:290:THR:HA	3:F:602:ATP:O1G	2.15	0.46
2:E:420:MET:SD	2:F:490:ILE:HG21	2.55	0.46
2:B:171:ARG:O	2:B:175:LEU:HG	2.16	0.46
2:C:25:MET:HE1	5:C:771:HOH:O	2.16	0.46
2:C:43:THR:HA	2:C:204:ASN:HB2	1.98	0.46
2:E:292:THR:O	2:E:470:TYR:OH	2.23	0.46
1:A:77:PHE:CD2	1:A:151:VAL:CG2	2.99	0.45
2:E:453:ILE:HD13	2:E:453:ILE:C	2.36	0.45
2:C:59:GLN:CG	2:C:93:TRP:CH2	2.98	0.45
1:A:283:ILE:HG12	1:A:404:LYS:HE2	1.98	0.45
2:B:46:SER:OG	2:B:183:THR:HG23	2.15	0.45
1:A:341:ARG:HA	1:A:341:ARG:HD2	1.80	0.45
2:B:454:ASN:HD21	2:B:456:PHE:HA	1.80	0.45
2:F:283:ILE:HG23	2:F:412:PHE:HE1	1.81	0.45
2:D:46:SER:HB3	2:D:183:THR:HG23	1.98	0.45
2:D:146:ASP:HA	2:D:147:SER:HA	1.73	0.45
2:D:433:ILE:HG22	2:D:433:ILE:O	2.17	0.45
2:F:384:ALA:HB2	2:F:392:PHE:CE1	2.52	0.45
2:B:71:PRO:HB2	2:B:140:ALA:HA	1.99	0.45
2:C:458:MET:HG2	2:C:461:SER:HB3	1.99	0.45
2:F:381:SER:HB3	2:F:414:ASN:ND2	2.32	0.45
2:C:203:ASP:OD1	2:C:227:ARG:NH1	2.43	0.44
2:C:375:VAL:HG23	2:C:408:ILE:CG2	2.46	0.44
2:E:341:ARG:O	2:E:341:ARG:HG3	2.17	0.44
1:A:231:HIS:HE1	3:F:601:ATP:O2'	2.01	0.44
1:A:485:ASN:HA	1:A:497:ILE:HD11	2.00	0.44
5:C:705:HOH:O	2:D:233:LYS:CE	2.65	0.44
2:E:469:GLU:HB2	2:E:483:PHE:CZ	2.53	0.44
2:B:107:LEU:HD11	2:B:130:ARG:NH2	2.33	0.44
1:A:149:THR:HG21	1:A:194:ARG:HE	1.81	0.44
1:A:441:GLN:HE22	1:A:490:ILE:HA	1.83	0.44
2:B:43:THR:HA	2:B:204:ASN:HB2	1.99	0.44
2:D:57:ALA:HB1	2:D:144:SER:HB3	2.00	0.44
2:F:285:LEU:HB2	2:F:434:THR:HG21	2.00	0.44
2:C:287:THR:HG21	2:C:425:ILE:HG23	2.00	0.44
2:E:433:ILE:HG22	2:E:433:ILE:O	2.18	0.44
2:C:321:ARG:HD2	2:C:346:ILE:HB	2.00	0.43
1:A:458:MET:HG3	1:A:463:HIS:HB3	1.99	0.43
2:F:44:LEU:HD11	2:F:183:THR:HG23	2.01	0.43
2:F:77:PHE:O	2:F:110:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:THR:HA	2:D:204:ASN:HB2	2.00	0.43
1:A:402:PHE:O	1:A:406:GLU:HG2	2.19	0.43
2:B:254:LEU:HD23	2:B:254:LEU:HA	1.89	0.43
2:D:393:ARG:HB2	2:D:393:ARG:NH1	2.34	0.43
2:D:412:PHE:CD1	2:D:412:PHE:N	2.86	0.43
2:E:303:GLU:OE2	2:E:333:ILE:HG12	2.18	0.43
2:D:323:GLN:OE1	2:E:404:LYS:NZ	2.49	0.43
2:E:412:PHE:CD2	2:E:412:PHE:N	2.87	0.43
2:F:483:PHE:HB2	2:F:489:ILE:HD11	2.01	0.43
2:C:289:ALA:CB	2:C:419:PHE:HA	2.48	0.42
2:F:161:VAL:O	2:F:165:ILE:HG13	2.18	0.42
2:B:469:GLU:HB2	2:B:483:PHE:CZ	2.55	0.42
2:E:435:ASP:HA	2:E:459:ARG:HD2	2.01	0.42
2:F:44:LEU:HD11	2:F:183:THR:CG2	2.49	0.42
2:F:132:GLN:OE1	2:F:171:ARG:NH2	2.50	0.42
2:E:44:LEU:HA	2:E:181:MET:O	2.20	0.42
1:A:302:LEU:HD22	1:A:312:ALA:HB1	2.01	0.42
1:A:376:ALA:HA	1:A:411:PHE:O	2.19	0.42
2:E:43:THR:HA	2:E:204:ASN:HB2	2.00	0.42
2:C:47:GLY:HA2	2:C:185:ARG:HD3	2.01	0.42
2:D:371:LYS:N	2:D:372:PRO:CD	2.82	0.42
1:A:231:HIS:CE1	3:F:601:ATP:O2'	2.72	0.42
2:F:211:VAL:HG23	5:F:753:HOH:O	2.20	0.42
2:F:435:ASP:HA	2:F:459:ARG:HD2	2.01	0.42
1:A:397:ILE:CD1	1:A:433:ILE:HD13	2.48	0.42
2:C:420:MET:SD	2:D:490:ILE:HG21	2.60	0.41
2:F:40:GLY:HA2	2:F:177:VAL:O	2.20	0.41
1:A:431:SEP:HB2	2:F:290:THR:HG21	2.02	0.41
2:C:415:THR:HG21	2:D:432:TPO:CG2	2.50	0.41
2:D:321:ARG:NH1	5:D:718:HOH:O	2.54	0.41
3:D:602:ATP:O2'	2:E:463:HIS:HE1	2.04	0.41
2:E:45:VAL:O	2:E:182:THR:HA	2.21	0.41
1:A:54:THR:OG1	1:A:146:ASP:OD2	2.38	0.41
2:E:376:ALA:HA	2:E:411:PHE:O	2.21	0.41
2:B:288:GLY:O	2:B:415:THR:HA	2.20	0.41
2:B:432:TPO:HG22	5:B:796:HOH:O	2.20	0.41
2:B:483:PHE:HB2	2:B:489:ILE:CD1	2.51	0.41
2:E:356:LEU:HD21	2:E:392:PHE:HA	2.02	0.41
2:F:378:ASP:HA	2:F:379:SER:HA	1.89	0.41
1:A:397:ILE:N	1:A:397:ILE:HD13	2.36	0.41
2:B:377:ILE:HG12	2:B:412:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:378:ASP:HA	2:C:379:SER:HA	1.83	0.41
2:B:375:VAL:HG23	2:B:408:ILE:HG21	2.03	0.40
2:C:55:LEU:HD23	2:C:55:LEU:HA	1.85	0.40
5:C:705:HOH:O	2:D:233:LYS:HE2	2.21	0.40
2:D:393:ARG:O	2:D:397:ILE:HG12	2.21	0.40
2:E:194:ARG:NH2	2:F:196:GLY:O	2.48	0.40
2:C:162:ARG:CB	2:C:197:VAL:HG11	2.51	0.40
1:A:444:GLU:O	1:A:494:PRO:HD2	2.20	0.40
2:B:377:ILE:HG12	2:B:412:PHE:CD1	2.57	0.40
2:B:474:GLU:H	2:B:474:GLU:CD	2.25	0.40
2:F:317:TYR:HA	2:F:349:ALA:O	2.22	0.40
1:A:77:PHE:CE2	1:A:151:VAL:HG21	2.57	0.40
1:A:143:VAL:O	1:A:179:THR:HA	2.22	0.40
2:E:70:GLU:CD	2:E:142:ARG:HE	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/518 (86%)	432 (97%)	14 (3%)	0	100	100
2	B	443/518 (86%)	430 (97%)	13 (3%)	0	100	100
2	C	446/518 (86%)	431 (97%)	14 (3%)	1 (0%)	47	55
2	D	450/518 (87%)	435 (97%)	15 (3%)	0	100	100
2	E	446/518 (86%)	432 (97%)	14 (3%)	0	100	100
2	F	446/518 (86%)	432 (97%)	14 (3%)	0	100	100
All	All	2677/3108 (86%)	2592 (97%)	84 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	C	124	LEU

### 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	361/440 (82%)	346 (96%)	15 (4%)	30	38
2	B	352/439 (80%)	337 (96%)	15 (4%)	29	36
2	C	353/439 (80%)	333 (94%)	20 (6%)	20	24
2	D	362/439 (82%)	337 (93%)	25 (7%)	15	16
2	E	362/439 (82%)	341 (94%)	21 (6%)	20	23
2	F	351/439 (80%)	338 (96%)	13 (4%)	34	43
All	All	2141/2635 (81%)	2032 (95%)	109 (5%)	24	29

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	82	GLN
1	A	151	VAL
1	A	194	ARG
1	A	233	LYS
1	A	245	ASN
1	A	258	SER
1	A	259	SER
1	A	294	LYS
1	A	303	GLU
1	A	326	ARG
1	A	341	ARG
1	A	446	ARG
1	A	490	ILE
1	A	497	ILE
2	B	69	ASN
2	B	89	LEU
2	B	96	GLN

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Mol	Chain	Res	Type
2	B	107	LEU
2	B	125	SER
2	B	130	ARG
2	B	187	ASP
2	B	202	SER
2	B	254	LEU
2	B	294	LYS
2	B	329	SER
2	B	373	SER
2	B	405	GLN
2	B	451	ARG
2	B	482	SER
2	C	18	GLU
2	C	55	LEU
2	C	69	ASN
2	C	103	LYS
2	C	107	LEU
2	C	188	GLU
2	C	199	GLU
2	C	245	ASN
2	C	259	SER
2	C	262	ARG
2	C	263	VAL
2	C	294	LYS
2	C	338	LEU
2	C	389	ASN
2	C	424	SER
2	C	439	LEU
2	C	458	MET
2	C	468	ARG
2	C	471	VAL
2	C	484	ARG
2	D	18	GLU
2	D	27	GLU
2	D	82	GLN
2	D	103	LYS
2	D	147	SER
2	D	148	VAL
2	D	159	SER
2	D	174	GLN
2	D	185	ARG
2	D	194	ARG

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Mol	Chain	Res	Type
2	D	197	VAL
2	D	202	SER
2	D	213	GLU
2	D	292	THR
2	D	294	LYS
2	D	331	TRP
2	D	341	ARG
2	D	364	LYS
2	D	385	ARG
2	D	423	ASN
2	D	424	SER
2	D	468	ARG
2	D	480	ARG
2	D	482	SER
2	D	497	ILE
2	E	25	MET
2	E	31	ASP
2	E	89	LEU
2	E	107	LEU
2	E	124	LEU
2	E	139	LYS
2	E	188	GLU
2	E	194	ARG
2	E	213	GLU
2	E	245	ASN
2	E	300	LYS
2	E	308	GLN
2	E	356	LEU
2	E	364	LYS
2	E	373	SER
2	E	381	SER
2	E	424	SER
2	E	451	ARG
2	E	453	ILE
2	E	468	ARG
2	E	497	ILE
2	F	69	ASN
2	F	103	LYS
2	F	159	SER
2	F	194	ARG
2	F	294	LYS
2	F	307	GLN

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Mol	Chain	Res	Type
2	F	321	ARG
2	F	338	LEU
2	F	364	LYS
2	F	404	LYS
2	F	420	MET
2	F	439	LEU
2	F	482	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	441	GLN
2	B	69	ASN
2	B	241	ASN
2	B	405	GLN
2	B	454	ASN
2	B	463	HIS
2	C	69	ASN
2	C	101	GLN
2	C	441	GLN
2	D	39	GLN
2	D	231	HIS
2	D	241	ASN
2	D	361	GLN
2	D	414	ASN
2	E	245	ASN
2	E	454	ASN
2	E	463	HIS
2	F	245	ASN
2	F	359	HIS
2	F	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPO	D	432	2	8,10,11	1.07	1 (12%)	10,14,16	0.99	1 (10%)
2	TPO	E	432	2	8,10,11	1.64	1 (12%)	10,14,16	0.86	0
2	TPO	B	432	2	8,10,11	1.77	1 (12%)	10,14,16	0.82	0
2	TPO	F	432	2	8,10,11	1.28	1 (12%)	10,14,16	0.82	0
2	TPO	C	432	2	8,10,11	1.62	1 (12%)	10,14,16	0.89	0
2	SEP	B	431	2	8,9,10	0.68	0	8,12,14	1.31	1 (12%)
2	SEP	D	431	2	8,9,10	0.82	0	8,12,14	1.13	1 (12%)
2	SEP	C	431	2	8,9,10	0.66	0	8,12,14	0.79	0
1	SEP	A	431	1	8,9,10	0.78	0	8,12,14	0.92	0
2	SEP	F	431	2	8,9,10	0.85	0	8,12,14	1.02	1 (12%)
2	SEP	E	431	2	8,9,10	0.73	0	8,12,14	1.00	1 (12%)

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	TPO	D	432	2	-	0/9/11/13	-
2	TPO	E	432	2	-	0/9/11/13	-
2	TPO	B	432	2	-	1/9/11/13	-
2	TPO	F	432	2	-	4/9/11/13	-
2	TPO	C	432	2	-	0/9/11/13	-
2	SEP	B	431	2	-	2/5/8/10	-
2	SEP	D	431	2	-	1/5/8/10	-
2	SEP	C	431	2	-	2/5/8/10	-
1	SEP	A	431	1	-	0/5/8/10	-
2	SEP	F	431	2	-	0/5/8/10	-
2	SEP	E	431	2	-	2/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	432	TPO	P-OG1	4.72	1.68	1.59
2	E	432	TPO	P-OG1	4.34	1.67	1.59
2	C	432	TPO	P-OG1	4.22	1.67	1.59
2	F	432	TPO	P-OG1	3.24	1.65	1.59
2	D	432	TPO	P-OG1	2.48	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	431	SEP	OG-CB-CA	2.83	110.90	108.14
2	D	431	SEP	OG-CB-CA	2.49	110.57	108.14
2	D	432	TPO	O-C-CA	-2.19	119.03	124.78
2	F	431	SEP	OG-CB-CA	2.11	110.20	108.14
2	E	431	SEP	OG-CB-CA	2.02	110.11	108.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	431	SEP	CB-OG-P-O1P
2	F	432	TPO	N-CA-CB-OG1
2	F	432	TPO	C-CA-CB-CG2
2	F	432	TPO	N-CA-CB-CG2
2	C	431	SEP	CB-OG-P-O3P
2	D	431	SEP	CA-CB-OG-P
2	E	431	SEP	CA-CB-OG-P
2	B	431	SEP	CB-OG-P-O1P
2	E	431	SEP	CB-OG-P-O1P
2	B	431	SEP	CA-CB-OG-P
2	B	432	TPO	CB-OG1-P-O3P
2	F	432	TPO	CB-OG1-P-O3P

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	432	TPO	3	0
2	B	432	TPO	2	0
1	A	431	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	$\# Z  > 2$
3	ATP	C	601	4	26,33,33	0.71	1 (3%)	31,52,52	1.01	1 (3%)
3	ATP	E	601	4	26,33,33	0.73	0	31,52,52	0.86	1 (3%)
3	ATP	B	601	4	26,33,33	0.62	0	31,52,52	1.09	2 (6%)
3	ATP	F	601	4	26,33,33	0.70	0	31,52,52	1.11	4 (12%)
3	ATP	B	602	4	26,33,33	0.68	0	31,52,52	0.89	1 (3%)
3	ATP	C	602	4	26,33,33	0.70	0	31,52,52	0.84	1 (3%)
3	ATP	A	602	4	26,33,33	0.73	0	31,52,52	0.99	2 (6%)
3	ATP	D	601	4	26,33,33	0.74	0	31,52,52	0.99	2 (6%)
3	ATP	E	602	4	26,33,33	0.85	0	31,52,52	0.72	0
3	ATP	F	602	4	26,33,33	0.65	0	31,52,52	0.86	1 (3%)
3	ATP	D	602	4	26,33,33	0.71	0	31,52,52	0.75	1 (3%)
3	ATP	A	601	4	26,33,33	0.72	0	31,52,52	1.11	1 (3%)

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
3	ATP	C	601	4	-	4/18/38/38	0/3/3/3
3	ATP	E	601	4	-	6/18/38/38	0/3/3/3
3	ATP	B	601	4	-	6/18/38/38	0/3/3/3
3	ATP	F	601	4	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	602	4	-	2/18/38/38	0/3/3/3
3	ATP	C	602	4	-	3/18/38/38	0/3/3/3
3	ATP	A	602	4	-	2/18/38/38	0/3/3/3
3	ATP	D	601	4	-	1/18/38/38	0/3/3/3
3	ATP	E	602	4	-	0/18/38/38	0/3/3/3
3	ATP	F	602	4	-	2/18/38/38	0/3/3/3
3	ATP	D	602	4	-	2/18/38/38	0/3/3/3
3	ATP	A	601	4	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ATP	C8-N7	-2.06	1.31	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	ATP	O3'-C3'-C4'	-2.74	103.12	111.05
3	B	602	ATP	C5-C6-N6	2.63	124.35	120.35
3	D	601	ATP	O3'-C3'-C4'	-2.46	103.92	111.05
3	F	601	ATP	O3'-C3'-C4'	-2.44	104.01	111.05
3	A	602	ATP	PA-O3A-PB	-2.43	124.50	132.83
3	F	602	ATP	C5-C6-N6	2.38	123.97	120.35
3	A	602	ATP	C5-C6-N6	2.36	123.94	120.35
3	D	602	ATP	C5-C6-N6	2.32	123.88	120.35
3	F	601	ATP	C5-C6-N6	2.25	123.77	120.35
3	B	601	ATP	C5-C6-N6	2.24	123.76	120.35
3	F	601	ATP	O2A-PA-O1A	2.23	123.27	112.24
3	C	602	ATP	C5-C6-N6	2.18	123.66	120.35
3	F	601	ATP	O3'-C3'-C2'	2.16	118.81	111.82
3	D	601	ATP	C5-C6-N6	2.12	123.58	120.35
3	B	601	ATP	C3'-C2'-C1'	2.11	104.15	100.98
3	A	601	ATP	O3G-PG-O2G	2.10	115.66	107.64
3	E	601	ATP	PB-O3B-PG	-2.04	125.83	132.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	601	ATP	C5'-O5'-PA-O1A
3	C	602	ATP	PB-O3B-PG-O2G
3	E	601	ATP	C5'-O5'-PA-O1A
3	B	601	ATP	C3'-C4'-C5'-O5'
3	A	602	ATP	PA-O3A-PB-O1B
3	B	601	ATP	C5'-O5'-PA-O3A
3	C	601	ATP	C5'-O5'-PA-O3A
3	E	601	ATP	C5'-O5'-PA-O3A
3	B	601	ATP	C5'-O5'-PA-O2A
3	C	601	ATP	C5'-O5'-PA-O2A
3	E	601	ATP	C5'-O5'-PA-O2A
3	C	601	ATP	C3'-C4'-C5'-O5'
3	A	602	ATP	PA-O3A-PB-O2B
3	B	602	ATP	PA-O3A-PB-O2B
3	D	602	ATP	PA-O3A-PB-O1B
3	F	602	ATP	PA-O3A-PB-O2B
3	E	601	ATP	C3'-C4'-C5'-O5'
3	F	602	ATP	PA-O3A-PB-O1B
3	B	601	ATP	PG-O3B-PB-O1B
3	B	601	ATP	PG-O3B-PB-O2B
3	B	602	ATP	PA-O3A-PB-O1B
3	C	602	ATP	PA-O3A-PB-O1B
3	D	601	ATP	PA-O3A-PB-O1B
3	D	602	ATP	PA-O3A-PB-O2B
3	E	601	ATP	PG-O3B-PB-O1B
3	E	601	ATP	PG-O3B-PB-O2B
3	C	602	ATP	PB-O3B-PG-O1G

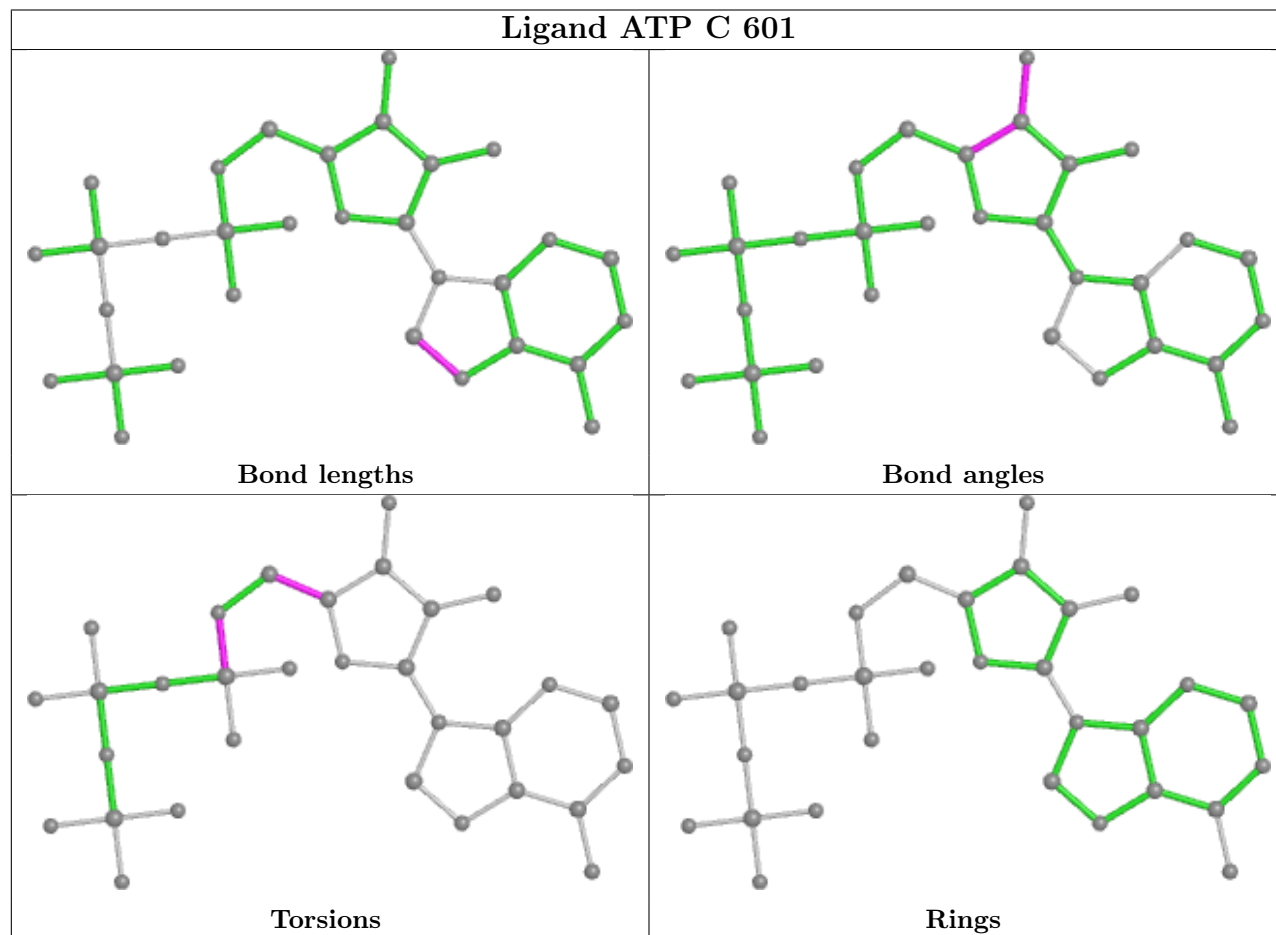
There are no ring outliers.

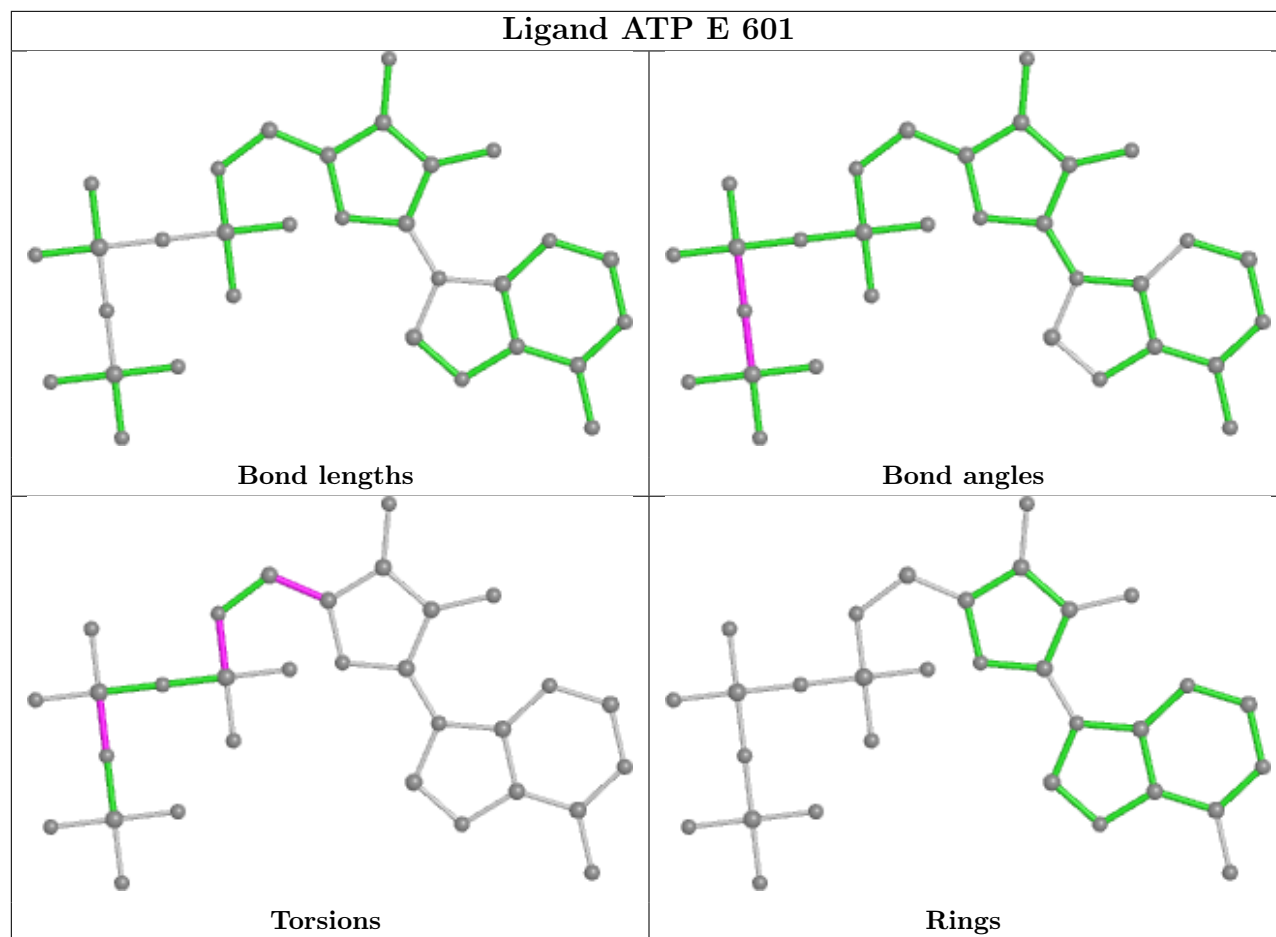
5 monomers are involved in 9 short contacts:

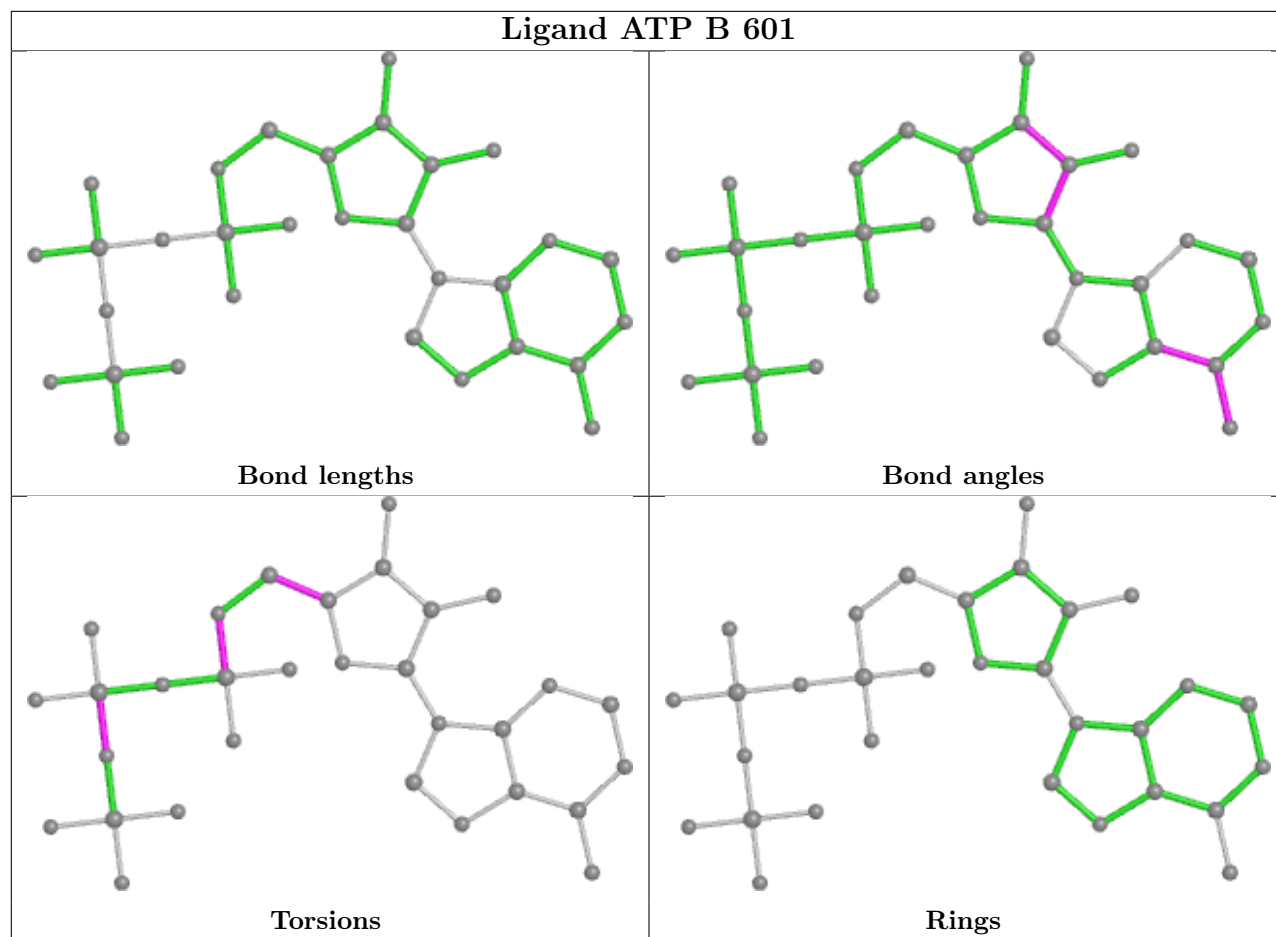
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	ATP	1	0
3	E	601	ATP	1	0
3	F	601	ATP	4	0
3	F	602	ATP	1	0
3	D	602	ATP	2	0

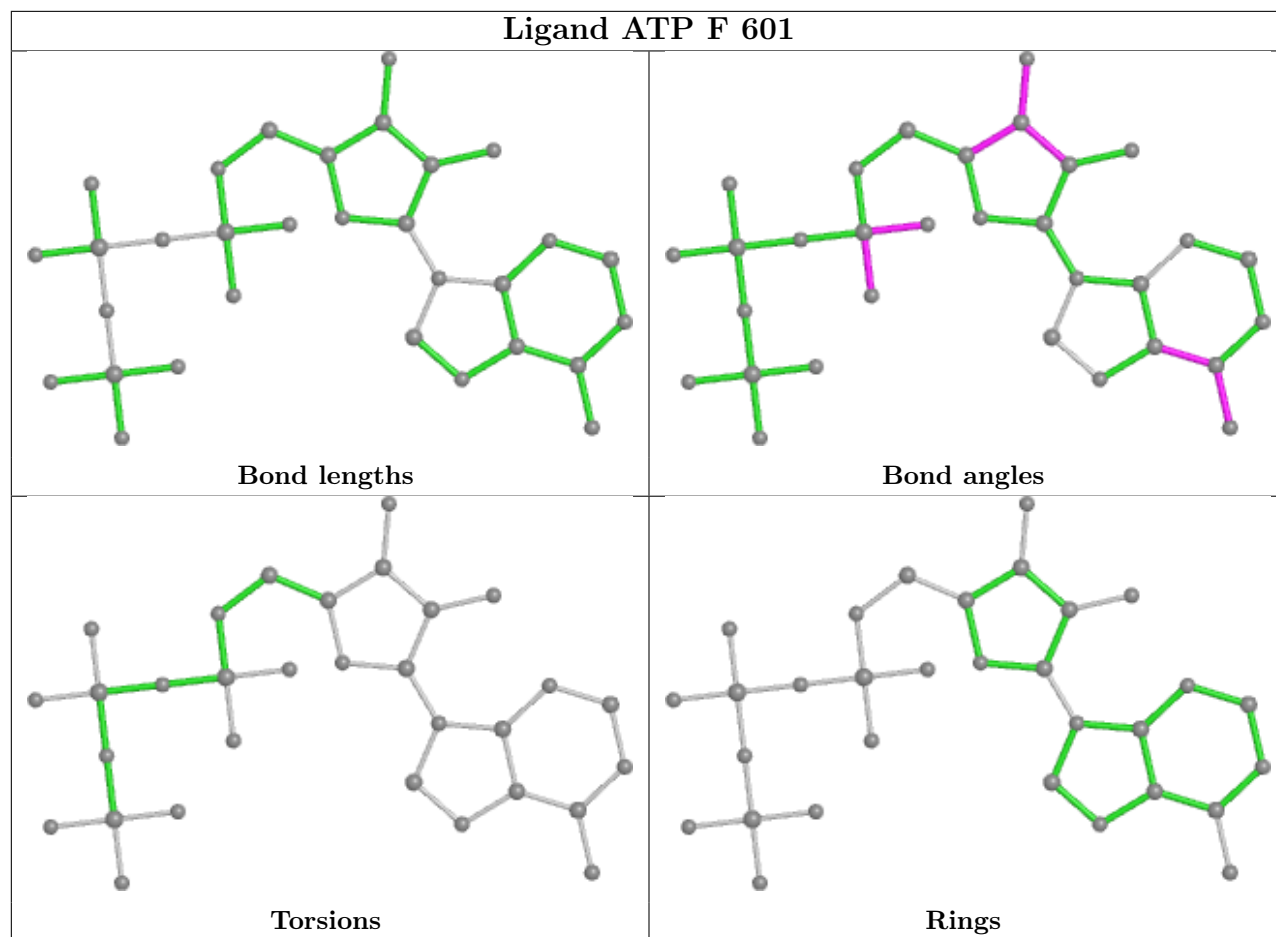
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

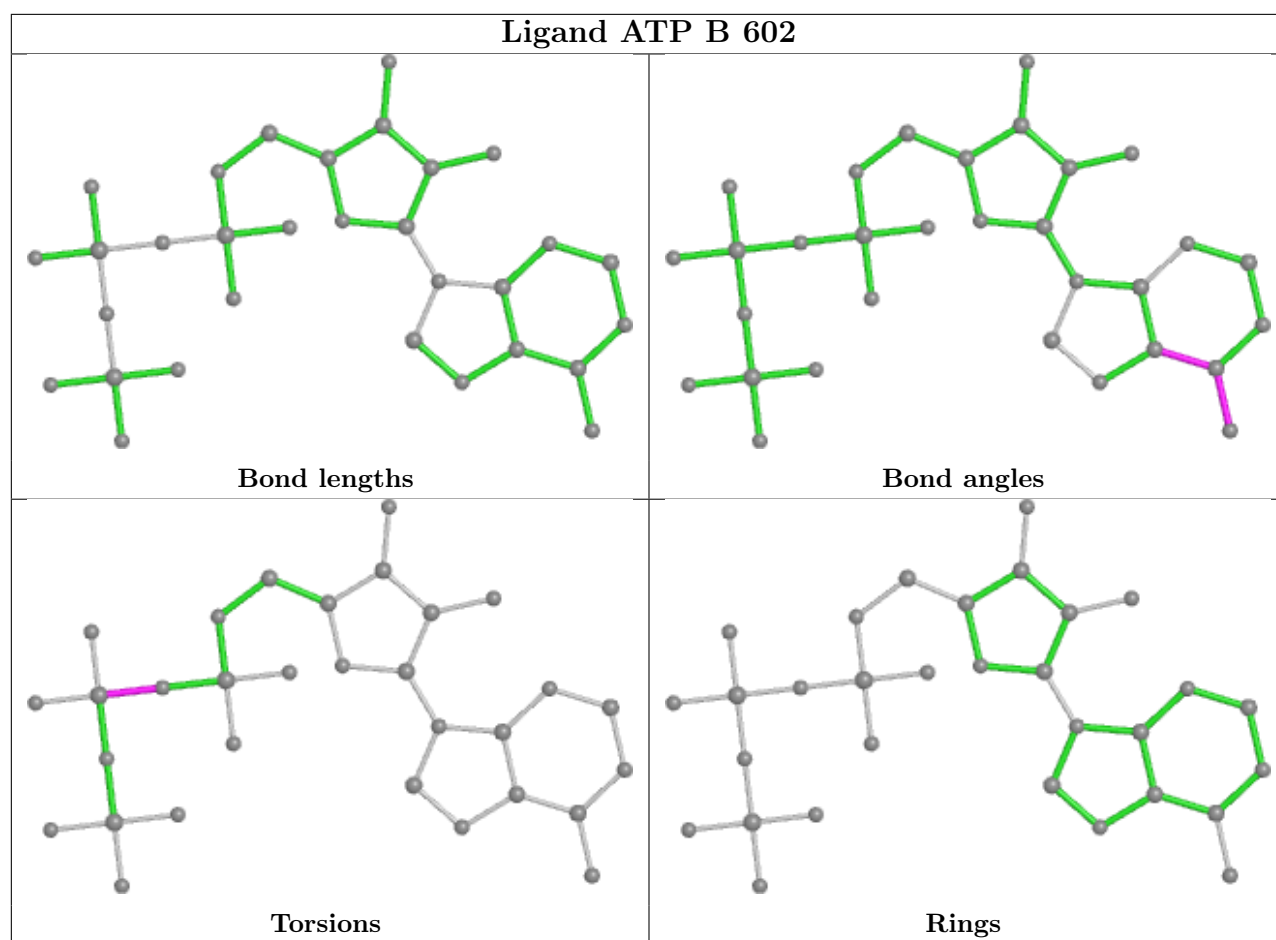
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

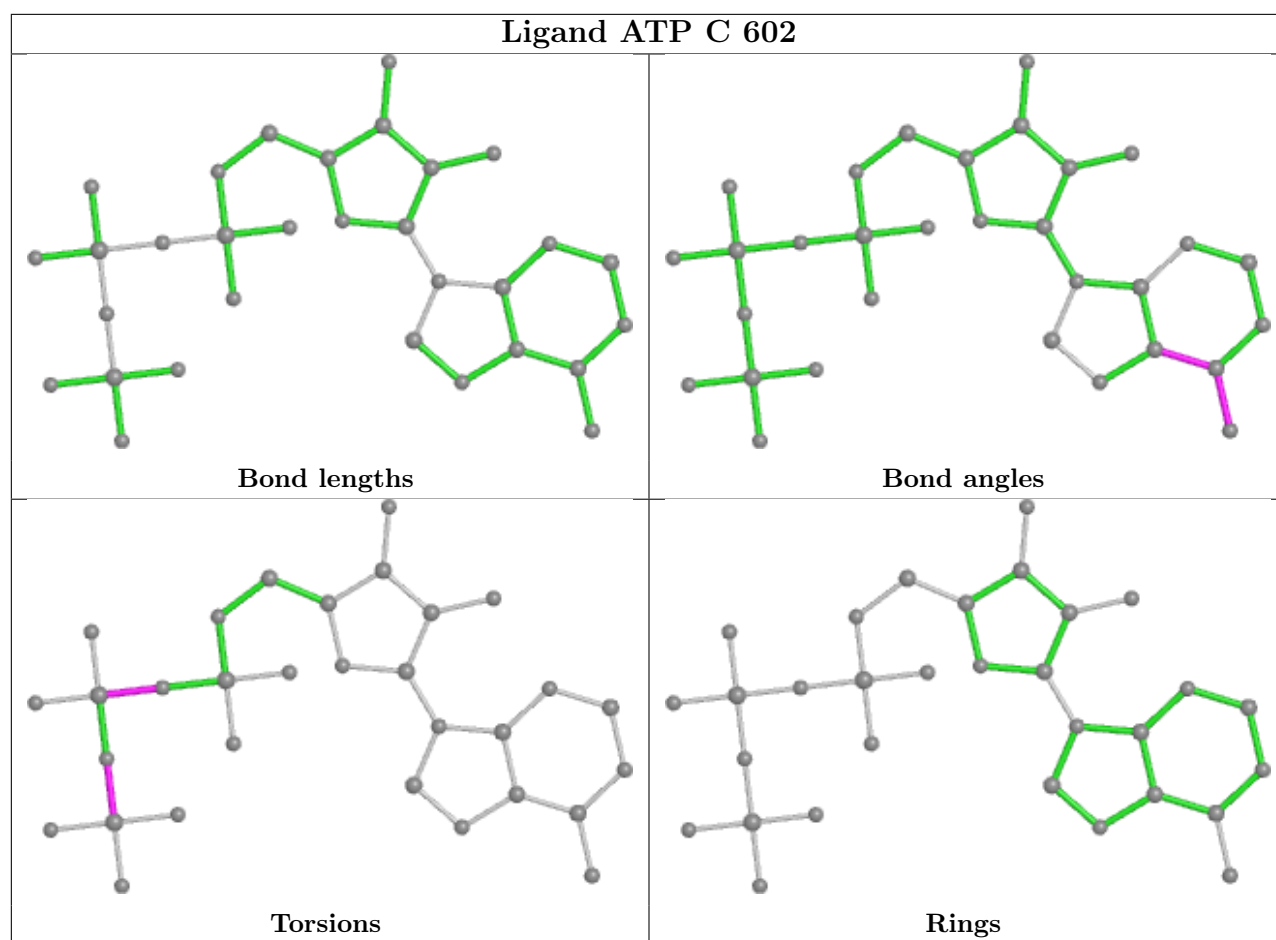


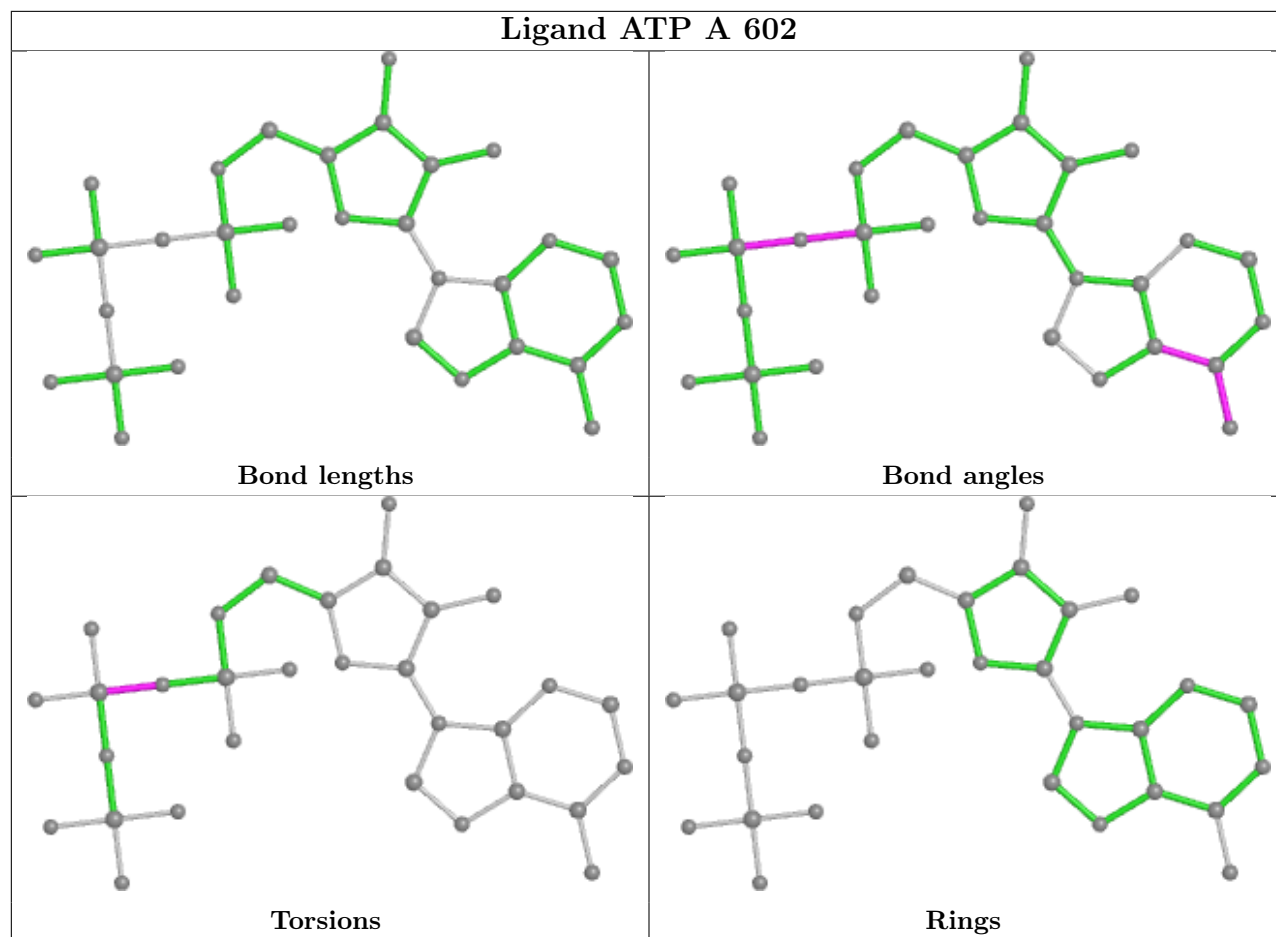




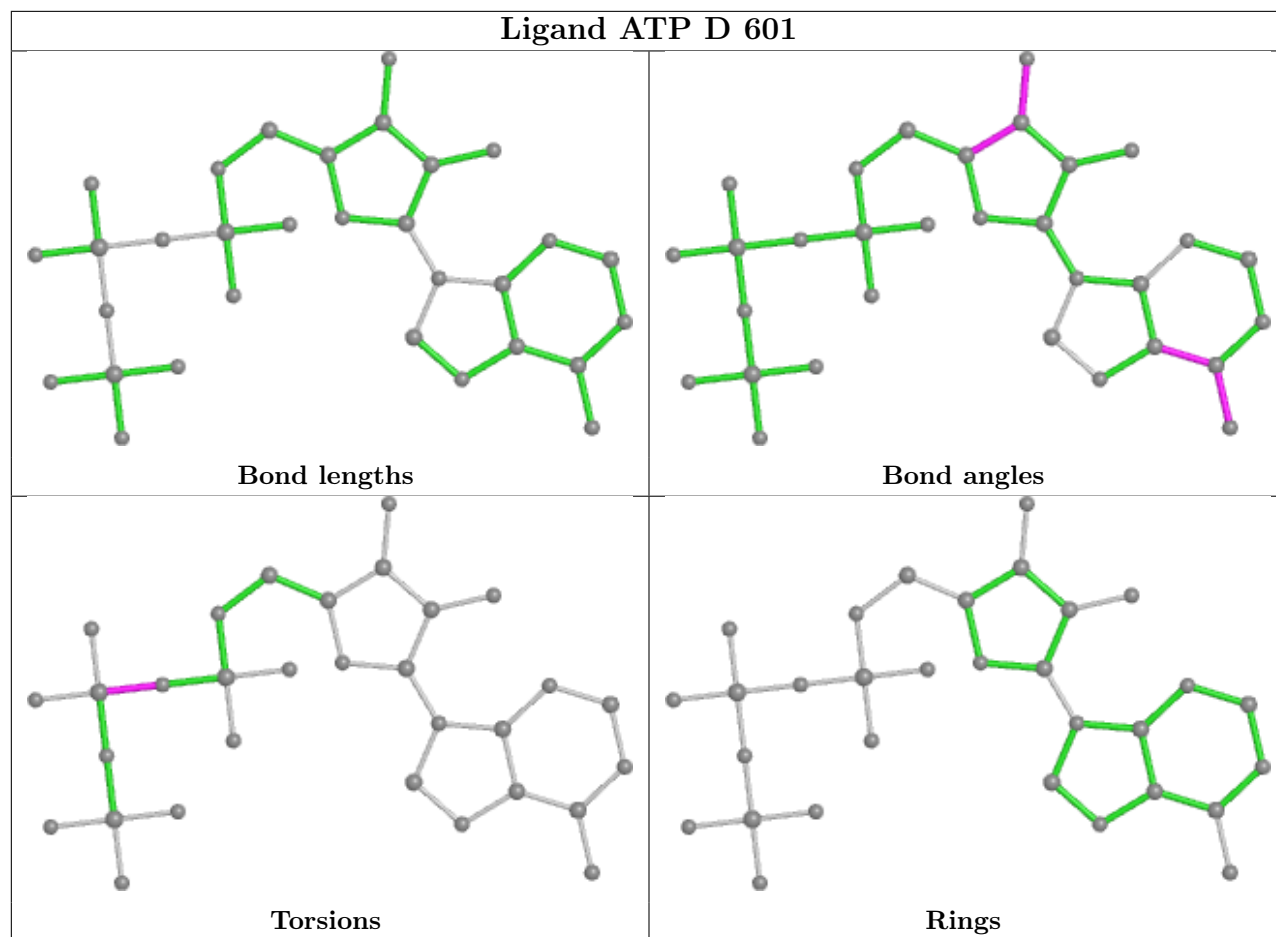


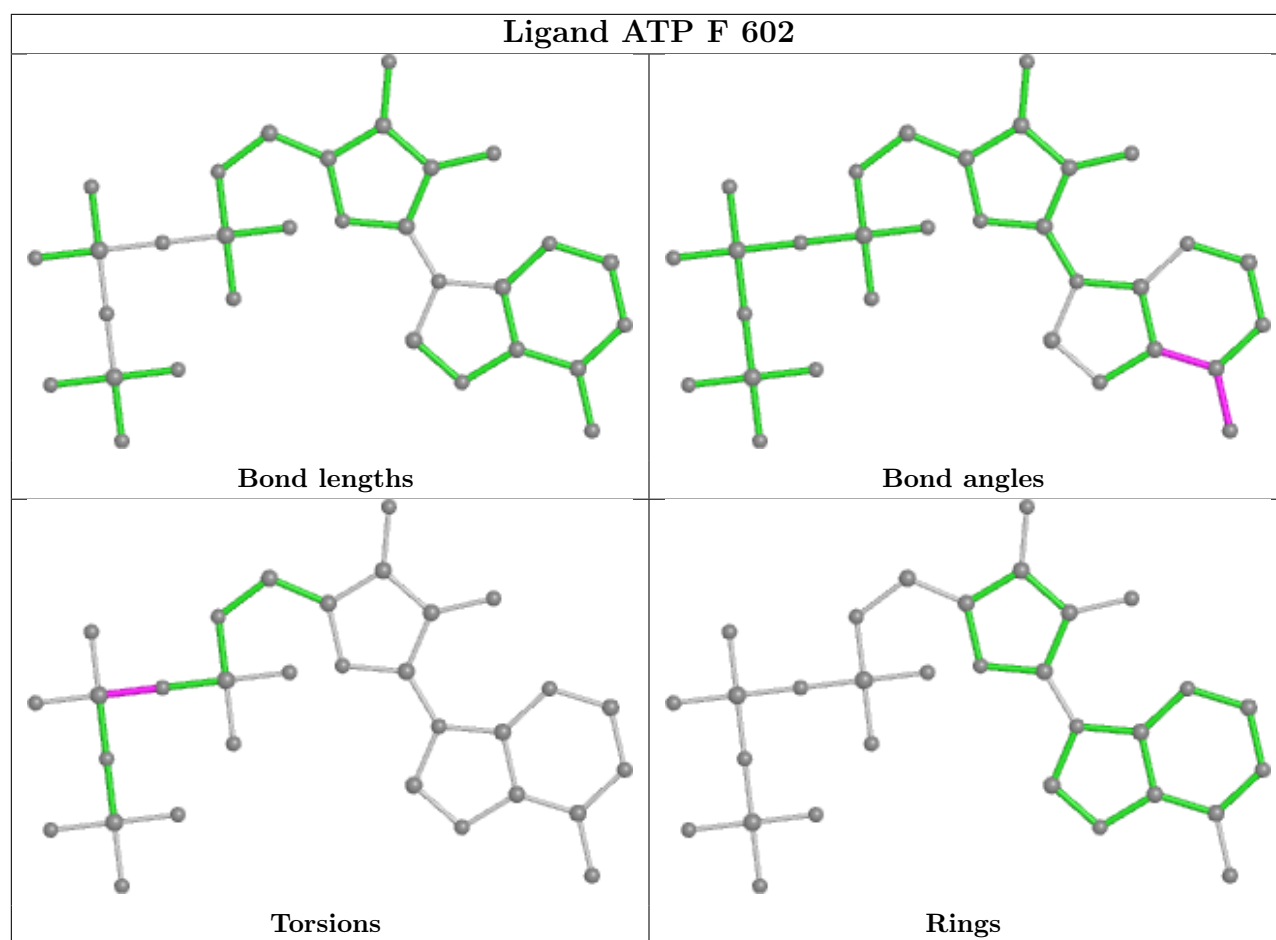


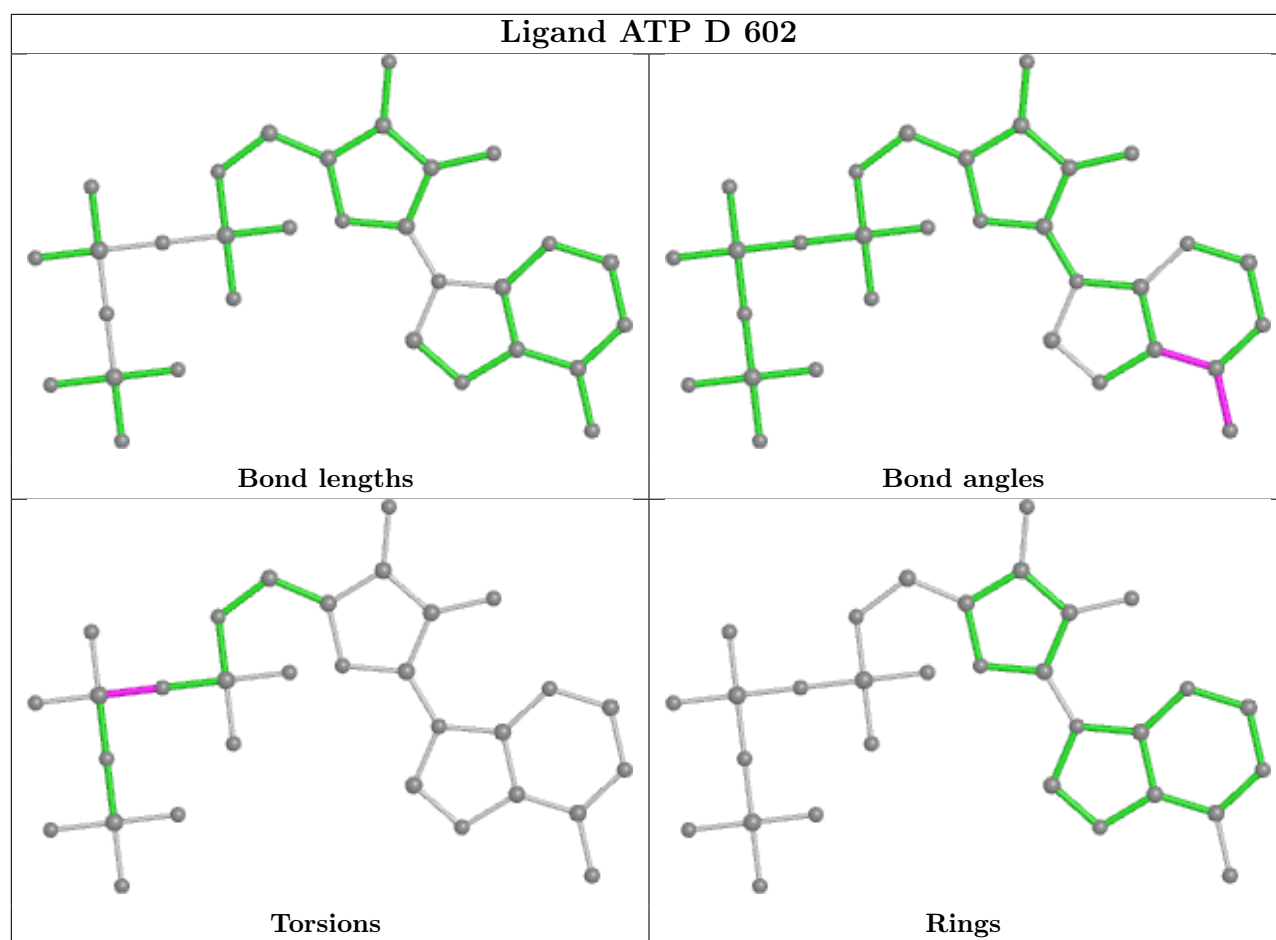


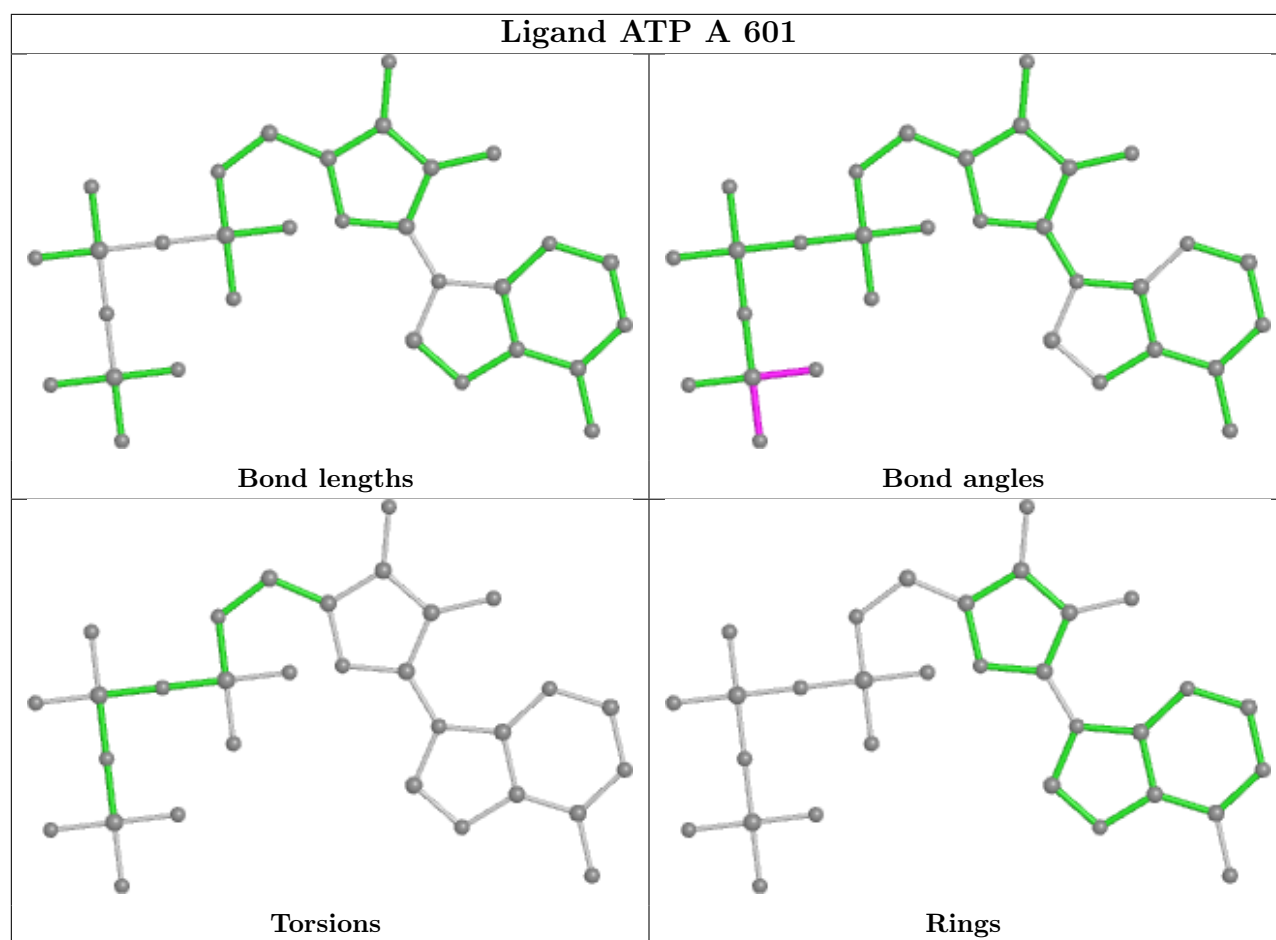












## 5.7 Other polymers [i](#)

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	453/518 (87%)	-0.19	5 (1%) 80 79	15, 27, 46, 68	0
2	B	450/518 (86%)	-0.16	6 (1%) 77 75	17, 30, 48, 66	0
2	C	454/518 (87%)	-0.14	1 (0%) 95 94	13, 29, 48, 87	0
2	D	456/518 (88%)	-0.15	4 (0%) 84 83	14, 26, 45, 78	0
2	E	453/518 (87%)	-0.16	5 (1%) 80 79	14, 29, 48, 74	0
2	F	454/518 (87%)	-0.13	4 (0%) 84 83	13, 29, 47, 69	0
All	All	2720/3108 (87%)	-0.15	25 (0%) 84 83	13, 29, 48, 87	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	111	PRO	4.3
2	D	157	ALA	4.0
1	A	111	PRO	3.9
2	C	484	ARG	3.5
2	D	254	LEU	3.3
2	B	423	ASN	3.0
2	B	77	PHE	2.8
2	E	255	THR	2.8
1	A	133	TYR	2.6
2	E	111	PRO	2.6
2	B	254	LEU	2.5
2	B	255	THR	2.4
2	B	127	LEU	2.3
2	E	164	GLU	2.3
2	F	111	PRO	2.3
2	E	157	ALA	2.3
1	A	77	PHE	2.3
2	B	370	PHE	2.3
2	F	160	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	152	PHE	2.2
1	A	497	ILE	2.1
1	A	420	MET	2.1
2	D	158	ALA	2.1
2	E	77	PHE	2.0
2	F	484	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	TPO	C	432	11/12	0.85	0.14	28,31,43,48	4
2	TPO	B	432	11/12	0.86	0.15	25,29,35,41	4
2	TPO	E	432	11/12	0.86	0.16	24,29,37,43	4
2	TPO	D	432	11/12	0.87	0.19	23,27,43,46	4
2	TPO	F	432	11/12	0.89	0.14	25,36,61,62	0
2	SEP	F	431	10/11	0.90	0.14	22,30,42,45	0
2	SEP	C	431	10/11	0.94	0.11	27,31,36,36	0
2	SEP	B	431	10/11	0.94	0.12	24,27,30,33	4
1	SEP	A	431	10/11	0.94	0.10	24,28,34,38	0
2	SEP	E	431	10/11	0.96	0.09	23,26,35,36	0
2	SEP	D	431	10/11	0.96	0.12	23,25,29,29	0

## 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(Å <sup>2</sup> )	Q<0.9
4	MG	B	603	1/1	0.91	0.14	30,30,30,30	0

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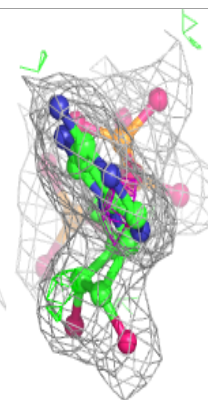
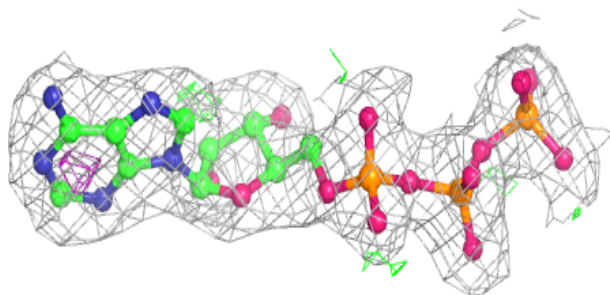
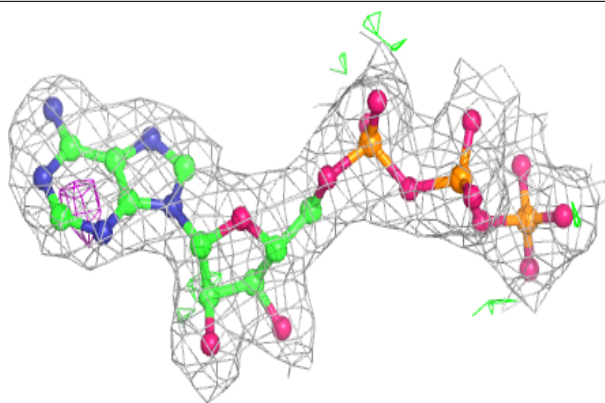
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	C	603	1/1	0.91	0.06	30,30,30,30	0
4	MG	F	604	1/1	0.91	0.04	24,24,24,24	0
4	MG	F	603	1/1	0.93	0.08	37,37,37,37	0
4	MG	A	604	1/1	0.95	0.09	19,19,19,19	0
3	ATP	D	601	31/31	0.96	0.11	15,22,26,27	0
3	ATP	F	601	31/31	0.96	0.11	17,23,29,31	0
3	ATP	F	602	31/31	0.96	0.10	19,23,27,32	0
3	ATP	B	601	31/31	0.96	0.10	17,23,28,29	0
3	ATP	B	602	31/31	0.97	0.11	15,22,26,29	0
3	ATP	C	601	31/31	0.97	0.10	18,23,31,35	0
3	ATP	C	602	31/31	0.97	0.10	16,21,32,37	0
3	ATP	A	601	31/31	0.97	0.12	16,23,29,34	0
4	MG	B	604	1/1	0.97	0.07	23,23,23,23	0
3	ATP	D	602	31/31	0.97	0.10	16,23,25,26	0
4	MG	D	604	1/1	0.97	0.11	17,17,17,17	0
4	MG	E	603	1/1	0.97	0.03	25,25,25,25	0
4	MG	E	604	1/1	0.97	0.07	26,26,26,26	0
3	ATP	E	601	31/31	0.97	0.11	17,25,31,33	0
3	ATP	E	602	31/31	0.97	0.11	16,22,26,26	0
4	MG	A	603	1/1	0.98	0.04	35,35,35,35	0
4	MG	C	604	1/1	0.98	0.05	25,25,25,25	0
4	MG	D	603	1/1	0.98	0.07	17,17,17,17	0
3	ATP	A	602	31/31	0.98	0.10	16,20,25,27	0

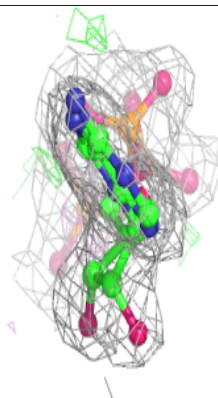
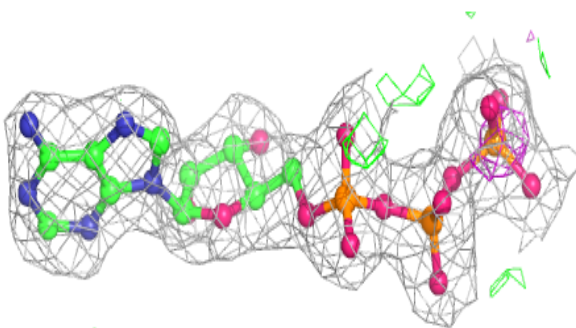
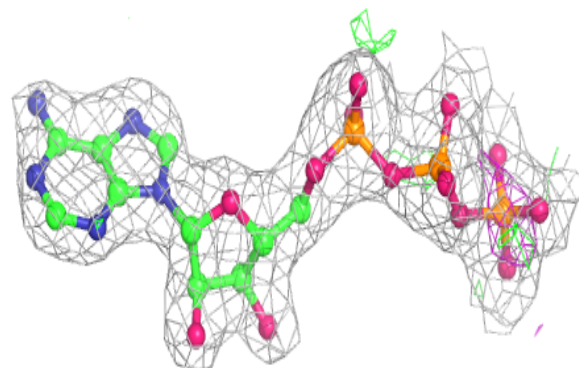
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP D 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 F 601:**

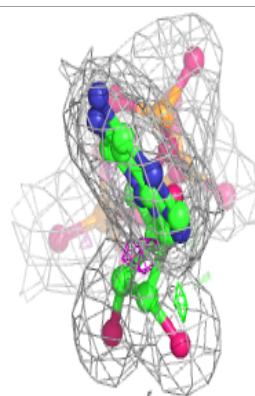
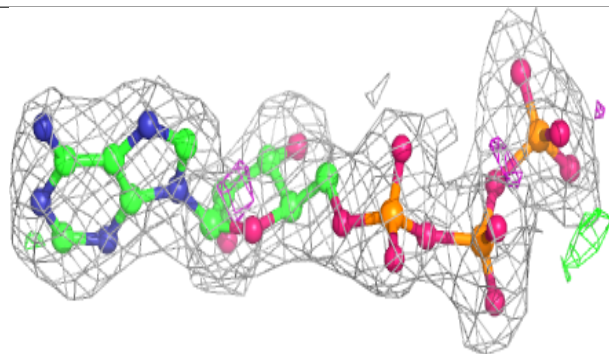
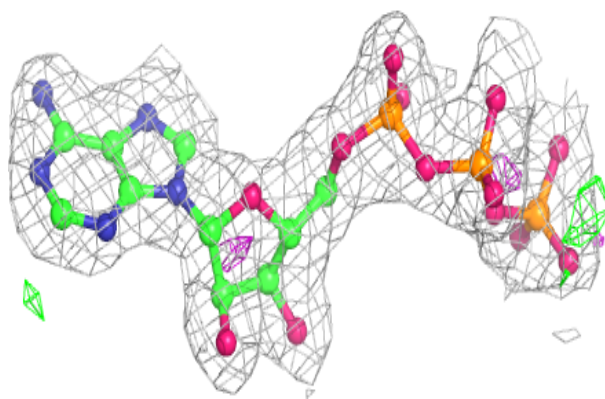
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



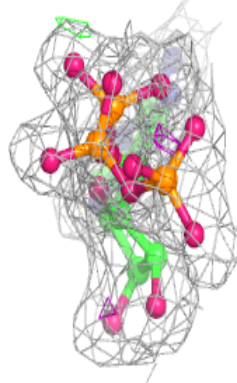
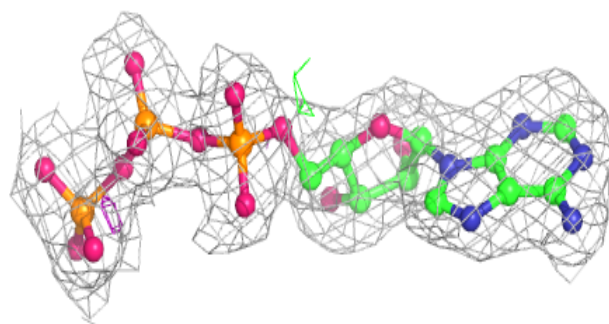
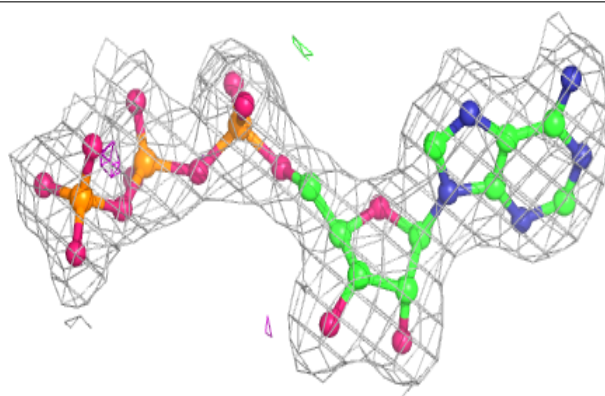


**Electron density around ATP F 602:**

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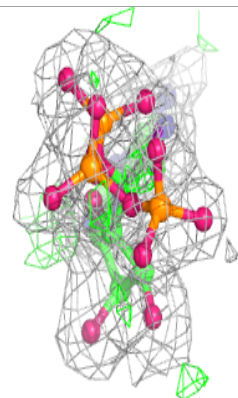
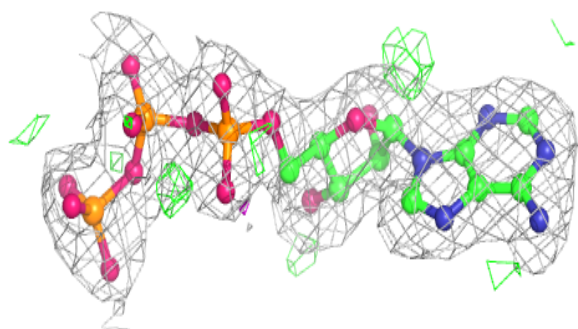
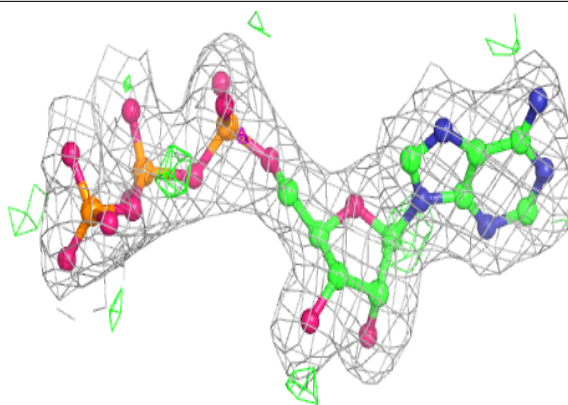
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and green (positive)

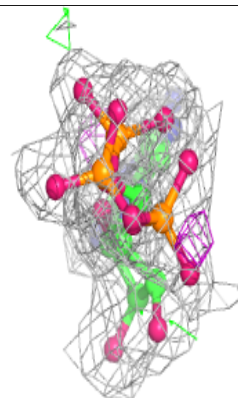
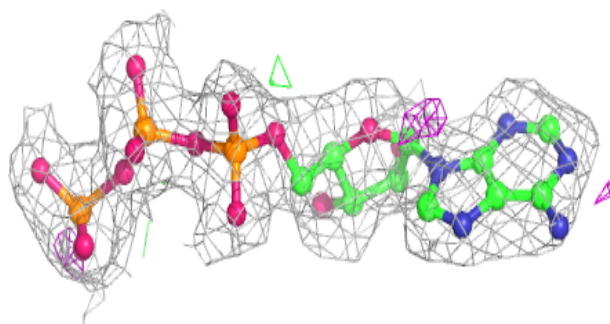
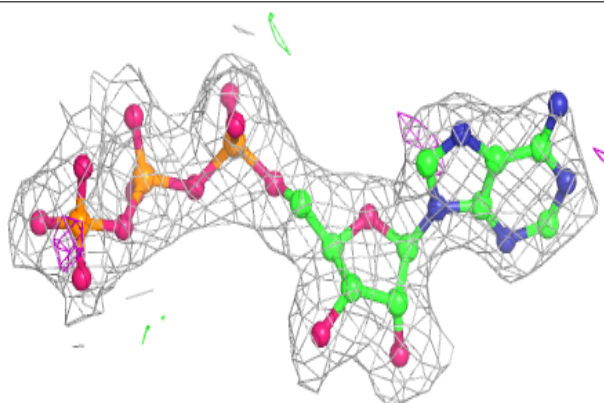


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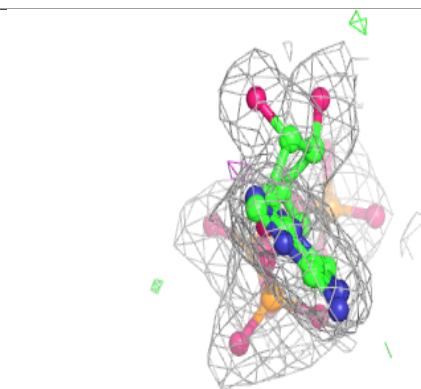
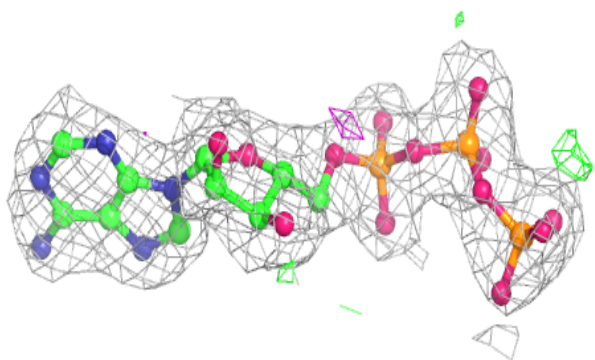
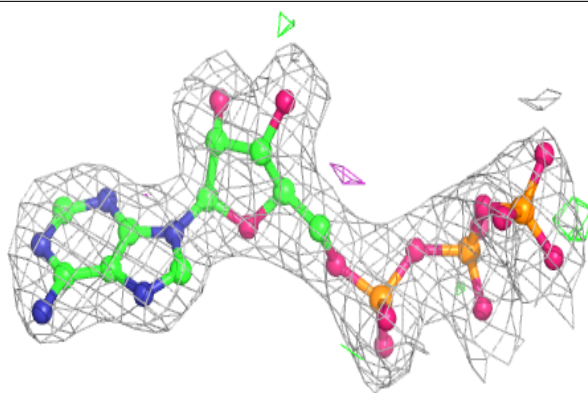
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and green (positive)

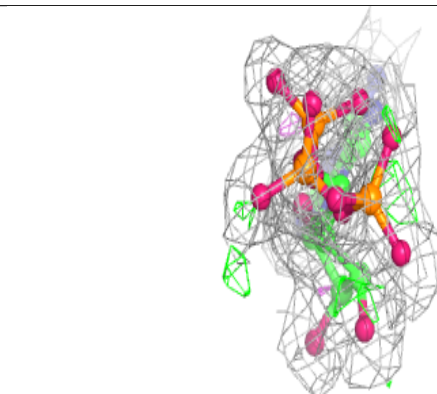
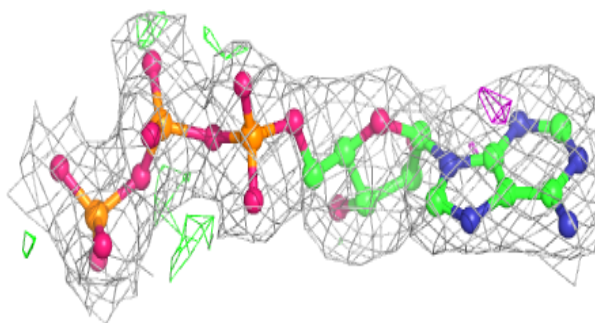
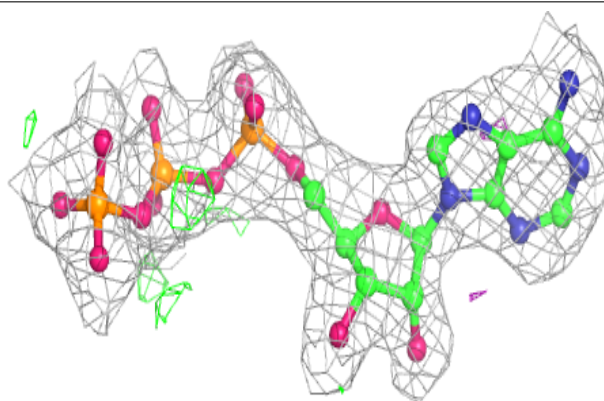


**Electron density around ATP C 602:**

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and green (positive)

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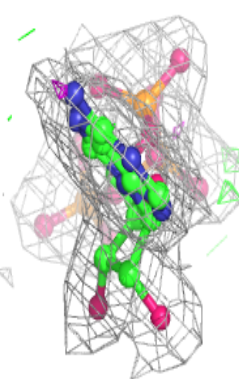
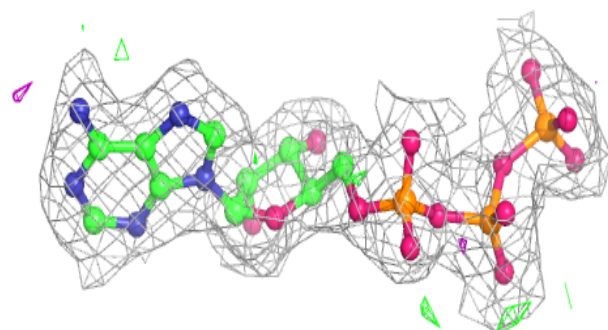
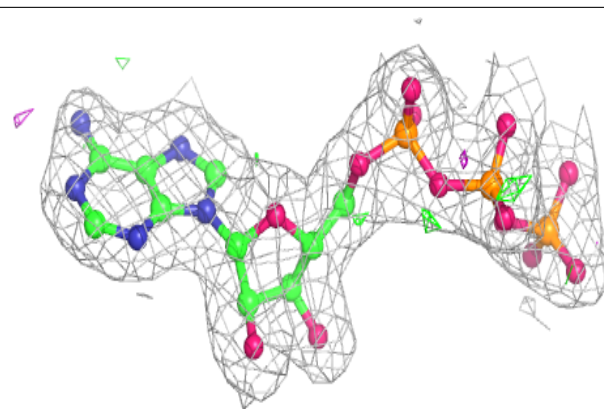
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



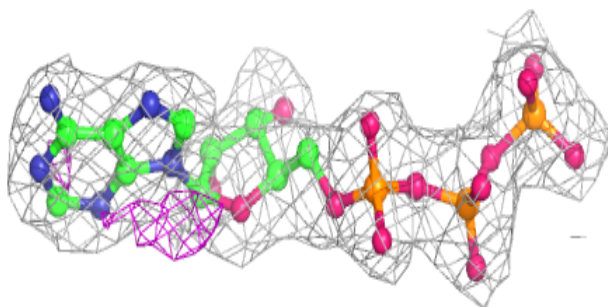
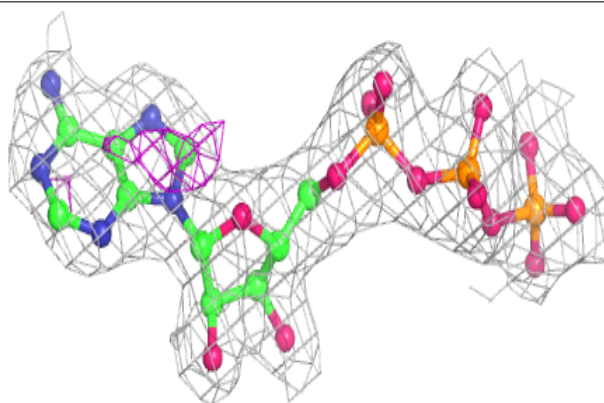


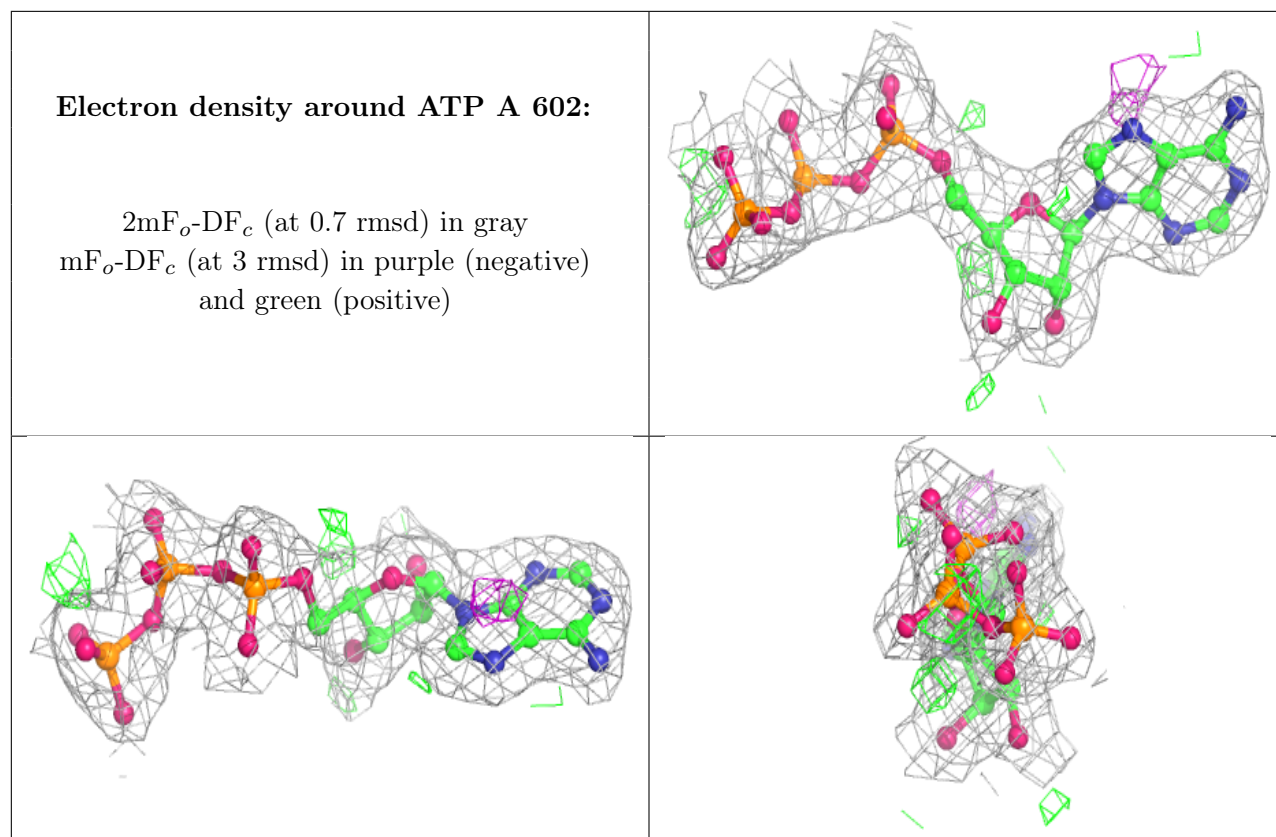
**Electron density around ATP D 602:**

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

**Electron density around ATP E 601:**

$2mF_o-DF_c$  (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.