



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:04 PM BST

PDB ID : 4TSF  
Title : The Pathway of Binding of the Intrinsically Disordered Mitochondrial Inhibitor Protein to F1-ATPase  
Authors : Bason, J.V.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2014-06-18  
Resolution : 3.20 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.

---

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

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

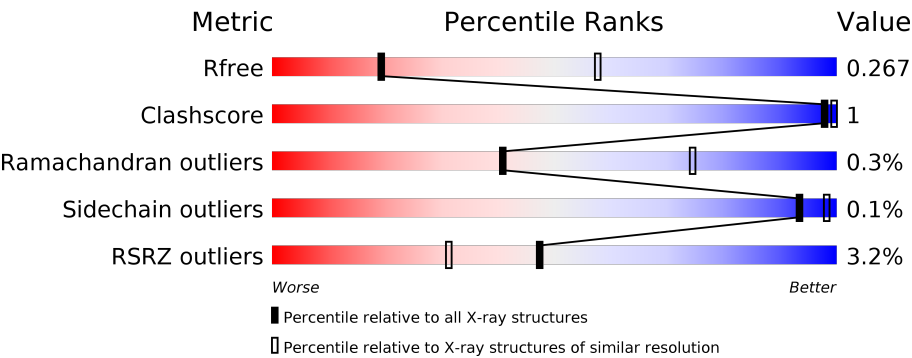
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	510	<div><div>%</div><div><div></div><div>95%</div><div>5%</div></div></div>
1	B	510	<div><div></div><div><div>93%</div><div>5%</div></div></div>
1	C	510	<div><div>%</div><div><div></div><div>93%</div><div>6%</div></div></div>
2	D	480	<div><div>%</div><div><div></div><div>95%</div><div>• •</div></div></div>
2	E	480	<div><div>2%</div><div><div></div><div>95%</div><div>• •</div></div></div>
2	F	480	<div><div>%</div><div><div></div><div>94%</div><div>• •</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	273	<div><div></div><div>22%</div><div></div><div>70%</div><div></div><div>28%</div></div>
4	H	66	<div><div></div><div>17%</div><div></div><div>24%</div><div></div><div>73%</div></div>
4	I	66	<div><div></div><div>2%</div><div></div><div>62%</div><div></div><div>38%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23887 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 ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	1	0
			3716	2345	655	704	12			
1	B	485	Total	C	N	O	S	0	0	0
			3693	2326	653	702	12			
1	C	479	Total	C	N	O	S	0	0	0
			3652	2301	647	692	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	see sequence details	UNP P19483
B	481	GLY	SER	see sequence details	UNP P19483
C	481	GLY	SER	see sequence details	UNP P19483

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	E	470	Total	C	N	O	S	0	0	0
			3564	2257	606	690	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	196	Total	C	N	O	S	0	0	0
			1525	955	277	286	7			

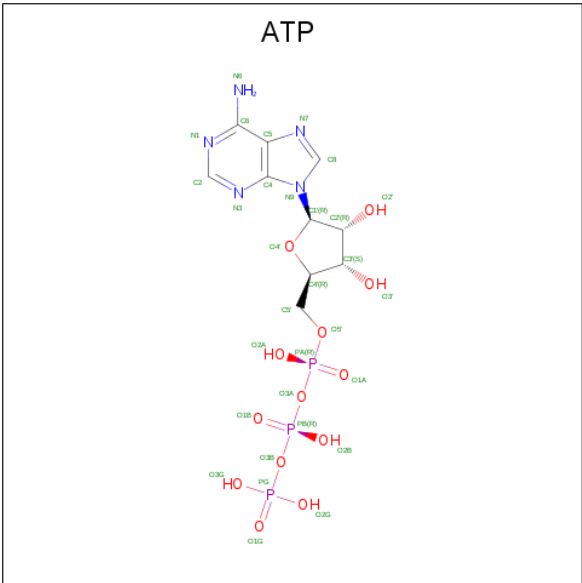
- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	41	Total	C	N	O	0	0	0
			323	196	67	60			
4	H	18	Total	C	N	O	0	0	0
			157	100	35	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	61	HIS	-	expression tag	UNP P01096
I	62	HIS	-	expression tag	UNP P01096
I	63	HIS	-	expression tag	UNP P01096
I	64	HIS	-	expression tag	UNP P01096
I	65	HIS	-	expression tag	UNP P01096
I	66	HIS	-	expression tag	UNP P01096
H	61	HIS	-	expression tag	UNP P01096
H	62	HIS	-	expression tag	UNP P01096
H	63	HIS	-	expression tag	UNP P01096
H	64	HIS	-	expression tag	UNP P01096
H	65	HIS	-	expression tag	UNP P01096
H	66	HIS	-	expression tag	UNP P01096

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



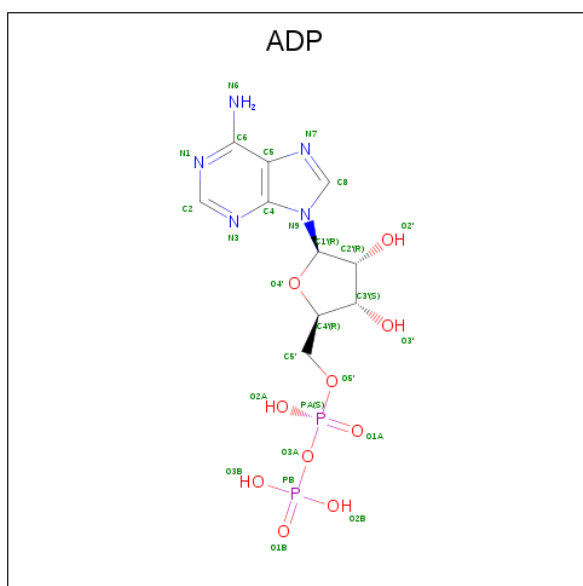
Continued from previous page...

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

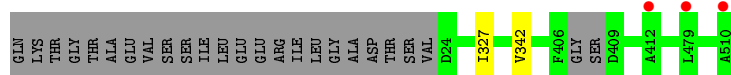
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total 3	O 3	0	0
8	B	3	Total 3	O 3	0	0
8	C	3	Total 3	O 3	0	0
8	D	4	Total 4	O 4	0	0
8	F	4	Total 4	O 4	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.

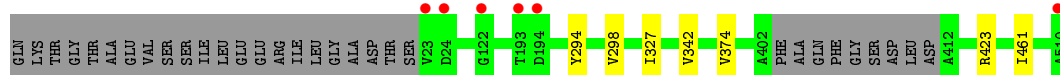
- Molecule 1: ATP synthase subunit alpha, mitochondrial



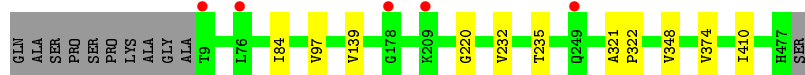
- Molecule 1: ATP synthase subunit alpha, mitochondrial



- Molecule 1: ATP synthase subunit alpha, mitochondrial



- Molecule 2: ATP synthase subunit beta, mitochondrial

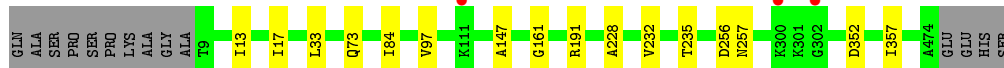


- Molecule 2: ATP synthase subunit beta, mitochondrial

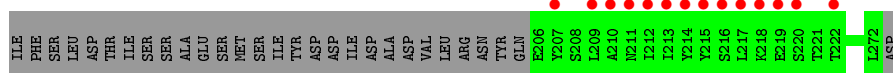
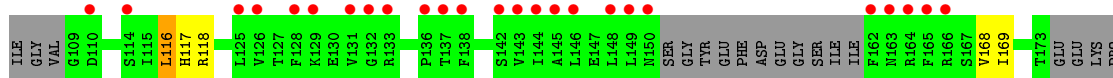
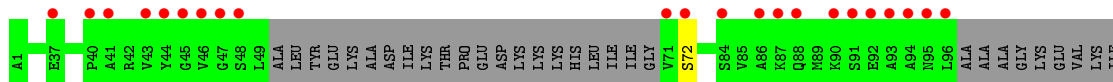


- Molecule 2: ATP synthase subunit beta, mitochondrial

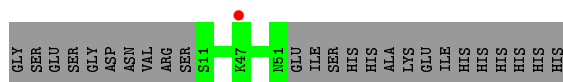




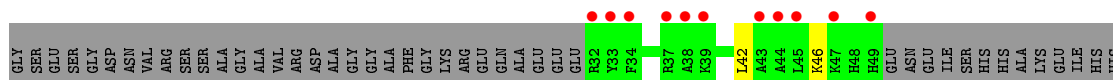
• Molecule 3: ATP synthase subunit gamma, mitochondrial



• Molecule 4: ATPase inhibitor, mitochondrial



• Molecule 4: ATPase inhibitor, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.02Å 154.42Å 269.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.73 – 3.20 62.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (134.73-3.20) 91.1 (62.81-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.234 , 0.272 0.233 , 0.267	Depositor DCC
$R_{free}$ test set	3386 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.7	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 19.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	0.25	0/3767	0.42	0/5080
1	B	0.25	0/3741	0.42	0/5046
1	C	0.25	0/3700	0.41	0/4990
2	D	0.25	0/3616	0.42	0/4906
2	E	0.25	0/3622	0.43	0/4914
2	F	0.25	0/3587	0.42	0/4867
3	G	0.26	0/1538	0.39	0/2057
4	H	0.29	0/160	0.34	0/210
4	I	0.28	0/327	0.40	0/432
All	All	0.25	0/24058	0.42	0/32502

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3716	0	3813	1	0
1	B	3693	0	3805	5	0
1	C	3652	0	3764	3	0
2	D	3558	0	3605	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3564	0	3611	9	0
2	F	3530	0	3586	6	0
3	G	1525	0	1595	2	0
4	H	157	0	165	2	0
4	I	323	0	312	0	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	D	27	0	12	0	0
7	F	27	0	12	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	4	0	0	0	0
8	F	4	0	0	0	0
All	All	23887	0	24316	32	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 1.

All (32) 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:97:VAL:HG22	2:D:232:VAL:HG13	1.79	0.64
2:E:473:LEU:HB3	4:H:42:LEU:HD11	1.85	0.57
2:D:97:VAL:HG22	2:D:232:VAL:CG1	2.34	0.57
2:E:474:ALA:O	2:E:477:HIS:ND1	2.39	0.56
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.88	0.56
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.89	0.54
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.89	0.53
2:E:61:ILE:HD11	2:E:272:LEU:HD21	1.91	0.53
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.90	0.53
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.93	0.50
2:F:97:VAL:HG22	2:F:232:VAL:HB	1.95	0.48
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.45	0.47
2:F:97:VAL:HG21	2:F:228:ALA:HB1	1.96	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.97	0.46
2:F:256:ASP:HA	2:F:257:ASN:HA	1.76	0.45
2:E:50:ALA:HB2	2:E:61:ILE:HD13	1.99	0.44
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.99	0.44
2:D:139:VAL:HG11	2:D:348:VAL:HB	1.98	0.44
2:E:474:ALA:HB1	4:H:46:LYS:HA	1.99	0.44
1:A:327:ILE:HD11	1:A:342:VAL:HG21	2.00	0.43
2:E:345:TYR:HA	2:E:346:PRO:C	2.39	0.43
2:D:374:VAL:HG13	2:D:410:ILE:HG21	2.01	0.42
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.50	0.42
2:F:147:ALA:HB2	2:F:357:ILE:HG21	2.02	0.42
2:F:13:ILE:HD12	2:F:73:GLN:HB3	2.00	0.42
1:B:327:ILE:HD11	1:B:342:VAL:HG21	2.01	0.41
3:G:116:LEU:O	3:G:118:ARG:N	2.53	0.41
1:B:246:ALA:HB3	1:B:247:PRO:HD3	2.03	0.41
3:G:168:VAL:HG23	3:G:169:ILE:HG13	2.03	0.41
1:B:423:ARG:NH1	1:B:454:ASP:O	2.54	0.41
2:F:84:ILE:HD13	2:F:235:THR:HG23	2.03	0.40
1:C:294:TYR:HB3	1:C:298:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/510 (94%)	470 (98%)	12 (2%)	0	100	100
1	B	481/510 (94%)	465 (97%)	16 (3%)	0	100	100
1	C	475/510 (93%)	459 (97%)	15 (3%)	1 (0%)	47	79
2	D	467/480 (97%)	442 (95%)	25 (5%)	0	100	100
2	E	468/480 (98%)	441 (94%)	27 (6%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	464/480 (97%)	437 (94%)	23 (5%)	4 (1%)	17	56
3	G	186/273 (68%)	180 (97%)	3 (2%)	3 (2%)	9	43
4	H	16/66 (24%)	15 (94%)	1 (6%)	0	100	100
4	I	39/66 (59%)	39 (100%)	0	0	100	100
All	All	3078/3375 (91%)	2948 (96%)	122 (4%)	8 (0%)	41	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	VAL
3	G	72	SER
3	G	116	LEU
3	G	117	HIS
2	F	33	LEU
2	F	352	ASP
2	F	161	GLY
2	F	17	ILE

### 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	393/412 (95%)	393 (100%)	0	100	100
1	B	392/412 (95%)	392 (100%)	0	100	100
1	C	387/412 (94%)	387 (100%)	0	100	100
2	D	379/386 (98%)	379 (100%)	0	100	100
2	E	380/386 (98%)	378 (100%)	2 (0%)	88	95
2	F	376/386 (97%)	375 (100%)	1 (0%)	92	96
3	G	166/231 (72%)	166 (100%)	0	100	100
4	H	14/50 (28%)	14 (100%)	0	100	100
4	I	28/50 (56%)	28 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2515/2725 (92%)	2512 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	330	ASP
2	E	477	HIS
2	F	191	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
5	ATP	A	600	6	26,33,33	0.97	2 (7%)	31,52,52	1.51	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ADP	F	600	6	24,29,29	1.01	2 (8%)	29,45,45	1.43	5 (17%)
5	ATP	C	600	6	26,33,33	0.98	2 (7%)	31,52,52	1.55	5 (16%)
5	ATP	B	600	6	26,33,33	0.97	2 (7%)	31,52,52	1.62	5 (16%)
7	ADP	D	600	6	24,29,29	0.99	1 (4%)	29,45,45	1.51	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	A	600	6	-	0/18/38/38	0/3/3/3
7	ADP	F	600	6	-	0/12/32/32	0/3/3/3
5	ATP	C	600	6	-	2/18/38/38	0/3/3/3
5	ATP	B	600	6	-	0/18/38/38	0/3/3/3
7	ADP	D	600	6	-	1/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	ATP	C5-C4	2.57	1.47	1.40
5	C	600	ATP	C5-C4	2.53	1.47	1.40
5	A	600	ATP	C5-C4	2.51	1.47	1.40
7	F	600	ADP	C5-C4	2.50	1.47	1.40
7	D	600	ADP	C5-C4	2.48	1.47	1.40
5	C	600	ATP	C2-N3	2.08	1.35	1.32
5	A	600	ATP	C2-N3	2.08	1.35	1.32
7	F	600	ADP	C2-N3	2.03	1.35	1.32
5	B	600	ATP	C2-N3	2.03	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ATP	N3-C2-N1	-3.75	122.81	128.68
5	C	600	ATP	N3-C2-N1	-3.71	122.88	128.68
7	F	600	ADP	N3-C2-N1	-3.71	122.88	128.68
7	D	600	ADP	N3-C2-N1	-3.71	122.88	128.68
5	B	600	ATP	N3-C2-N1	-3.68	122.93	128.68
7	D	600	ADP	C3'-C2'-C1'	3.52	106.28	100.98
5	B	600	ATP	PB-O3B-PG	-3.52	120.75	132.83
5	B	600	ATP	C3'-C2'-C1'	3.48	106.22	100.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	ATP	C3'-C2'-C1'	3.39	106.08	100.98
5	B	600	ATP	PA-O3A-PB	-3.32	121.42	132.83
5	C	600	ATP	PA-O3A-PB	-3.23	121.73	132.83
5	A	600	ATP	PB-O3B-PG	-3.19	121.89	132.83
7	D	600	ADP	PA-O3A-PB	-3.06	122.33	132.83
7	F	600	ADP	PA-O3A-PB	-3.06	122.33	132.83
5	A	600	ATP	PA-O3A-PB	-3.02	122.45	132.83
5	C	600	ATP	PB-O3B-PG	-3.02	122.47	132.83
7	F	600	ADP	C3'-C2'-C1'	2.99	105.48	100.98
7	D	600	ADP	C4-C5-N7	-2.82	106.46	109.40
5	A	600	ATP	C4-C5-N7	-2.77	106.51	109.40
5	B	600	ATP	C4-C5-N7	-2.77	106.51	109.40
5	C	600	ATP	C4-C5-N7	-2.75	106.54	109.40
7	F	600	ADP	C4-C5-N7	-2.65	106.64	109.40
5	A	600	ATP	C3'-C2'-C1'	2.56	104.83	100.98
7	F	600	ADP	C2-N1-C6	2.02	122.20	118.75
5	A	600	ATP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

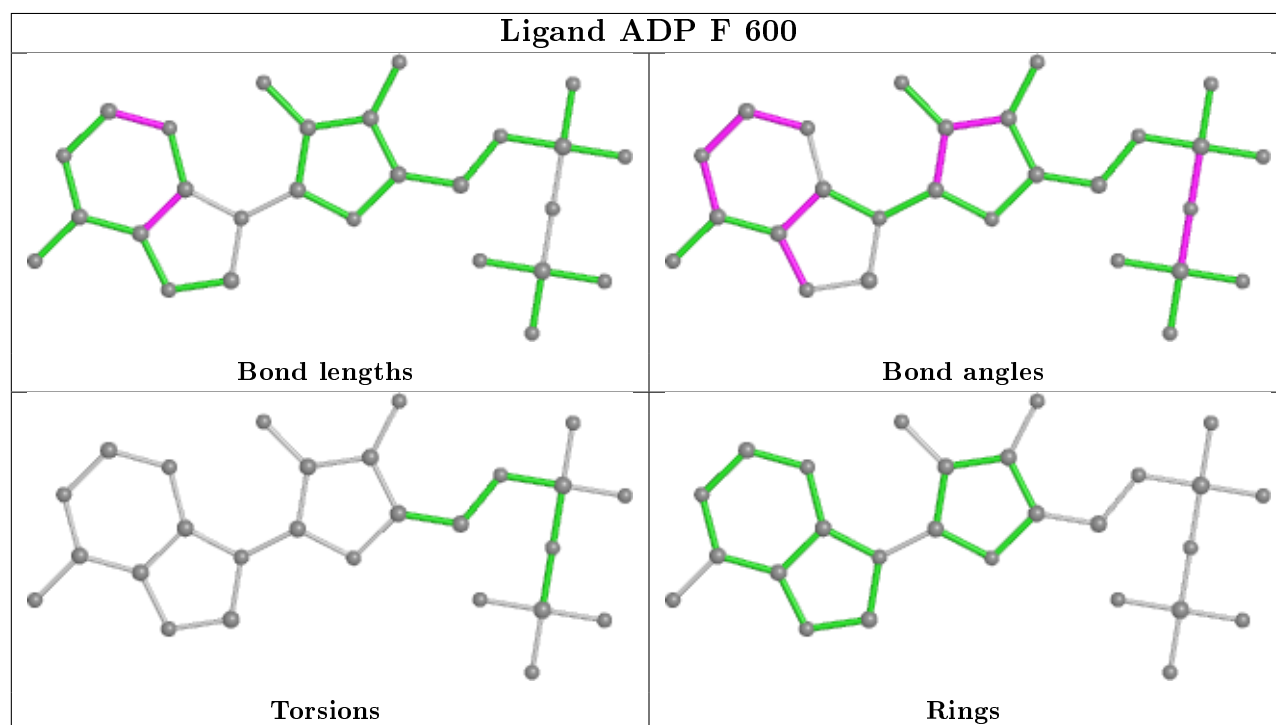
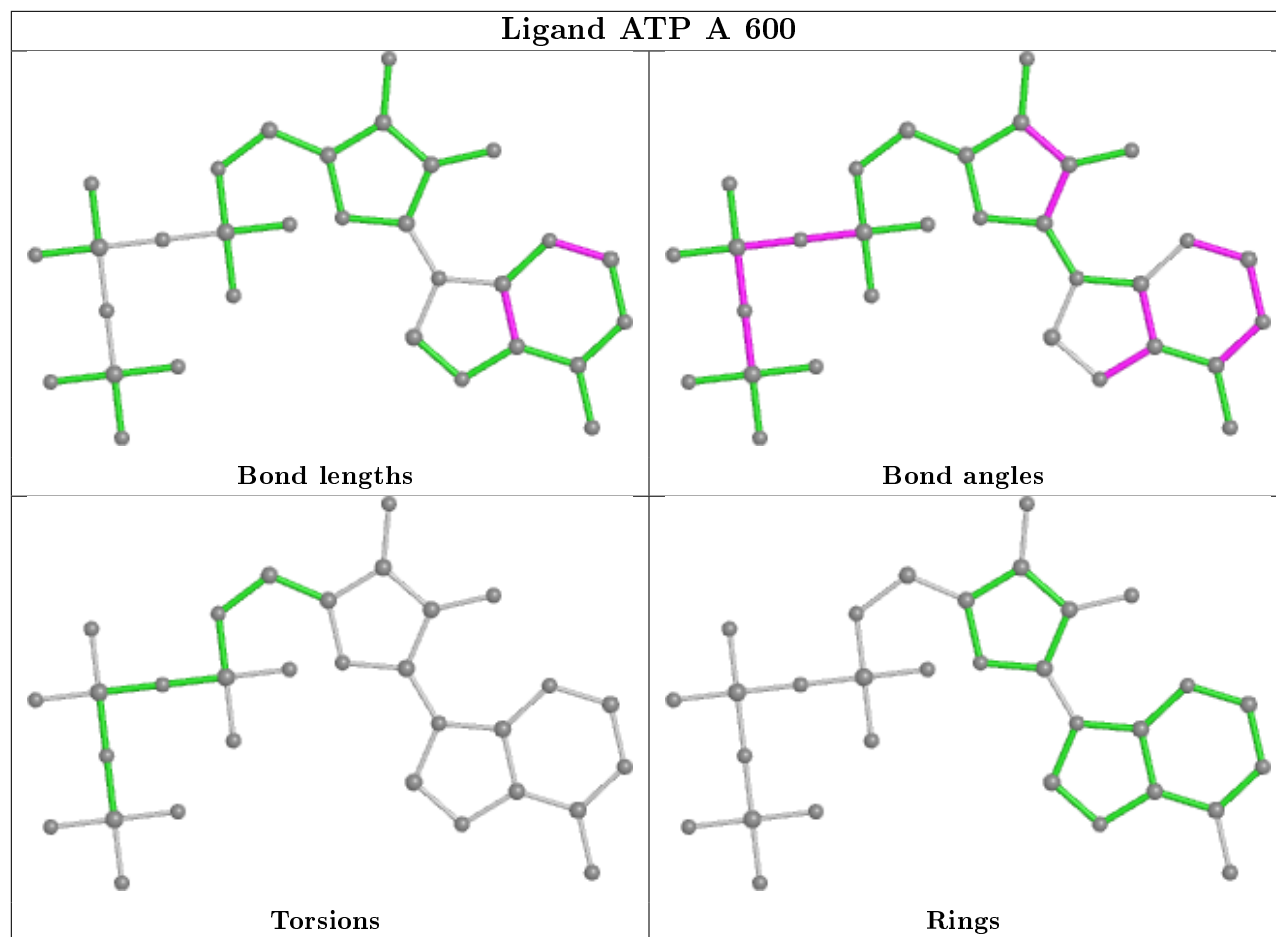
All (3) torsion outliers are listed below:

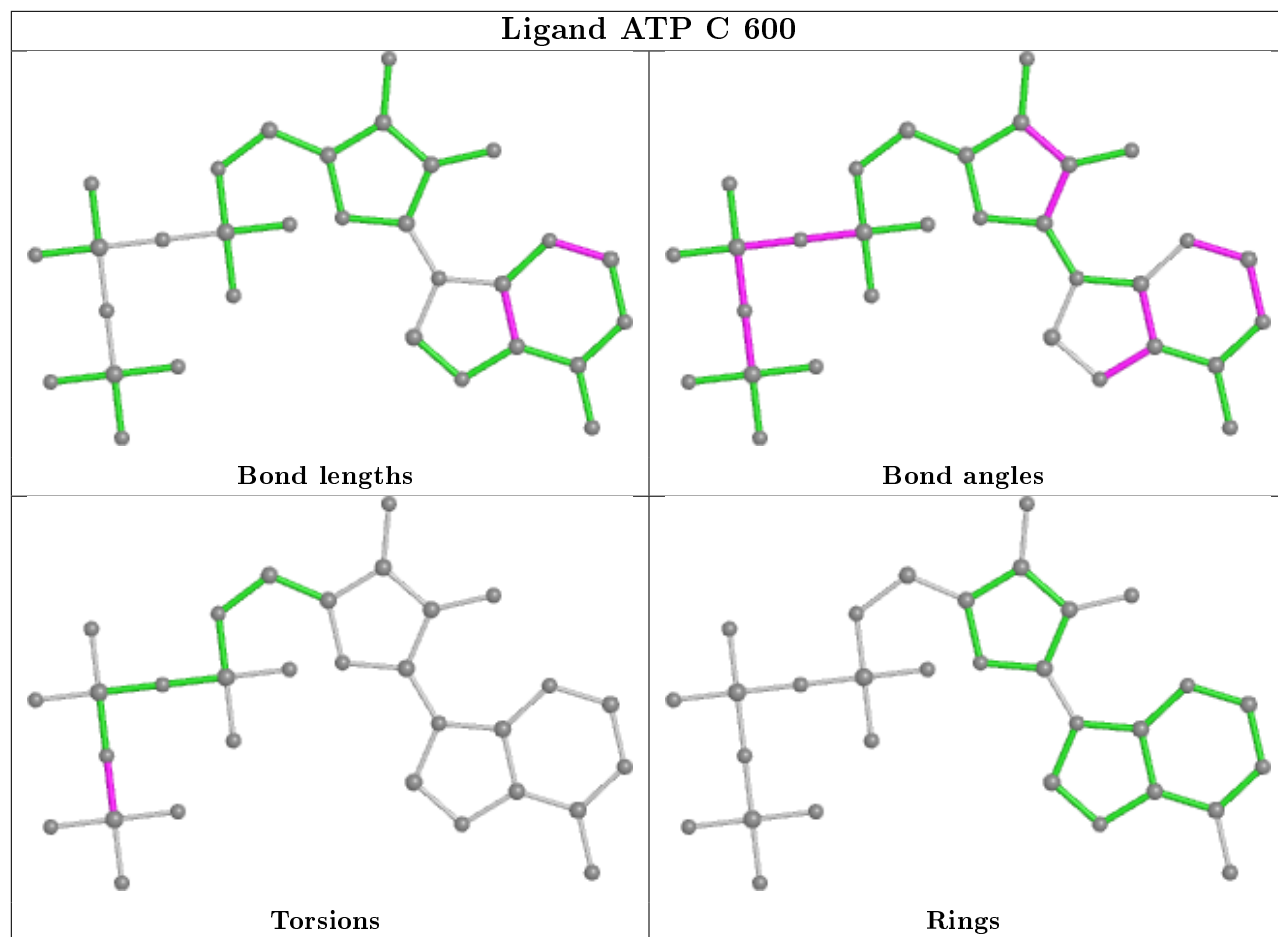
Mol	Chain	Res	Type	Atoms
5	C	600	ATP	PB-O3B-PG-O2G
5	C	600	ATP	PB-O3B-PG-O1G
7	D	600	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

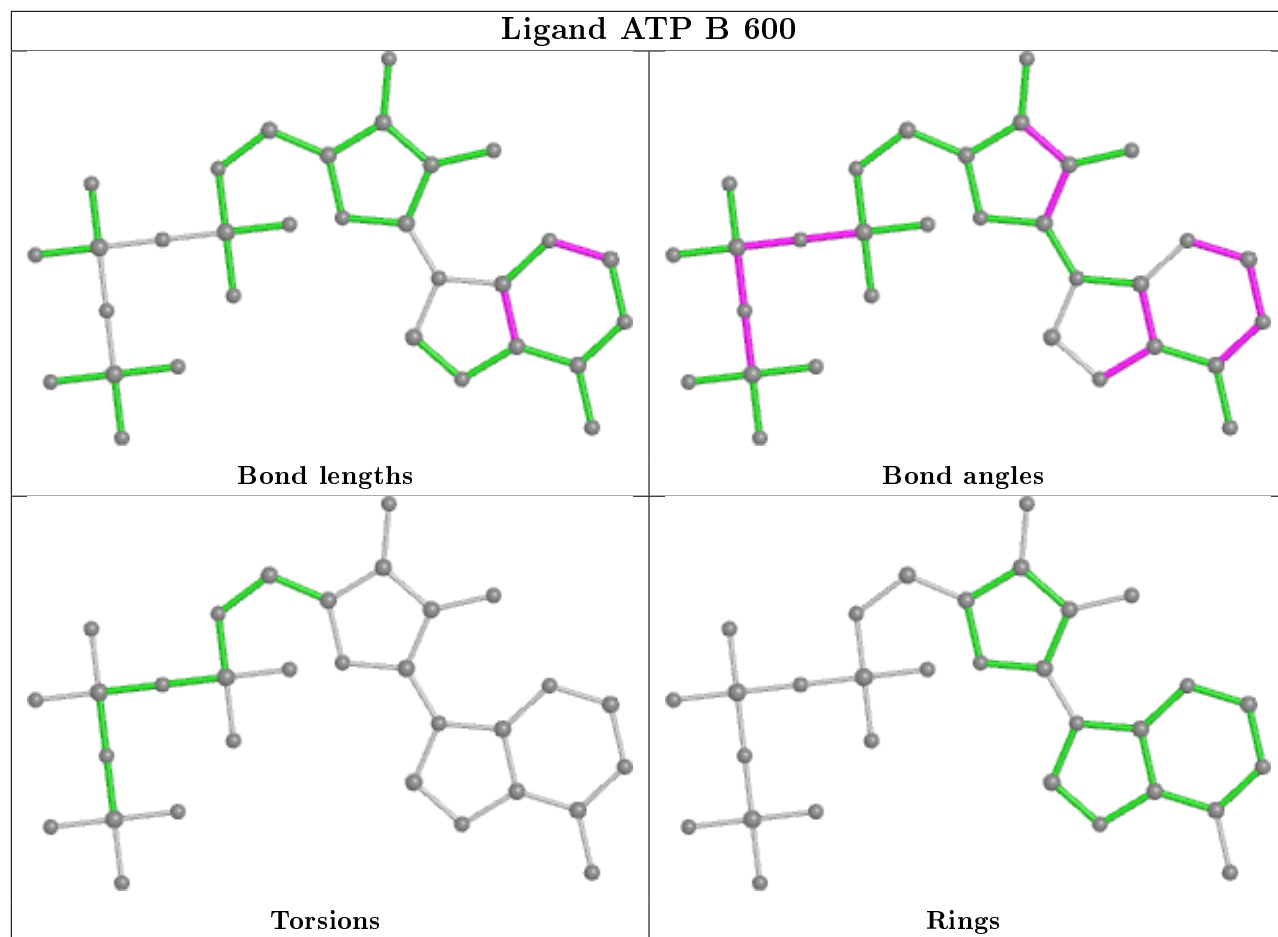
No monomer is involved in short contacts.

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

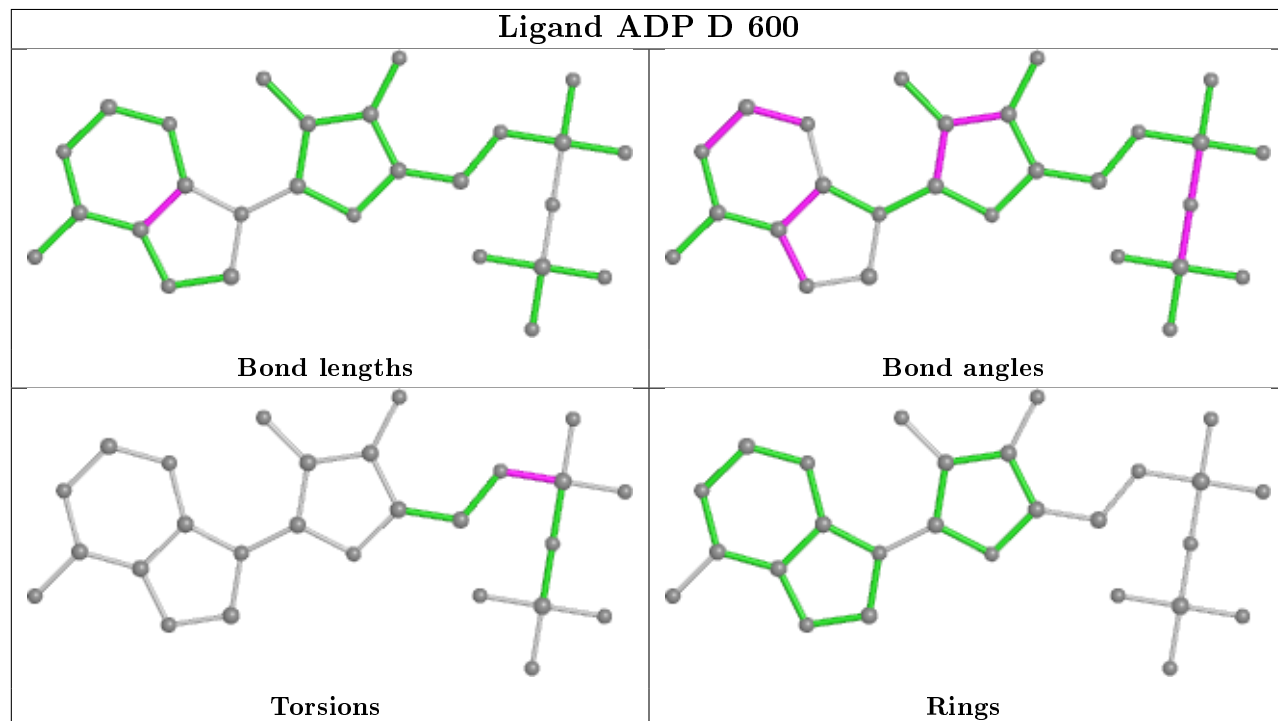




## Ligand ATP B 600



## Ligand ADP D 600



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	485/510 (95%)	-0.02	3 (0%) 89 83	53, 67, 102, 137	0
1	B	485/510 (95%)	-0.10	1 (0%) 95 94	49, 64, 94, 123	0
1	C	479/510 (93%)	0.14	6 (1%) 77 65	60, 84, 105, 124	0
2	D	469/480 (97%)	0.06	5 (1%) 80 69	61, 80, 106, 118	0
2	E	470/480 (97%)	0.07	8 (1%) 70 57	50, 64, 110, 138	0
2	F	466/480 (97%)	0.11	3 (0%) 89 83	58, 80, 100, 107	0
3	G	196/273 (71%)	1.29	61 (31%) 0 0	59, 130, 156, 163	0
4	H	18/66 (27%)	2.28	11 (61%) 0 0	141, 149, 154, 154	0
4	I	41/66 (62%)	0.37	1 (2%) 59 44	78, 90, 113, 119	0
All	All	3109/3375 (92%)	0.14	99 (3%) 47 31	49, 75, 121, 163	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	217	LEU	5.5
3	G	162	PHE	5.2
2	E	393	MET	5.0
3	G	145	ALA	4.9
3	G	138	PHE	4.4
3	G	48	SER	4.4
3	G	209	LEU	4.2
3	G	95	ASN	4.0
3	G	210	ALA	4.0
4	H	43	ALA	3.9
3	G	211	ASN	3.7
3	G	166	ARG	3.7
4	H	34	PHE	3.7
3	G	46	VAL	3.6
4	H	37	ARG	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	71	VAL	3.5
3	G	126	VAL	3.5
3	G	213	ILE	3.4
1	A	510	ALA	3.4
1	C	510	ALA	3.4
3	G	136	PRO	3.3
3	G	47	GLY	3.3
3	G	149	LEU	3.2
3	G	215	TYR	3.1
3	G	146	LEU	3.1
2	E	478	SER	3.1
3	G	163	ASN	3.1
4	H	39	LYS	3.1
3	G	143	VAL	3.1
2	E	394	ASP	3.0
3	G	133	ARG	3.0
3	G	86	ALA	3.0
1	A	412	ALA	2.9
3	G	94	ALA	2.9
2	D	178	GLY	2.9
1	C	23	VAL	2.9
2	E	391	LEU	2.9
3	G	214	TYR	2.8
3	G	142	SER	2.8
3	G	129	LYS	2.8
3	G	165	PHE	2.8
4	H	38	ALA	2.7
2	D	209	LYS	2.6
3	G	43	VAL	2.6
3	G	72	SER	2.6
1	C	24	ASP	2.6
3	G	84	SER	2.6
2	E	387	ILE	2.6
3	G	96	LEU	2.6
3	G	41	ALA	2.6
4	H	47	LYS	2.6
3	G	87	LYS	2.5
3	G	110	ASP	2.5
3	G	137	THR	2.5
4	H	32	ARG	2.5
3	G	218	LYS	2.5
3	G	216	SER	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	91	SER	2.5
4	H	49	HIS	2.5
3	G	164	ARG	2.5
3	G	150	ASN	2.4
1	C	122	GLY	2.4
2	F	111	LYS	2.4
1	C	193	THR	2.4
3	G	144	ILE	2.4
3	G	220	SER	2.4
3	G	222	THR	2.4
3	G	88	GLN	2.4
2	F	302	GLY	2.3
3	G	114	SER	2.3
1	A	479	LEU	2.3
2	D	76	LEU	2.2
2	D	249	GLN	2.2
3	G	212	ILE	2.2
3	G	207	TYR	2.2
3	G	45	GLY	2.2
3	G	44	TYR	2.2
3	G	148	LEU	2.2
2	D	9	THR	2.2
3	G	93	ALA	2.2
4	H	44	ALA	2.2
1	B	16	ILE	2.1
3	G	128	PHE	2.1
3	G	92	GLU	2.1
1	C	194	ASP	2.1
3	G	131	VAL	2.1
3	G	90	LYS	2.1
3	G	125	LEU	2.1
3	G	37	GLU	2.1
3	G	132	GLY	2.1
2	F	300	LYS	2.1
2	E	403	THR	2.1
2	E	474	ALA	2.1
2	E	386	ASP	2.0
3	G	219	GLU	2.0
4	H	45	LEU	2.0
3	G	40	PRO	2.0
4	I	47	LYS	2.0
4	H	33	TYR	2.0



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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

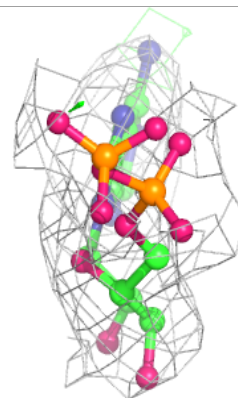
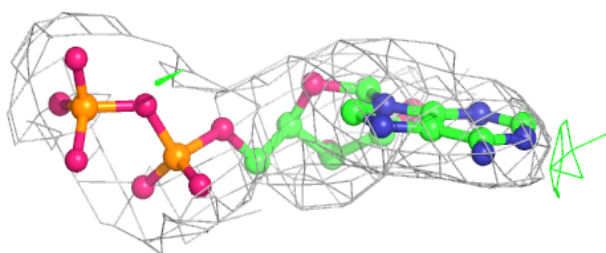
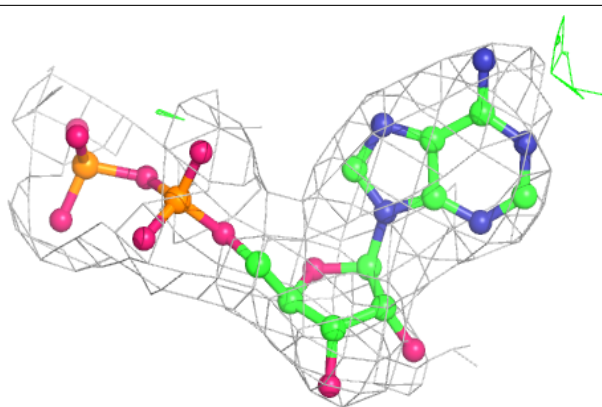
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	MG	D	601	1/1	0.77	0.17	73,73,73,73	0
6	MG	B	601	1/1	0.90	0.14	54,54,54,54	0
6	MG	A	601	1/1	0.91	0.22	57,57,57,57	0
7	ADP	D	600	27/27	0.94	0.19	71,71,72,73	0
6	MG	C	601	1/1	0.95	0.22	72,72,72,72	0
5	ATP	A	600	31/31	0.95	0.17	56,57,58,58	4
5	ATP	C	600	31/31	0.95	0.18	72,79,83,83	4
5	ATP	B	600	31/31	0.95	0.18	54,60,62,62	0
7	ADP	F	600	27/27	0.95	0.21	60,63,66,66	0
6	MG	F	601	1/1	0.97	0.21	62,62,62,62	0

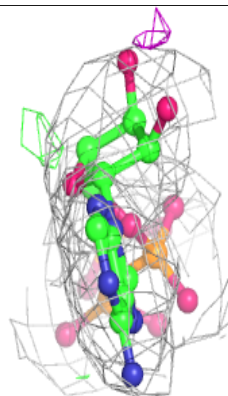
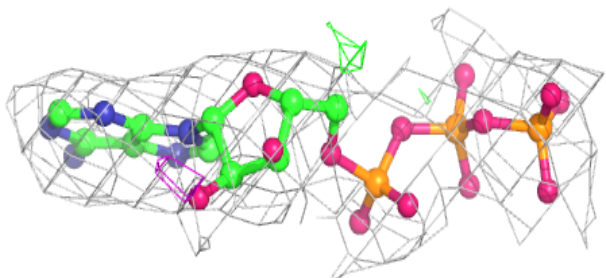
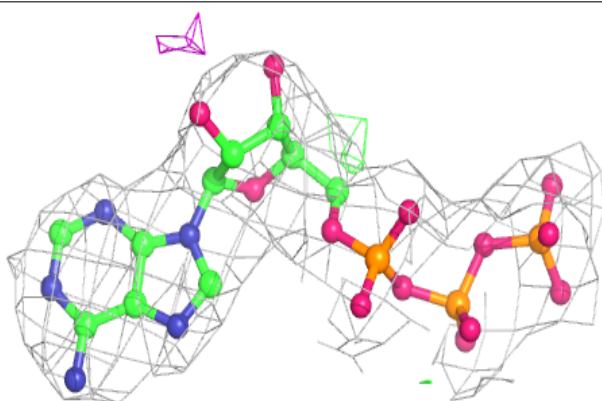
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP D 600:**

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

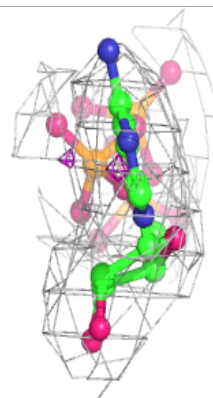
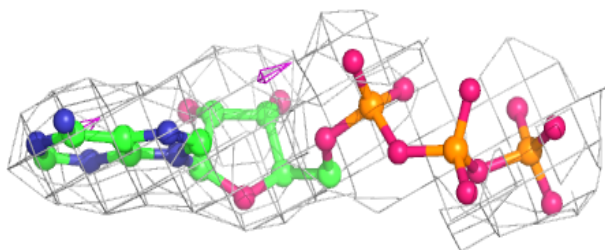
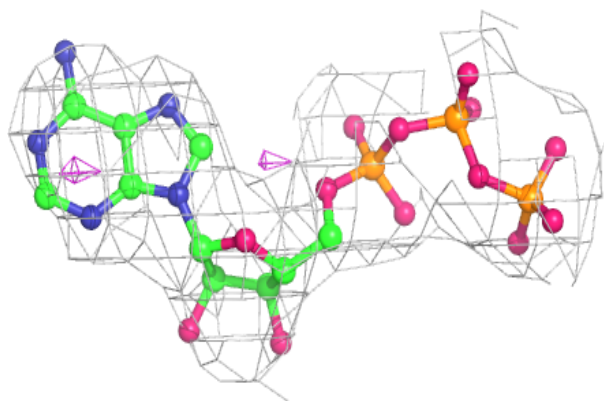
**Electron density around ATP A 600:**

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

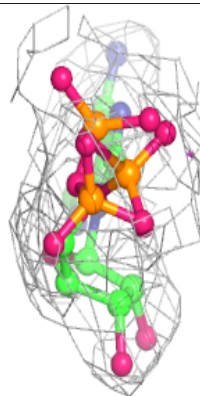
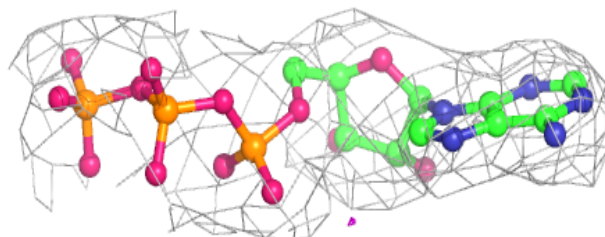
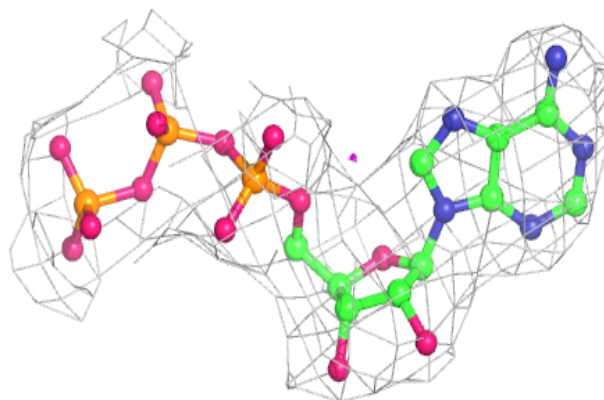


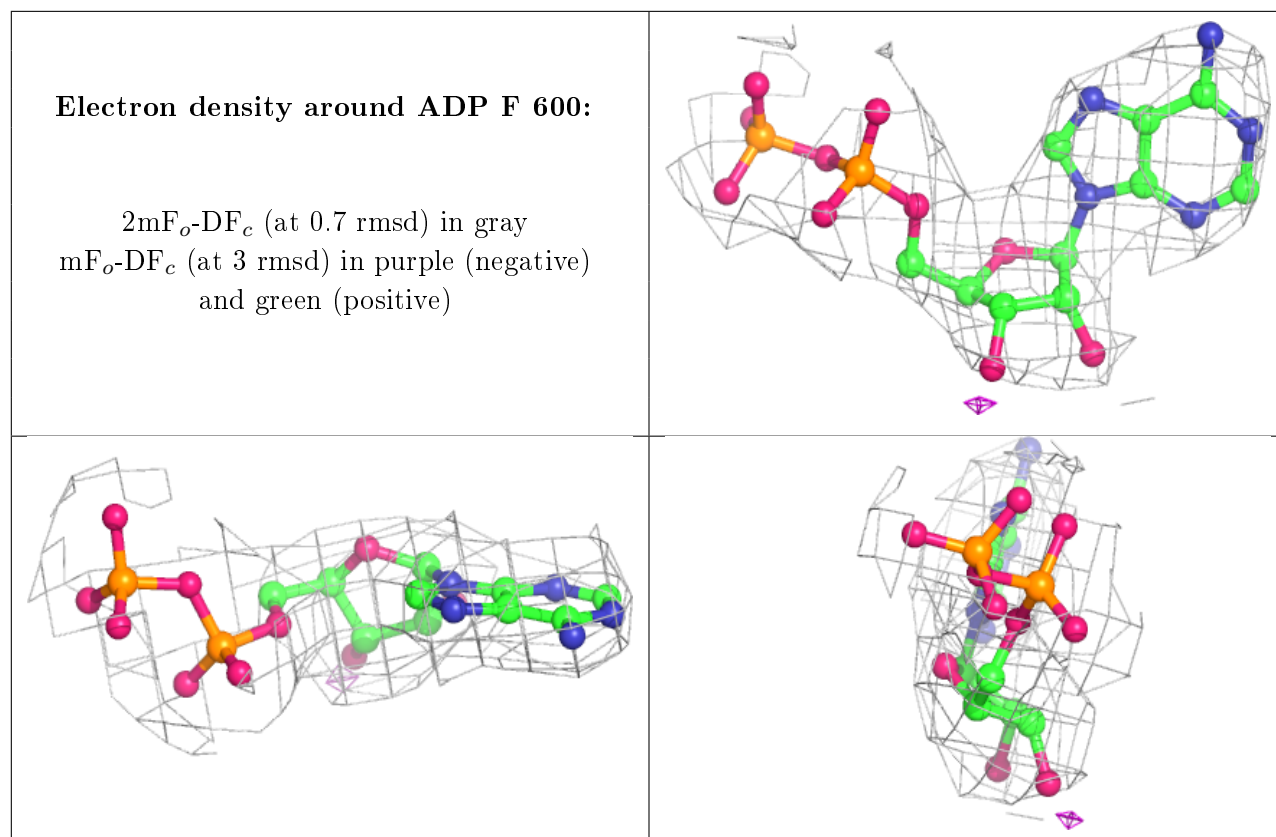
**Electron density around ATP C 600:**

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

**Electron density around ATP B 600:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.