



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:51 am BST

PDB ID : 4Z1M
Title : Bovine F1-ATPase inhibited by three copies of the inhibitor protein IF1 crystallised in the presence of thiophosphate.
Authors : Bason, J.V.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2015-03-27
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

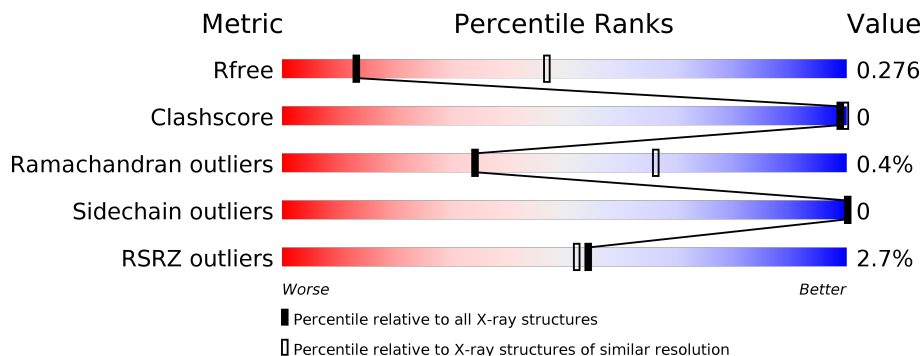
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



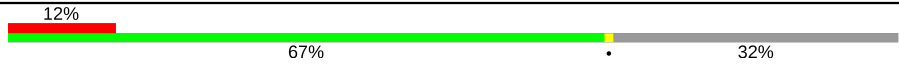



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 ≥ 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	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	

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Mol	Chain	Length	Quality of chain
3	G	273	
4	H	66	
4	I	66	
4	J	66	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 24201 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
			Total	C	N	O	S			
1	A	487	Total	C	N	O	S	0	1	0
			3723	2349	656	706	12			
1	B	487	Total	C	N	O	S	0	0	0
			3706	2333	655	706	12			
1	C	483	Total	C	N	O	S	0	0	0
			3684	2323	651	698	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	variant	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	variant	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	variant	UNP P19483

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			3563	2257	606	689	11			
2	F	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	187	Total	C	N	O	S	0	0	0
			1467	919	267	274	7			

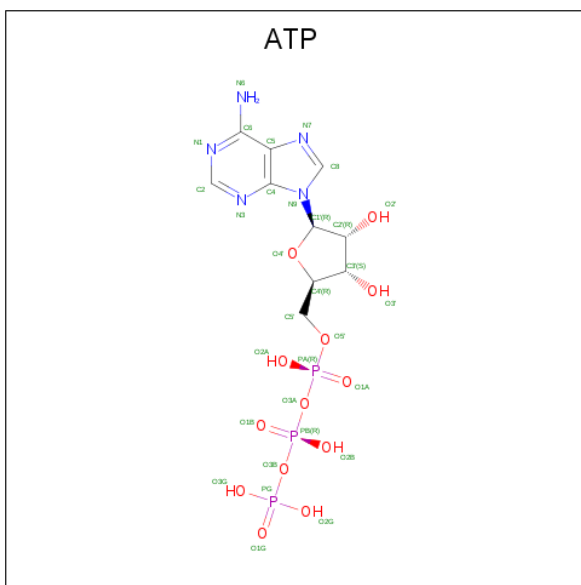
- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	41	317	192	65	60	0	0	0
4	I	28	236	144	49	43	0	0	0
4	J	22	189	117	38	34	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	39	ALA	LYS	engineered mutation	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
I	39	ALA	LYS	engineered mutation	UNP P01096
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
J	39	ALA	LYS	engineered mutation	UNP P01096
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

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

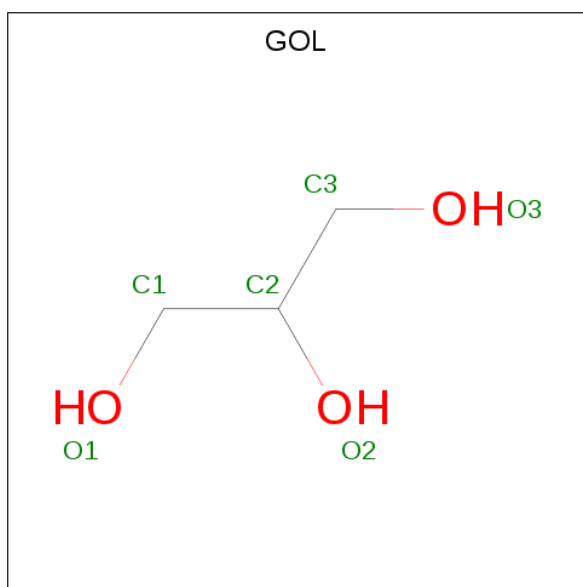


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0
5	B	1	31	10	5	13	3	0	0
5	C	1	31	10	5	13	3	0	0

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

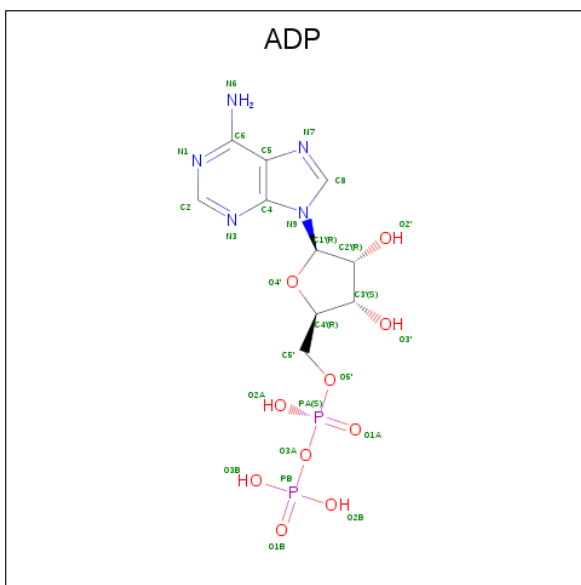


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	2	Total Cl 2 2	0	0
8	B	1	Total Cl 1 1	0	0
8	C	2	Total Cl 2 2	0	0
8	F	2	Total Cl 2 2	0	0
8	E	4	Total Cl 4 4	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	O	0	0
			4	4		
10	B	4	Total	O	0	0
			4	4		
10	C	5	Total	O	0	0
			5	5		
10	D	5	Total	O	0	0
			5	5		
10	E	3	Total	O	0	0
			3	3		
10	F	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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

Chain A:  94% 5%



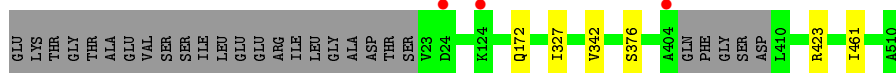
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain B:  94% 5%



- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:  94% 5%



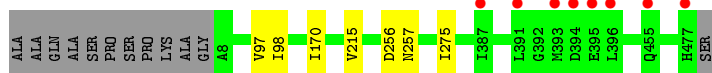
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D:  96% 2% 2%



- Molecule 2: ATP synthase subunit beta, mitochondrial

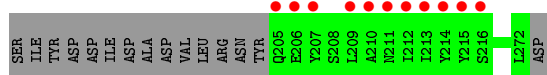
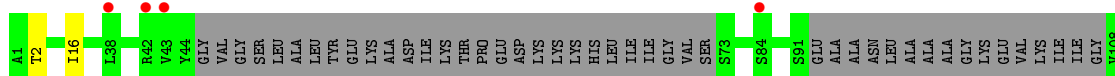
Chain E:  96% 2% 2%



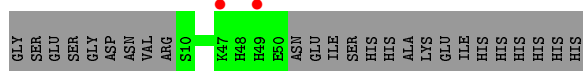
- Molecule 2: ATP synthase subunit beta, mitochondrial



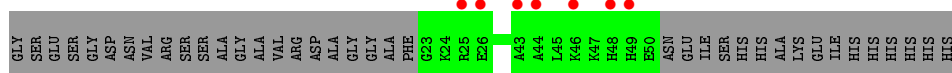
• Molecule 3: ATP synthase subunit gamma, mitochondrial



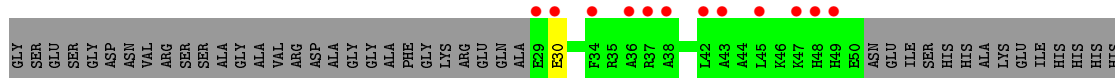
• Molecule 4: ATPase inhibitor, mitochondrial



• 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, α , β , γ	108.77Å 155.29Å 271.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 3.30 46.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (46.31-3.30) 95.8 (46.31-3.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.32Å)	Xtrriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.239 , 0.275 0.239 , 0.276	Depositor DCC
R_{free} test set	3346 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24201	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/3778	0.46	0/5096
1	B	0.28	0/3754	0.46	0/5064
1	C	0.29	0/3733	0.45	0/5035
2	D	0.29	0/3616	0.45	0/4906
2	E	0.28	0/3621	0.46	0/4913
2	F	0.28	0/3616	0.46	0/4906
3	G	0.30	0/1480	0.45	0/1978
4	H	0.29	0/321	0.37	0/425
4	I	0.32	0/239	0.41	0/315
4	J	0.30	0/192	0.42	0/254
All	All	0.29	0/24350	0.46	0/32892

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	3723	0	3823	3	0
1	B	3706	0	3814	4	0
1	C	3684	0	3793	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3558	0	3605	6	0
2	E	3563	0	3611	4	0
2	F	3558	0	3605	2	0
3	G	1467	0	1536	1	0
4	H	317	0	303	0	0
4	I	236	0	229	0	0
4	J	189	0	181	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	A	6	0	8	0	0
7	B	6	0	8	0	0
8	B	1	0	0	0	0
8	C	2	0	0	0	0
8	E	4	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
9	D	27	0	12	0	0
9	F	27	0	12	0	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
10	C	5	0	0	1	0
10	D	5	0	0	0	0
10	E	3	0	0	0	0
10	F	4	0	0	0	0
All	All	24201	0	24576	21	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 0.

All (21) 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:63:MET:CE	2:D:227:GLY:O	2.11	0.98
2:D:63:MET:HE1	2:D:227:GLY:O	1.69	0.92
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:MET:CE	2:D:227:GLY:C	2.74	0.56
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.91	0.52
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.93	0.51
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.93	0.51
1:B:383:MET:HG3	1:B:438:ILE:HD11	1.92	0.50
2:F:13:ILE:HD12	2:F:73:GLN:HB3	1.97	0.47
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.95	0.47
1:A:265:LEU:HD11	1:A:324:LEU:HD13	1.96	0.46
2:D:256:ASP:HA	2:D:257:ASN:HA	1.78	0.46
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.99	0.45
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.97	0.45
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.98	0.45
2:D:390:ILE:HD11	3:G:16:ILE:HG23	1.99	0.45
2:D:63:MET:HE2	2:D:227:GLY:C	2.37	0.44
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.00	0.43
2:F:163:THR:HA	2:F:166:ILE:HG22	2.02	0.42
1:C:172:GLN:NE2	10:C:701:HOH:O	2.52	0.41
2:E:256:ASP:HA	2:E:257:ASN:HA	1.80	0.41

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	486/510 (95%)	467 (96%)	17 (4%)	2 (0%)	34	66
1	B	483/510 (95%)	462 (96%)	21 (4%)	0	100	100
1	C	479/510 (94%)	460 (96%)	18 (4%)	1 (0%)	47	77
2	D	467/482 (97%)	432 (92%)	33 (7%)	2 (0%)	34	66
2	E	468/482 (97%)	439 (94%)	29 (6%)	0	100	100
2	F	467/482 (97%)	437 (94%)	28 (6%)	2 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	177/273 (65%)	165 (93%)	9 (5%)	3 (2%)	9	35
4	H	39/66 (59%)	39 (100%)	0	0	100	100
4	I	26/66 (39%)	26 (100%)	0	0	100	100
4	J	20/66 (30%)	18 (90%)	1 (5%)	1 (5%)	2	14
All	All	3112/3447 (90%)	2945 (95%)	156 (5%)	11 (0%)	34	66

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ALA
3	G	2	THR
2	D	220	GLY
3	G	126	VAL
4	J	30	GLU
3	G	127	THR
1	A	408	SER
2	D	352	ASP
2	F	352	ASP
1	C	376	SER
2	F	161	GLY

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	394/412 (96%)	394 (100%)	0	100	100
1	B	393/412 (95%)	393 (100%)	0	100	100
1	C	390/412 (95%)	390 (100%)	0	100	100
2	D	379/386 (98%)	379 (100%)	0	100	100
2	E	379/386 (98%)	379 (100%)	0	100	100
2	F	379/386 (98%)	379 (100%)	0	100	100
3	G	160/231 (69%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	27/49 (55%)	27 (100%)	0	100	100
4	I	21/49 (43%)	21 (100%)	0	100	100
4	J	17/49 (35%)	17 (100%)	0	100	100
All	All	2539/2772 (92%)	2539 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	405	GLN
1	B	432	GLN
3	G	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 16 are monoatomic - leaving 7 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	C	601	6	26,33,33	0.98	1 (3%)	31,52,52	1.47	5 (16%)
5	ATP	B	601	6	26,33,33	1.00	2 (7%)	31,52,52	1.52	5 (16%)
7	GOL	B	604	-	5,5,5	0.27	0	5,5,5	0.37	0
9	ADP	D	600	6	24,29,29	1.00	1 (4%)	29,45,45	1.43	4 (13%)
5	ATP	A	601	6	26,33,33	0.98	2 (7%)	31,52,52	1.48	5 (16%)
7	GOL	A	603	-	5,5,5	0.23	0	5,5,5	0.27	0
9	ADP	F	501	6	24,29,29	1.01	1 (4%)	29,45,45	1.40	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	C	601	6	-	0/18/38/38	0/3/3/3
5	ATP	B	601	6	-	0/18/38/38	0/3/3/3
7	GOL	B	604	-	-	2/4/4/4	-
9	ADP	D	600	6	-	2/12/32/32	0/3/3/3
5	ATP	A	601	6	-	0/18/38/38	0/3/3/3
7	GOL	A	603	-	-	2/4/4/4	-
9	ADP	F	501	6	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	ATP	C5-C4	2.64	1.47	1.40
5	C	601	ATP	C5-C4	2.62	1.47	1.40
9	F	501	ADP	C5-C4	2.60	1.47	1.40
9	D	600	ADP	C5-C4	2.57	1.47	1.40
5	A	601	ATP	C5-C4	2.56	1.47	1.40
5	A	601	ATP	C2-N3	2.11	1.35	1.32
5	B	601	ATP	C2-N3	2.02	1.35	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	ATP	N3-C2-N1	-3.57	123.10	128.68
5	B	601	ATP	N3-C2-N1	-3.46	123.27	128.68
9	F	501	ADP	N3-C2-N1	-3.43	123.32	128.68
9	F	501	ADP	C3'-C2'-C1'	3.42	106.13	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	ATP	N3-C2-N1	-3.42	123.33	128.68
9	D	600	ADP	C3'-C2'-C1'	3.38	106.07	100.98
9	D	600	ADP	N3-C2-N1	-3.37	123.42	128.68
5	B	601	ATP	PA-O3A-PB	-3.35	121.32	132.83
5	A	601	ATP	PB-O3B-PG	-3.18	121.92	132.83
5	B	601	ATP	C3'-C2'-C1'	3.17	105.75	100.98
5	A	601	ATP	C3'-C2'-C1'	3.07	105.60	100.98
5	C	601	ATP	C3'-C2'-C1'	3.05	105.57	100.98
5	B	601	ATP	PB-O3B-PG	-3.01	122.49	132.83
9	D	600	ADP	PA-O3A-PB	-2.96	122.67	132.83
5	C	601	ATP	PA-O3A-PB	-2.93	122.76	132.83
9	F	501	ADP	PA-O3A-PB	-2.88	122.95	132.83
5	B	601	ATP	C4-C5-N7	-2.80	106.48	109.40
5	A	601	ATP	PA-O3A-PB	-2.79	123.25	132.83
5	A	601	ATP	C4-C5-N7	-2.75	106.53	109.40
9	D	600	ADP	C4-C5-N7	-2.69	106.60	109.40
5	C	601	ATP	PB-O3B-PG	-2.61	123.88	132.83
9	F	501	ADP	C4-C5-N7	-2.50	106.79	109.40
5	C	601	ATP	C4-C5-N7	-2.46	106.83	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

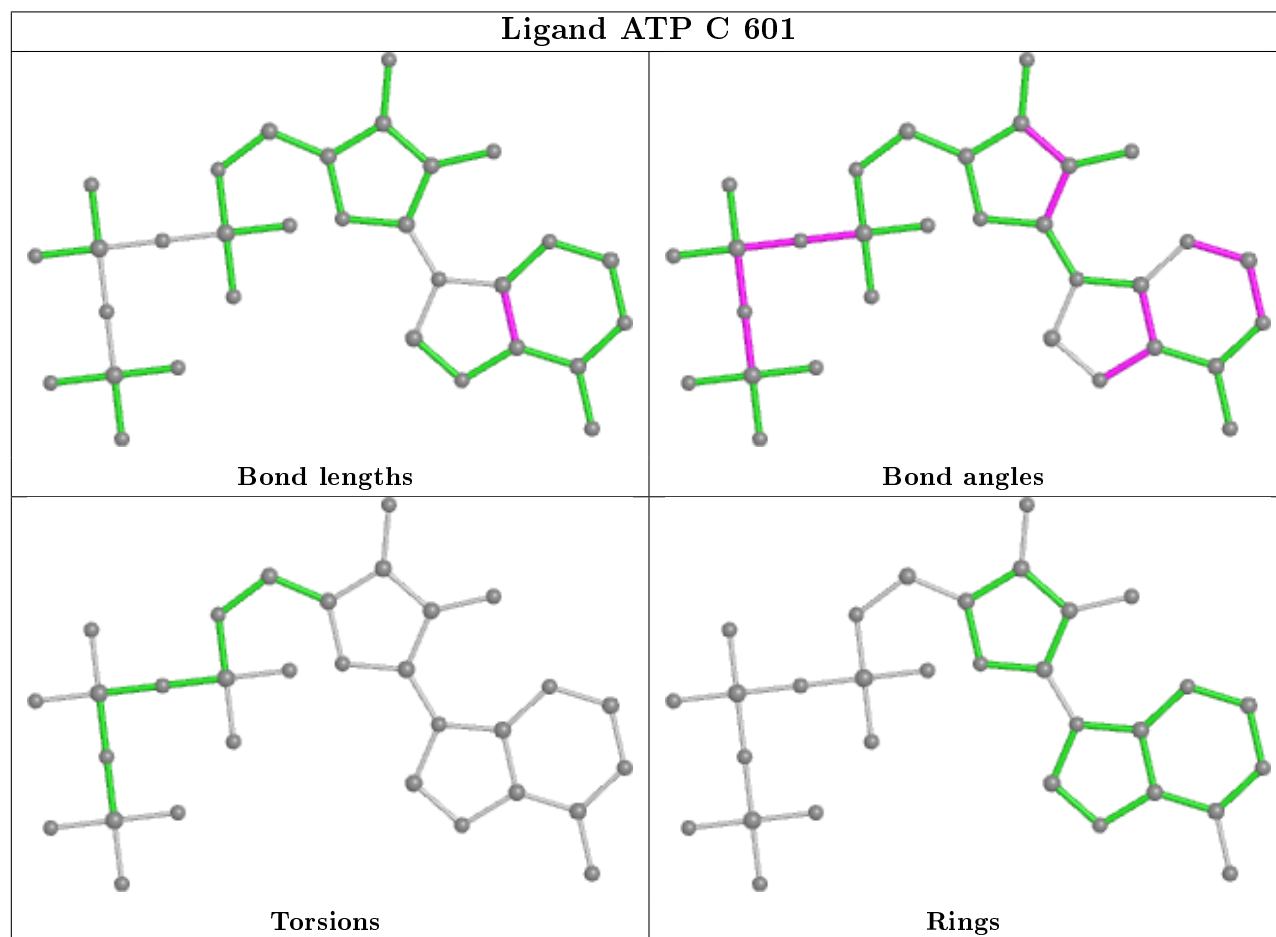
Mol	Chain	Res	Type	Atoms
7	A	603	GOL	C1-C2-C3-O3
9	D	600	ADP	C5'-O5'-PA-O1A
7	A	603	GOL	O2-C2-C3-O3
7	B	604	GOL	C1-C2-C3-O3
7	B	604	GOL	O2-C2-C3-O3
9	D	600	ADP	C5'-O5'-PA-O3A

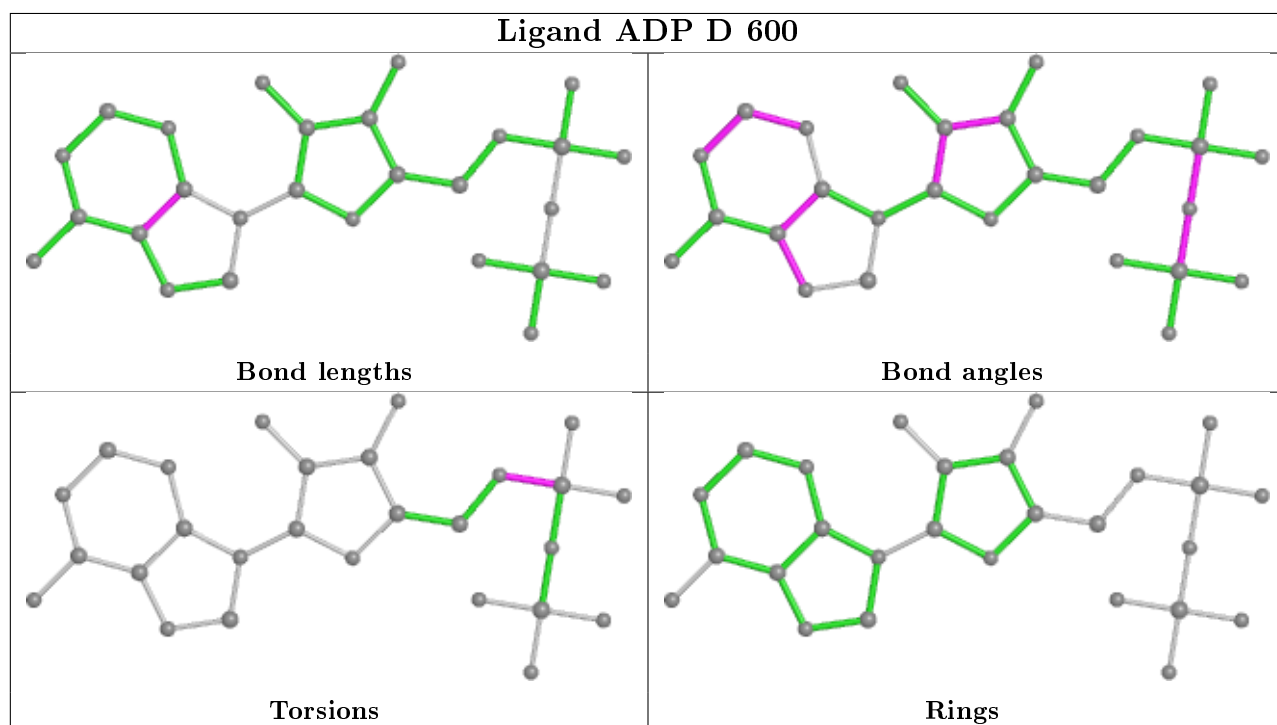
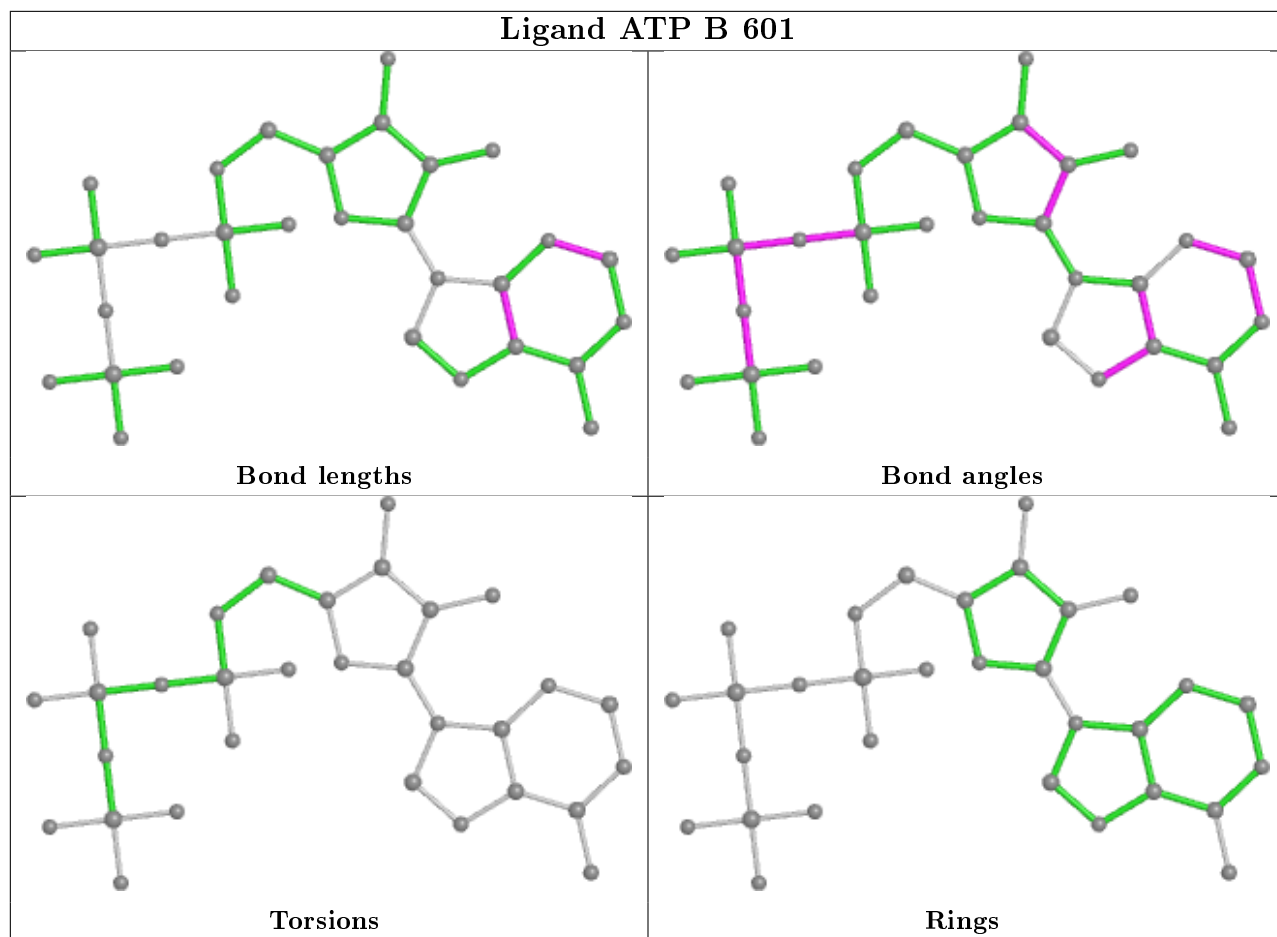
There are no ring outliers.

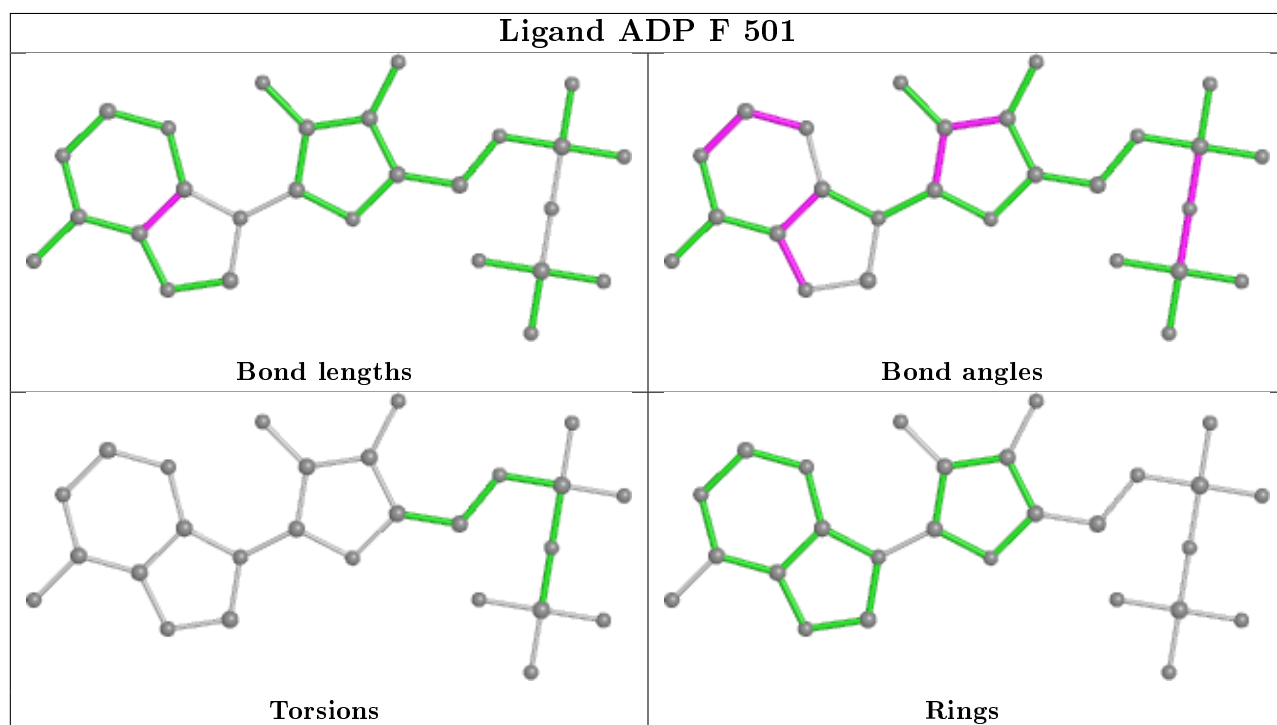
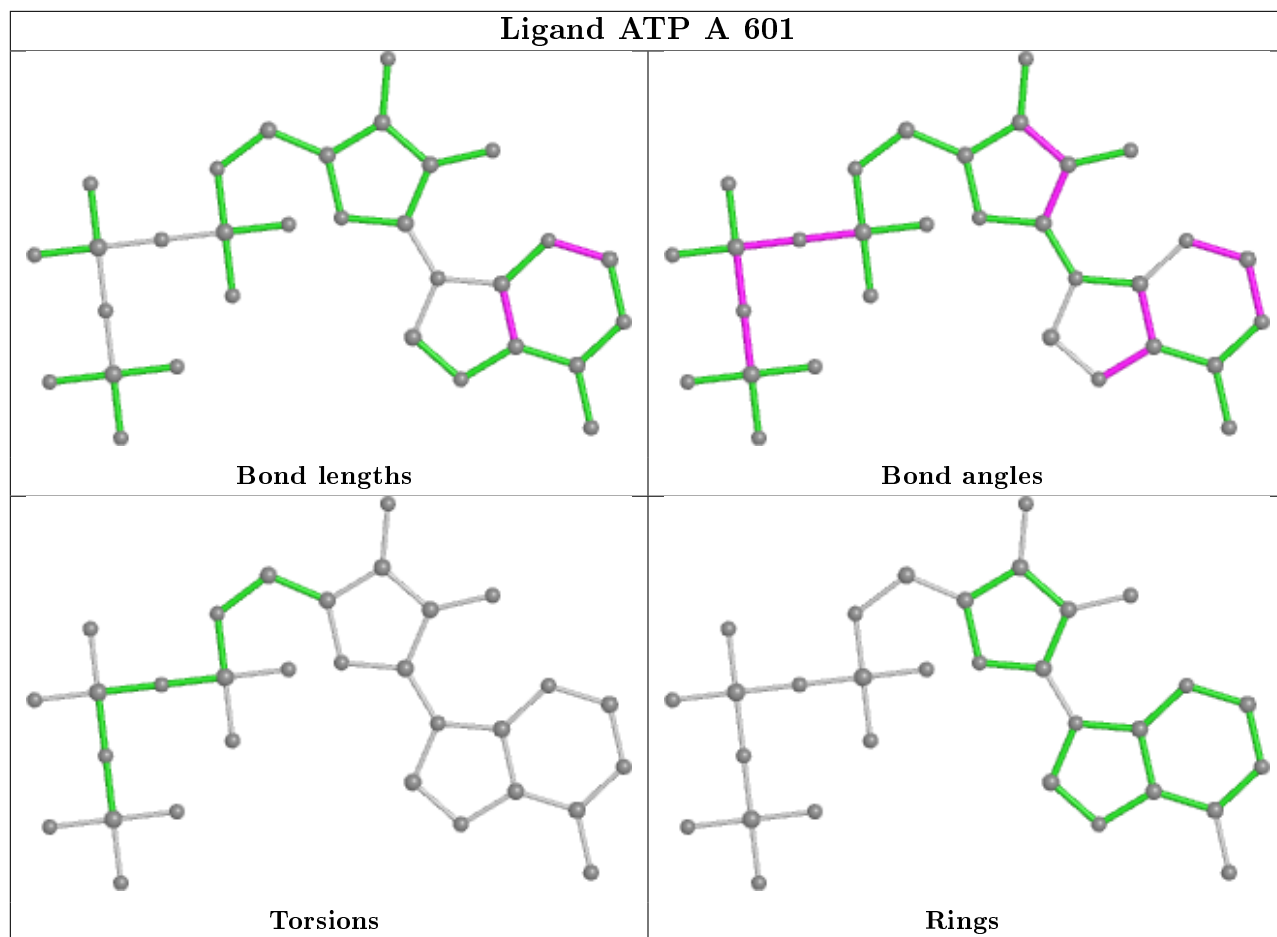
No monomer is involved in short contacts.

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.







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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/510 (95%)	-0.20	2 (0%) 92 93	47, 63, 95, 140	0
1	B	487/510 (95%)	-0.25	1 (0%) 95 96	41, 60, 92, 122	0
1	C	483/510 (94%)	0.02	3 (0%) 89 90	54, 83, 109, 142	0
2	D	469/482 (97%)	0.05	11 (2%) 60 59	56, 81, 112, 123	0
2	E	470/482 (97%)	-0.07	8 (1%) 70 68	40, 62, 109, 152	0
2	F	469/482 (97%)	0.01	4 (0%) 84 84	50, 79, 108, 134	0
3	G	187/273 (68%)	1.03	34 (18%) 1 1	56, 120, 160, 180	0
4	H	41/66 (62%)	0.27	2 (4%) 29 27	66, 90, 124, 138	0
4	I	28/66 (42%)	1.50	7 (25%) 0 0	110, 128, 146, 158	0
4	J	22/66 (33%)	2.21	12 (54%) 0 0	123, 134, 141, 144	0
All	All	3143/3447 (91%)	0.02	84 (2%) 54 52	40, 75, 124, 180	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	211	ASN	5.6
3	G	138	PHE	5.5
4	I	48	HIS	4.9
3	G	149	LEU	4.9
3	G	213	ILE	4.8
3	G	207	TYR	4.6
1	C	404	ALA	4.5
2	E	393	MET	4.4
4	J	43	ALA	4.4
3	G	215	TYR	4.2
2	E	394	ASP	4.1
3	G	136	PRO	4.1
2	E	391	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	G	205	GLN	4.0
3	G	151	SER	3.9
2	D	209	LYS	3.8
3	G	209	LEU	3.8
3	G	166	ARG	3.7
3	G	142	SER	3.6
3	G	212	ILE	3.5
3	G	43	VAL	3.5
2	D	477	HIS	3.5
4	J	47	LYS	3.5
3	G	126	VAL	3.4
4	J	42	LEU	3.3
2	F	477	HIS	3.3
3	G	210	ALA	3.3
4	J	37	ARG	3.3
2	E	477	HIS	3.3
2	E	387	ILE	3.2
3	G	206	GLU	3.2
3	G	42	ARG	3.0
1	C	24	ASP	2.9
4	J	49	HIS	2.9
4	J	30	GLU	2.8
4	I	46	LYS	2.8
4	H	49	HIS	2.8
2	D	429	GLY	2.8
2	F	108	ILE	2.8
2	E	396	LEU	2.7
3	G	123	GLN	2.7
3	G	120	HIS	2.7
4	J	48	HIS	2.7
4	I	25	ARG	2.7
4	I	26	GLU	2.6
4	J	34	PHE	2.6
3	G	148	LEU	2.6
4	I	44	ALA	2.6
2	F	111	LYS	2.5
3	G	165	PHE	2.5
4	H	47	LYS	2.5
4	J	29	GLU	2.5
2	E	395	GLU	2.5
3	G	214	TYR	2.5
4	J	38	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	J	45	LEU	2.4
2	D	451	HIS	2.4
3	G	137	THR	2.4
2	D	110	THR	2.4
3	G	216	SER	2.3
4	I	43	ALA	2.3
2	D	210	ASP	2.3
3	G	146	LEU	2.3
3	G	139	GLY	2.3
3	G	140	ASP	2.2
2	D	180	TYR	2.2
3	G	119	THR	2.2
4	I	49	HIS	2.2
2	D	211	ALA	2.2
1	C	124	LYS	2.2
2	D	76	LEU	2.1
2	D	443	GLN	2.1
1	B	16	ILE	2.1
2	E	455	GLN	2.1
3	G	109	GLY	2.1
1	A	510	ALA	2.1
3	G	150	ASN	2.1
2	F	243	PHE	2.0
3	G	84	SER	2.0
1	A	403	PHE	2.0
2	D	301	LYS	2.0
4	J	36	ALA	2.0
3	G	38	LEU	2.0
3	G	112	ILE	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

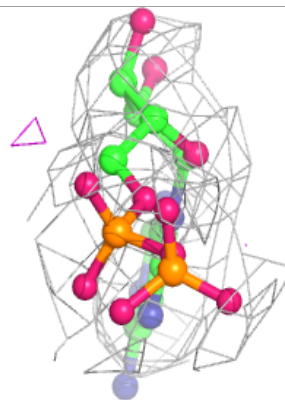
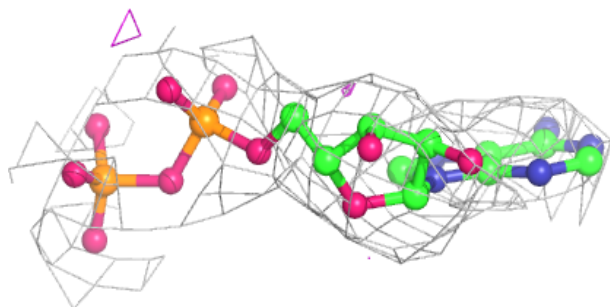
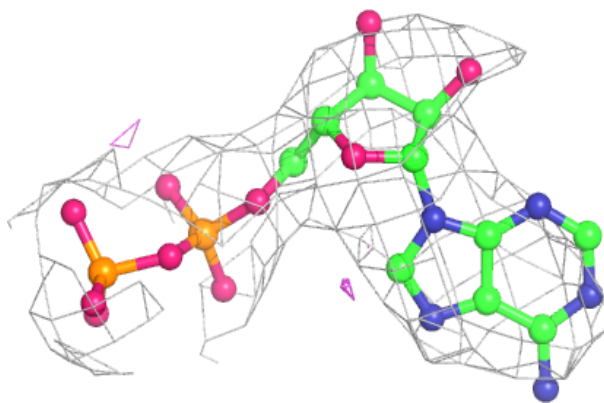
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CL	C	604	1/1	0.74	0.24	52,52,52,52	0
6	MG	F	502	1/1	0.81	0.20	67,67,67,67	0
8	CL	F	503	1/1	0.84	0.48	60,60,60,60	0
6	MG	D	601	1/1	0.86	0.20	85,85,85,85	0
8	CL	E	502	1/1	0.86	0.23	52,52,52,52	0
8	CL	G	302	1/1	0.87	0.38	86,86,86,86	0
6	MG	C	602	1/1	0.87	0.18	72,72,72,72	0
8	CL	G	301	1/1	0.88	0.25	70,70,70,70	0
8	CL	F	504	1/1	0.89	0.17	51,51,51,51	0
8	CL	B	603	1/1	0.90	0.21	52,52,52,52	0
8	CL	C	603	1/1	0.90	0.22	85,85,85,85	0
8	CL	E	504	1/1	0.90	0.19	69,69,69,69	0
9	ADP	D	600	27/27	0.91	0.24	88,93,96,98	0
7	GOL	A	603	6/6	0.92	0.25	47,48,48,49	0
6	MG	A	602	1/1	0.92	0.15	60,60,60,60	0
7	GOL	B	604	6/6	0.92	0.23	51,51,51,51	0
5	ATP	C	601	31/31	0.92	0.20	72,81,90,91	4
8	CL	E	503	1/1	0.92	0.16	54,54,54,54	0
5	ATP	A	601	31/31	0.94	0.18	59,61,64,65	4
9	ADP	F	501	27/27	0.95	0.24	63,70,76,76	0
5	ATP	B	601	31/31	0.96	0.18	53,62,71,72	0
6	MG	B	602	1/1	0.97	0.24	50,50,50,50	0
8	CL	E	501	1/1	0.98	0.09	44,44,44,44	0

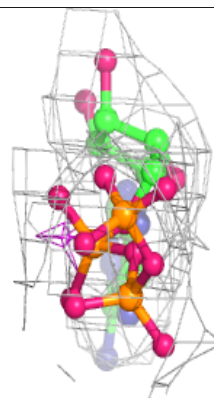
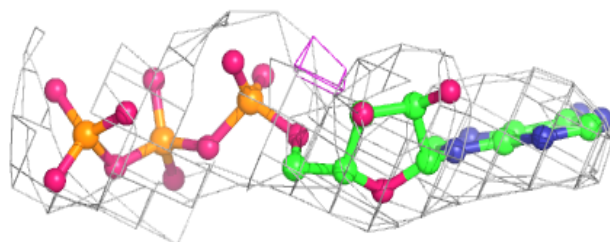
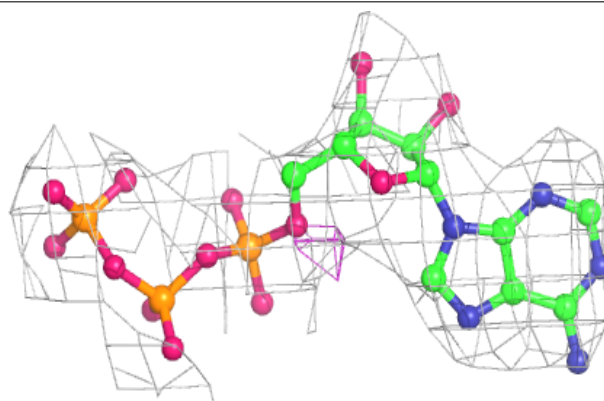
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

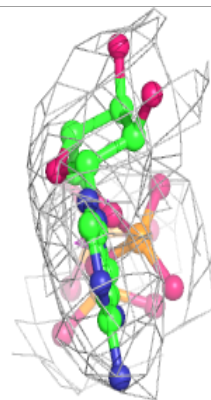
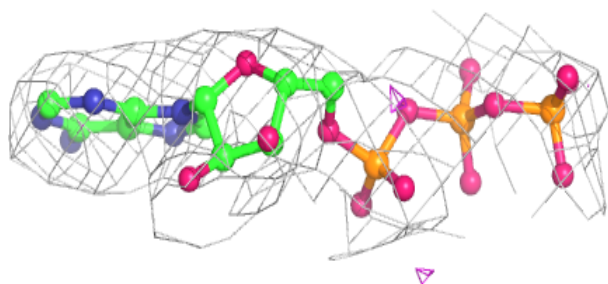
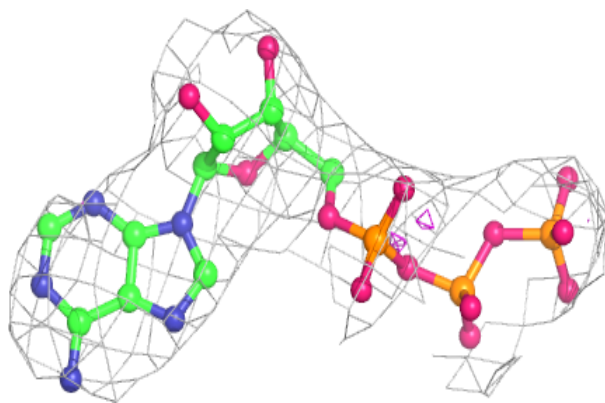
**Electron density around ATP C 601:**

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

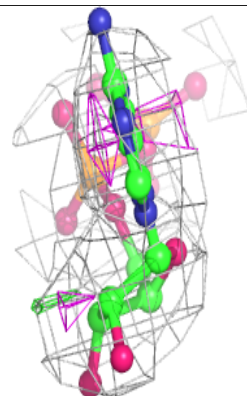
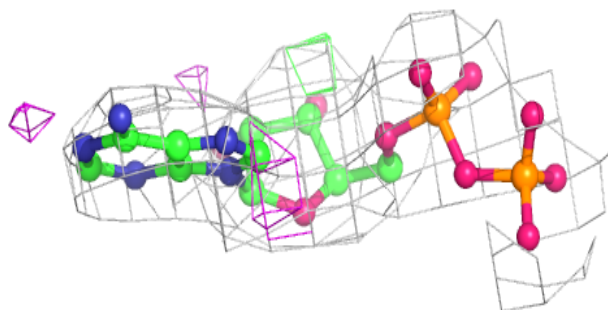
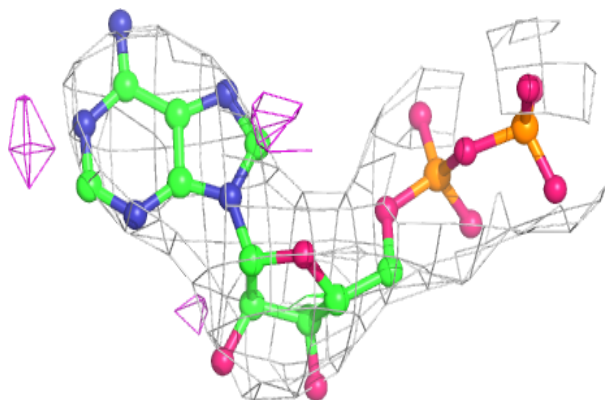


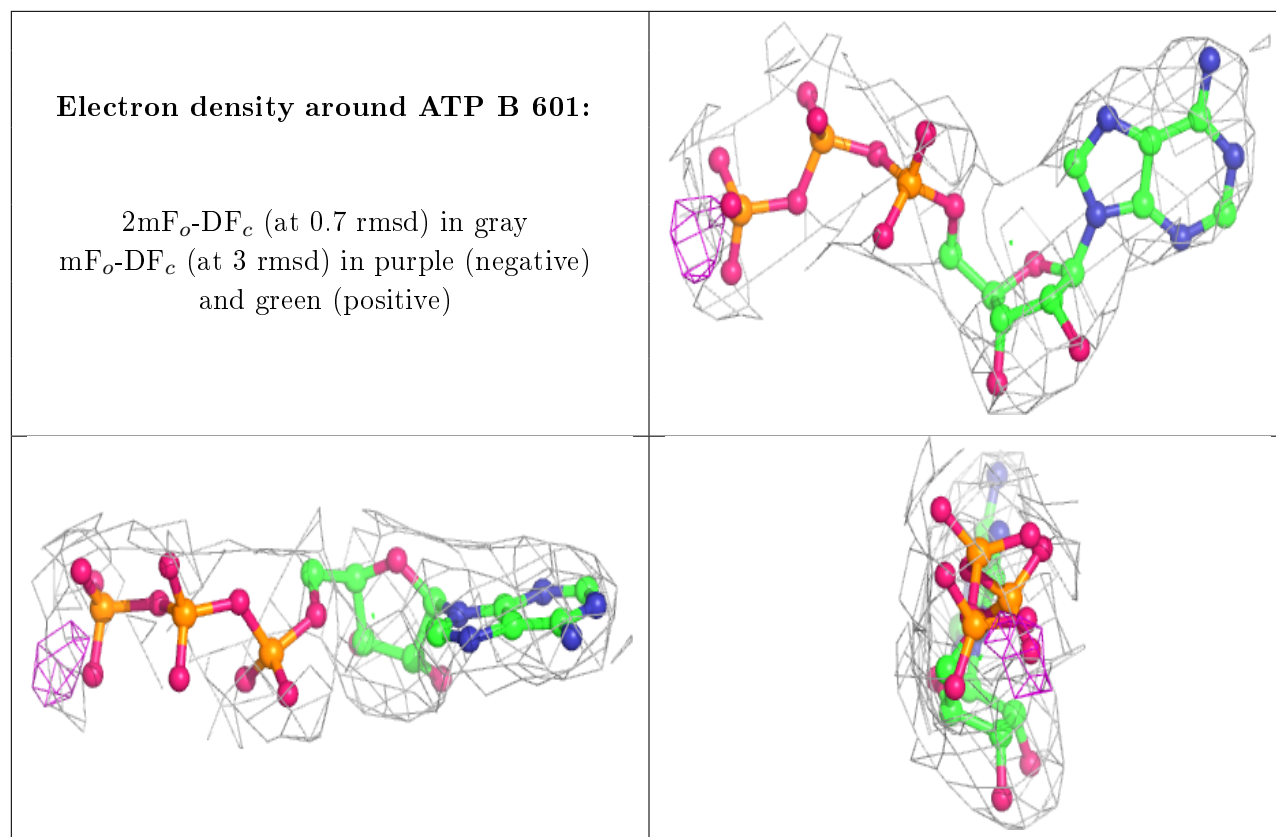
Electron density around ATP A 601:

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

**Electron density around ADP F 501:**

$2mF_o-DF_c$ (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.