



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 04:09 AM EDT

PDB ID : 6MW7 / pdb\_00006mw7  
Title : Crystal structure of ATPase module of SMCHD1 bound to ATP  
Authors : Pedersen, L.C.; Inoue, K.; Kim, S.; Perera, L.; Shaw, N.D.  
Deposited on : 2018-10-29  
Resolution : 2.19 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

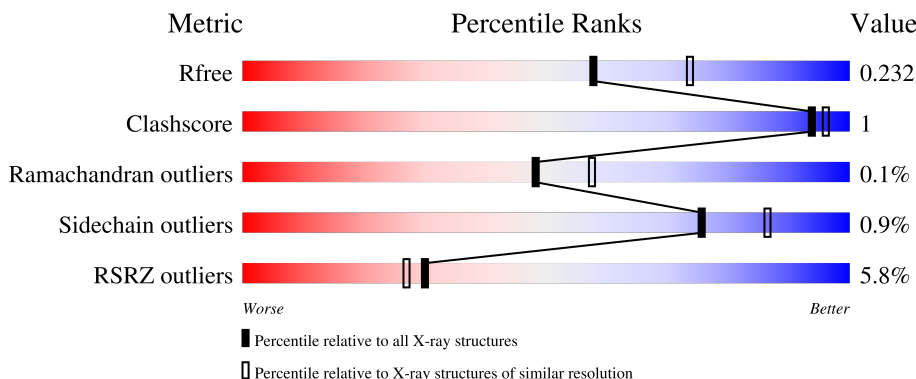
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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	562	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	562	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	562	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	562	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17288 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 Structural maintenance of chromosomes flexible hinge domain-containing protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	Se	0	2	0
			4119	2631	704	769	8	7			
1	B	502	Total	C	N	O	S	Se	0	0	0
			3972	2539	679	740	8	6			
1	C	519	Total	C	N	O	S	Se	0	0	0
			4123	2637	703	769	8	6			
1	D	505	Total	C	N	O	S	Se	0	1	0
			4011	2563	680	753	8	7			

There are 24 discrepancies between the modelled and reference sequences:

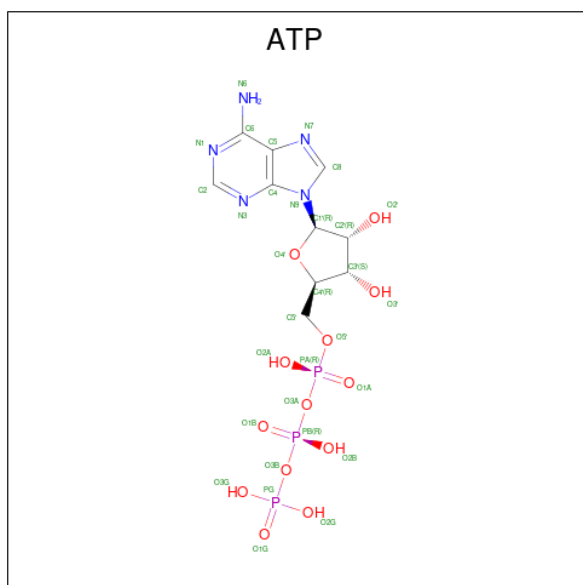
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP A6NHR9
A	20	SER	-	expression tag	UNP A6NHR9
A	21	ALA	-	expression tag	UNP A6NHR9
A	22	ALA	-	expression tag	UNP A6NHR9
A	23	ALA	-	expression tag	UNP A6NHR9
A	147	ALA	GLU	engineered mutation	UNP A6NHR9
B	19	GLY	-	expression tag	UNP A6NHR9
B	20	SER	-	expression tag	UNP A6NHR9
B	21	ALA	-	expression tag	UNP A6NHR9
B	22	ALA	-	expression tag	UNP A6NHR9
B	23	ALA	-	expression tag	UNP A6NHR9
B	147	ALA	GLU	engineered mutation	UNP A6NHR9
C	19	GLY	-	expression tag	UNP A6NHR9
C	20	SER	-	expression tag	UNP A6NHR9
C	21	ALA	-	expression tag	UNP A6NHR9
C	22	ALA	-	expression tag	UNP A6NHR9
C	23	ALA	-	expression tag	UNP A6NHR9
C	147	ALA	GLU	engineered mutation	UNP A6NHR9
D	19	GLY	-	expression tag	UNP A6NHR9
D	20	SER	-	expression tag	UNP A6NHR9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	21	ALA	-	expression tag	UNP A6NHR9
D	22	ALA	-	expression tag	UNP A6NHR9
D	23	ALA	-	expression tag	UNP A6NHR9
D	147	ALA	GLU	engineered mutation	UNP A6NHR9

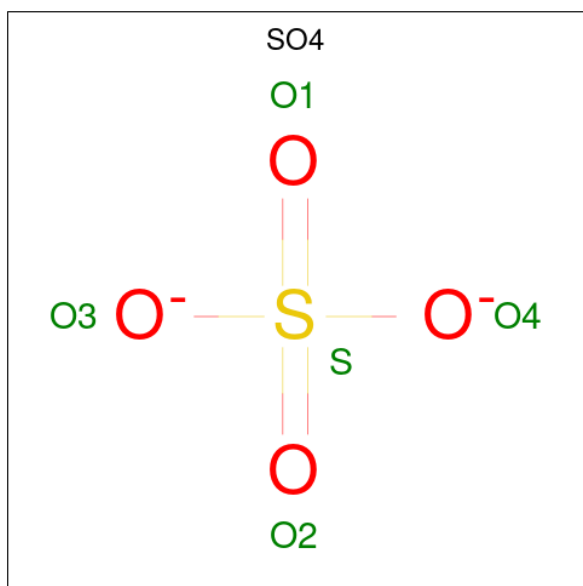
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na	0	0
			1	1		

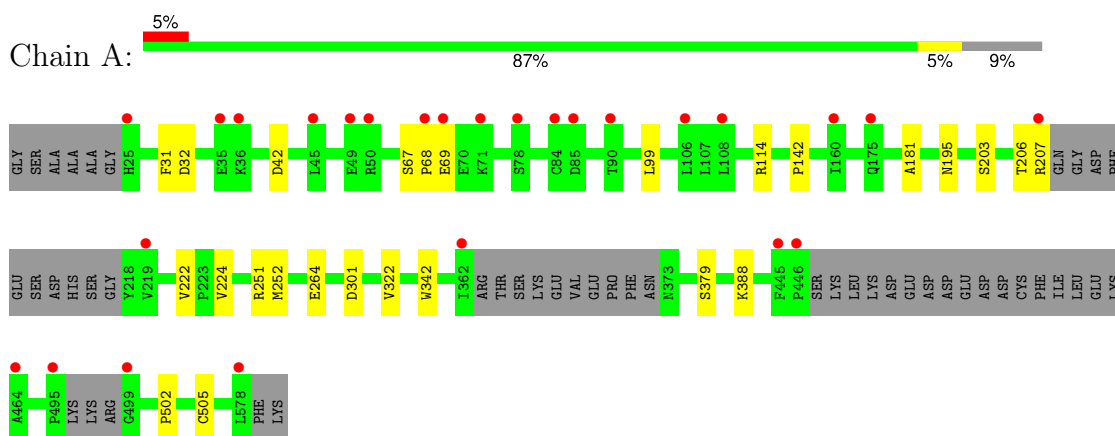
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	272	Total	O	0	1
			273	273		
6	B	217	Total	O	0	0
			217	217		
6	C	235	Total	O	0	1
			236	236		
6	D	203	Total	O	0	0
			203	203		

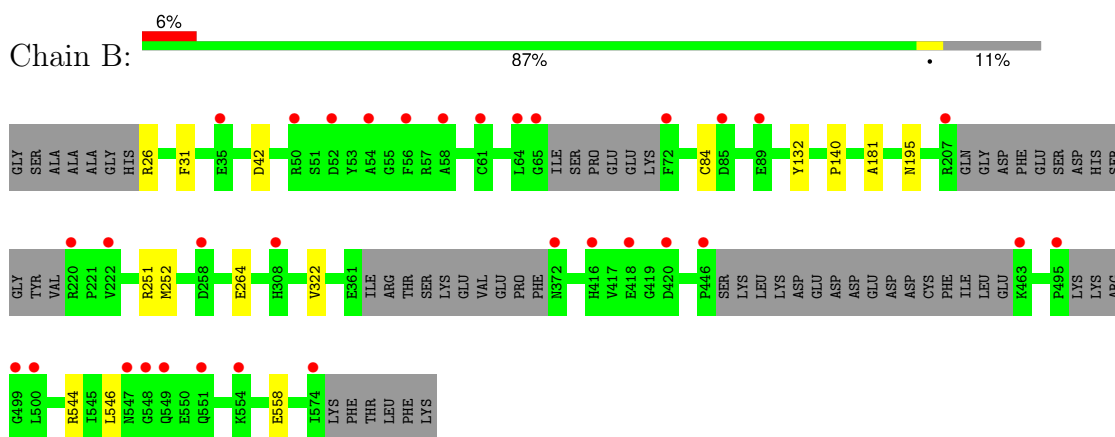
### 3 Residue-property plots

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.

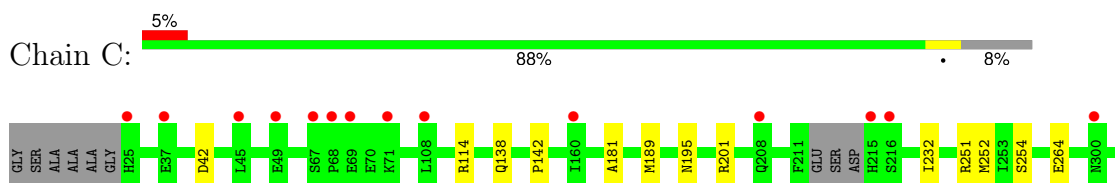
- Molecule 1: Structural maintenance of chromosomes flexible hinge domain-containing protein 1

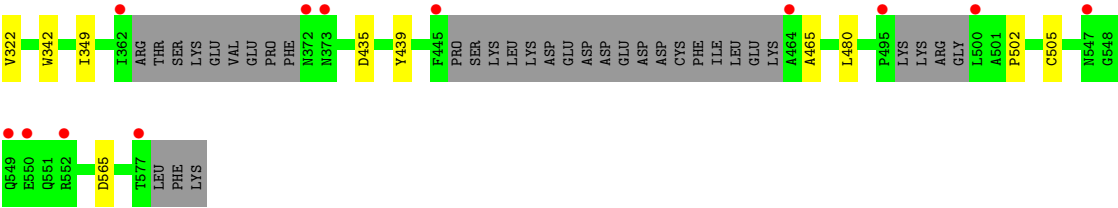


- Molecule 1: Structural maintenance of chromosomes flexible hinge domain-containing protein 1

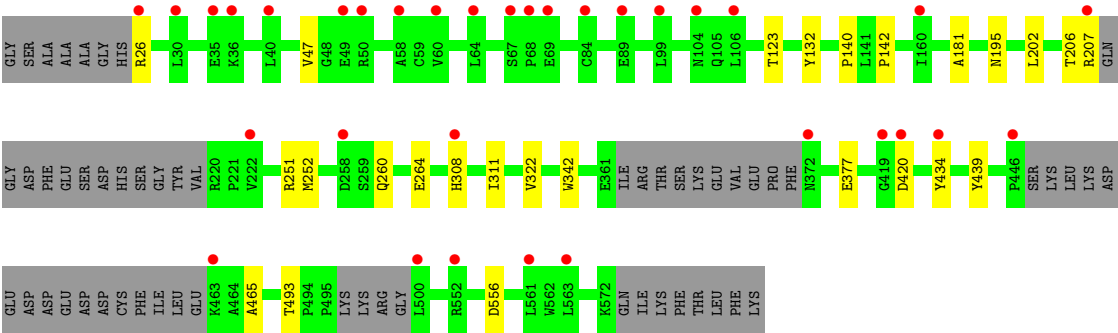
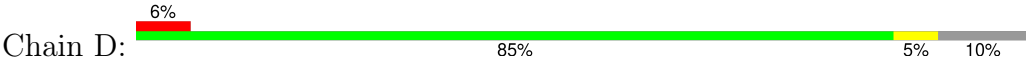


- Molecule 1: Structural maintenance of chromosomes flexible hinge domain-containing protein 1





- Molecule 1: Structural maintenance of chromosomes flexible hinge domain-containing protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.76Å 148.01Å 191.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.19 47.78 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.78-2.19) 89.6 (47.78-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.197 , 0.230 0.198 , 0.232	Depositor DCC
$R_{free}$ test set	7778 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.851	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.2	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	0.96	EDS
Total number of atoms	17288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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 30.58 % 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 1.2779e-03. 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, ATP, SO4

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	0.30	0/4206	0.49	0/5682
1	B	0.26	0/4055	0.46	0/5483
1	C	0.28	0/4211	0.48	0/5693
1	D	0.28	0/4096	0.47	0/5541
All	All	0.28	0/16568	0.47	0/22399

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	4119	0	3984	13	0
1	B	3972	0	3808	6	0
1	C	4123	0	3955	13	0
1	D	4011	0	3840	11	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	5	0	0	0	0
5	C	1	0	0	0	0
6	A	273	0	0	0	0
6	B	217	0	0	0	0
6	C	236	0	0	1	0
6	D	203	0	0	1	0
All	All	17288	0	15635	42	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 (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ASP:OD2	1:C:114:ARG:NH1	2.20	0.75
1:C:138:GLN:NE2	6:C:702:HOH:O	2.26	0.67
1:D:377:GLU:OE1	6:D:701:HOH:O	2.13	0.66
1:C:251:ARG:NH1	1:C:264:GLU:OE2	2.29	0.63
1:C:232:ILE:HG22	1:C:232:ILE:O	2.01	0.60
1:A:251:ARG:NH1	1:A:264:GLU:OE2	2.35	0.56
1:B:544:ARG:HH11	1:B:558:GLU:HG3	1.71	0.55
1:A:42:ASP:OD2	1:A:114:ARG:NH1	2.42	0.53
1:D:251:ARG:NH1	1:D:264:GLU:OE2	2.44	0.48
1:A:67:SER:C	1:A:69:GLU:H	2.17	0.47
1:D:202:LEU:HD11	1:D:207:ARG:HB3	1.97	0.47
1:B:181:ALA:HA	1:B:322:VAL:O	2.15	0.46
1:C:181:ALA:HA	1:C:322:VAL:O	2.15	0.46
1:A:32:ASP:HA	1:A:99:LEU:HB2	1.97	0.45
1:D:252:MSE:HE1	1:D:322:VAL:HG22	1.98	0.45
1:B:252:MSE:HE1	1:B:322:VAL:HG22	1.99	0.45
1:C:142:PRO:HG3	1:C:342:TRP:HB2	1.99	0.44
1:A:252:MSE:HE1	1:A:322:VAL:HG22	1.99	0.44
1:A:379:SER:HA	1:A:388:LYS:O	2.18	0.43
1:A:203:SER:O	1:A:207:ARG:HG2	2.19	0.43
1:A:181:ALA:HA	1:A:322:VAL:O	2.19	0.43
1:D:142:PRO:HG3	1:D:342:TRP:HB2	2.01	0.43
1:D:181:ALA:HA	1:D:322:VAL:O	2.19	0.43
1:D:26:ARG:O	1:D:47:VAL:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:PRO:HG2	1:A:505:CYS:SG	2.59	0.42
1:D:132:TYR:HB3	1:D:140:PRO:HB2	2.01	0.42
1:A:142:PRO:HG3	1:A:342:TRP:HB2	2.01	0.42
1:B:132:TYR:HB3	1:B:140:PRO:HB2	2.02	0.42
1:A:31:PHE:CZ	1:A:42:ASP:HB3	2.55	0.41
1:B:31:PHE:CZ	1:B:42:ASP:HB3	2.56	0.41
1:C:189:MSE:N	1:C:254:SER:OG	2.51	0.41
1:C:252:MSE:O	1:C:264:GLU:HA	2.21	0.41
1:A:222:VAL:O	1:A:224:VAL:HG13	2.21	0.41
1:C:502:PRO:HG2	1:C:505:CYS:SG	2.60	0.41
1:D:439:TYR:HB2	1:D:465:ALA:HB1	2.02	0.41
1:C:435:ASP:OD1	1:C:435:ASP:N	2.53	0.41
1:C:349:ILE:HA	1:C:480:LEU:HB3	2.02	0.41
1:B:251:ARG:NH1	1:B:264:GLU:OE2	2.53	0.41
1:D:308:HIS:O	1:D:311:ILE:HG22	2.21	0.40
1:C:439:TYR:HB2	1:C:465:ALA:HB1	2.03	0.40
1:A:252:MSE:O	1:A:264:GLU:HA	2.21	0.40
1:C:201:ARG:HG3	1:D:123:THR:HA	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	506/562 (90%)	491 (97%)	14 (3%)	1 (0%)	44	52
1	B	490/562 (87%)	473 (96%)	17 (4%)	0	100	100
1	C	509/562 (91%)	496 (97%)	13 (3%)	0	100	100
1	D	496/562 (88%)	482 (97%)	13 (3%)	1 (0%)	44	52
All	All	2001/2248 (89%)	1942 (97%)	57 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	434	TYR
1	A	68	PRO

### 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	441/495 (89%)	438 (99%)	3 (1%)	81	90
1	B	418/495 (84%)	414 (99%)	4 (1%)	73	84
1	C	435/495 (88%)	433 (100%)	2 (0%)	86	93
1	D	425/495 (86%)	419 (99%)	6 (1%)	62	77
All	All	1719/1980 (87%)	1704 (99%)	15 (1%)	75	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	206	THR
1	A	301	ASP
1	B	26	ARG
1	B	84	CYS
1	B	195	ASN
1	B	546	LEU
1	C	195	ASN
1	C	565	ASP
1	D	195	ASN
1	D	206	THR
1	D	260	GLN
1	D	420	ASP
1	D	493	THR
1	D	556	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
2	ATP	D	601	3	28,33,33	0.96	1 (3%)	34,52,52	1.19	2 (5%)
2	ATP	B	601	3	28,33,33	0.96	1 (3%)	34,52,52	1.16	1 (2%)
4	SO4	C	602	5	4,4,4	0.23	0	6,6,6	0.12	0
2	ATP	A	901	3	28,33,33	1.01	1 (3%)	34,52,52	1.14	1 (2%)
2	ATP	C	601	3	28,33,33	0.99	1 (3%)	34,52,52	1.19	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	601	3	-	4/18/38/38	0/3/3/3
2	ATP	B	601	3	-	5/18/38/38	0/3/3/3
2	ATP	A	901	3	-	5/18/38/38	0/3/3/3
2	ATP	C	601	3	-	4/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	ATP	PB-O3B	2.52	1.62	1.59
2	C	601	ATP	PB-O3B	2.47	1.62	1.59
2	A	901	ATP	PB-O3B	2.44	1.62	1.59
2	B	601	ATP	PB-O3B	2.24	1.61	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ATP	N3-C2-N1	-4.44	122.65	128.67
2	C	601	ATP	N3-C2-N1	-4.26	122.89	128.67
2	B	601	ATP	N3-C2-N1	-4.24	122.92	128.67
2	D	601	ATP	N3-C2-N1	-4.22	122.94	128.67
2	D	601	ATP	C4-C5-N7	-2.12	107.09	109.34
2	C	601	ATP	C4-C5-N7	-2.05	107.17	109.34

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ATP	PB-O3B-PG-O2G
2	A	901	ATP	PB-O3B-PG-O3G
2	B	601	ATP	PB-O3B-PG-O2G
2	B	601	ATP	PB-O3B-PG-O3G
2	C	601	ATP	PB-O3B-PG-O2G
2	D	601	ATP	PB-O3B-PG-O3G
2	D	601	ATP	PB-O3B-PG-O2G
2	C	601	ATP	PA-O3A-PB-O2B
2	D	601	ATP	PA-O3A-PB-O2B
2	A	901	ATP	PA-O3A-PB-O2B
2	B	601	ATP	PA-O3A-PB-O2B
2	D	601	ATP	PB-O3B-PG-O1G
2	C	601	ATP	PB-O3B-PG-O3G
2	A	901	ATP	PA-O3A-PB-O1B

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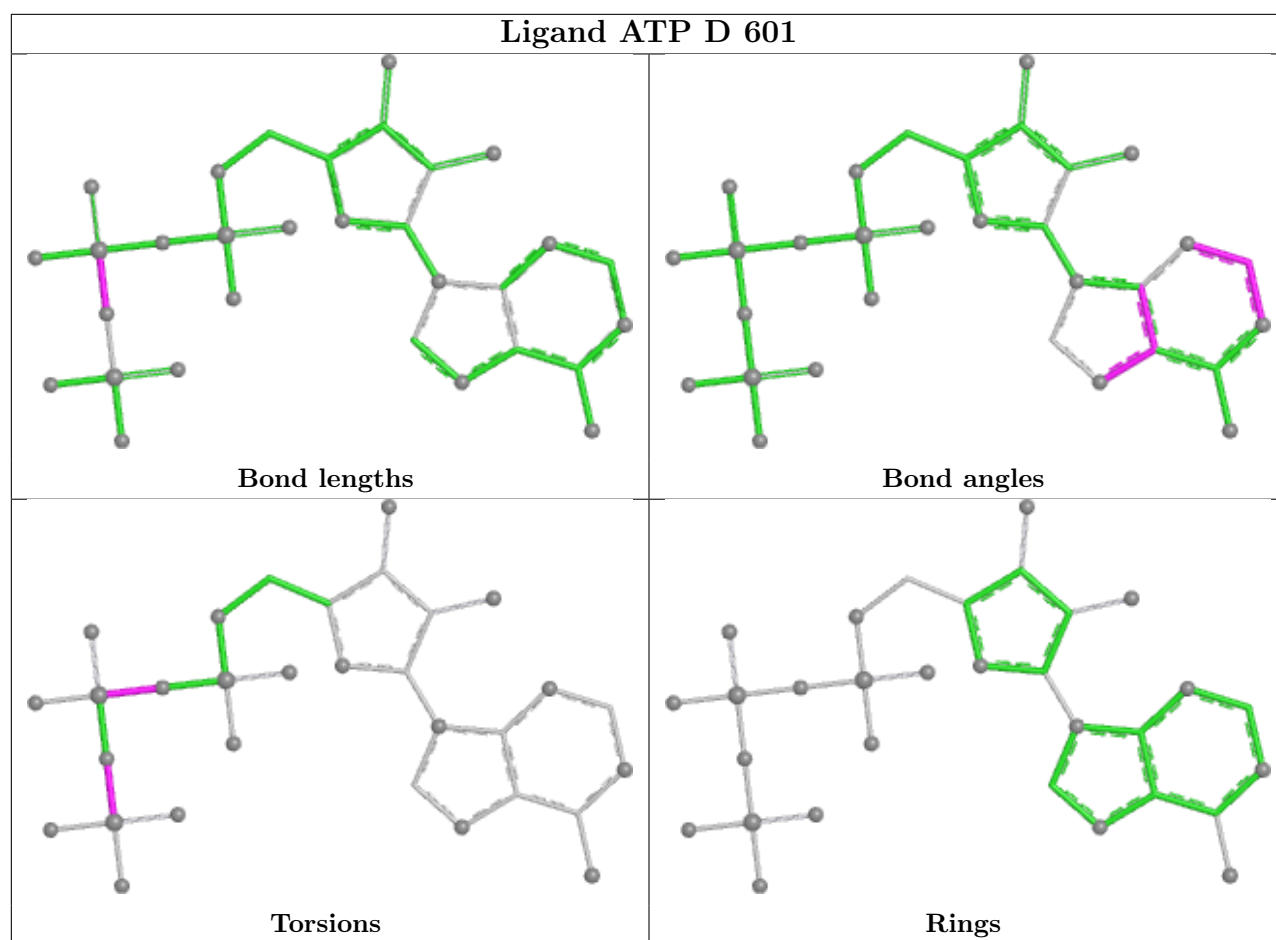
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Mol	Chain	Res	Type	Atoms
2	C	601	ATP	PA-O3A-PB-O1B
2	A	901	ATP	PB-O3B-PG-O1G
2	B	601	ATP	PB-O3B-PG-O1G
2	B	601	ATP	PA-O3A-PB-O1B

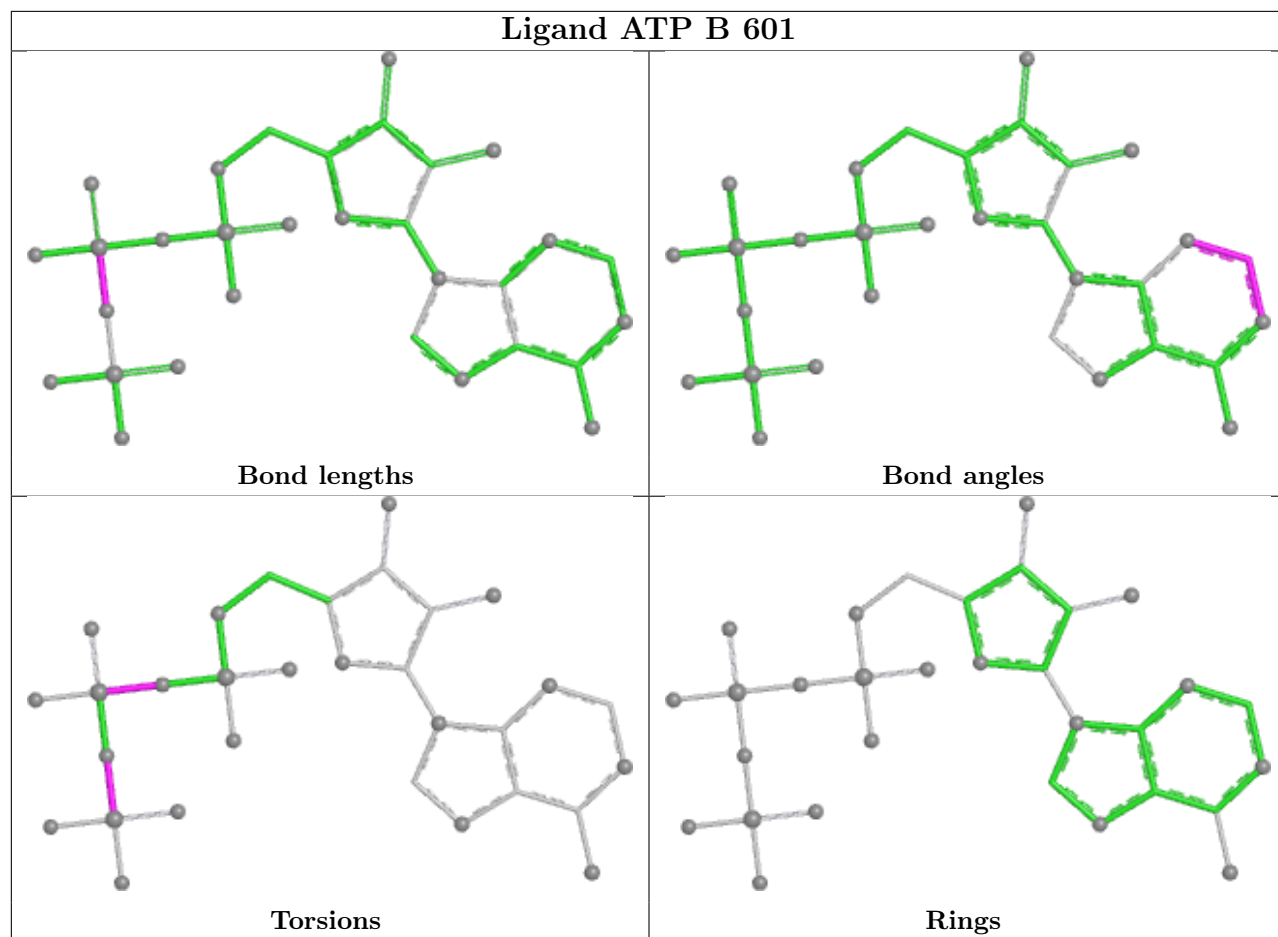
There are no ring outliers.

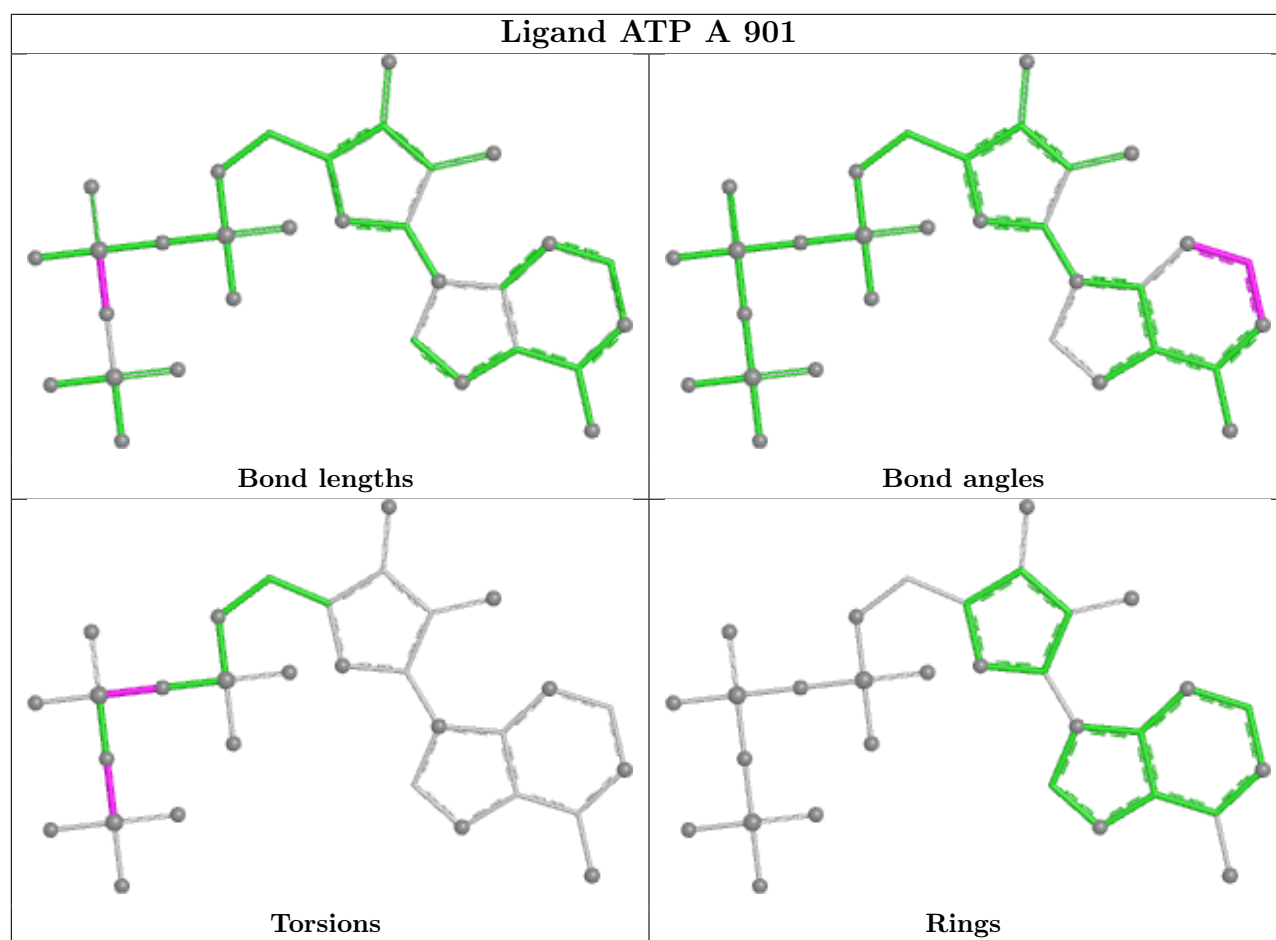
No monomer is involved in short contacts.

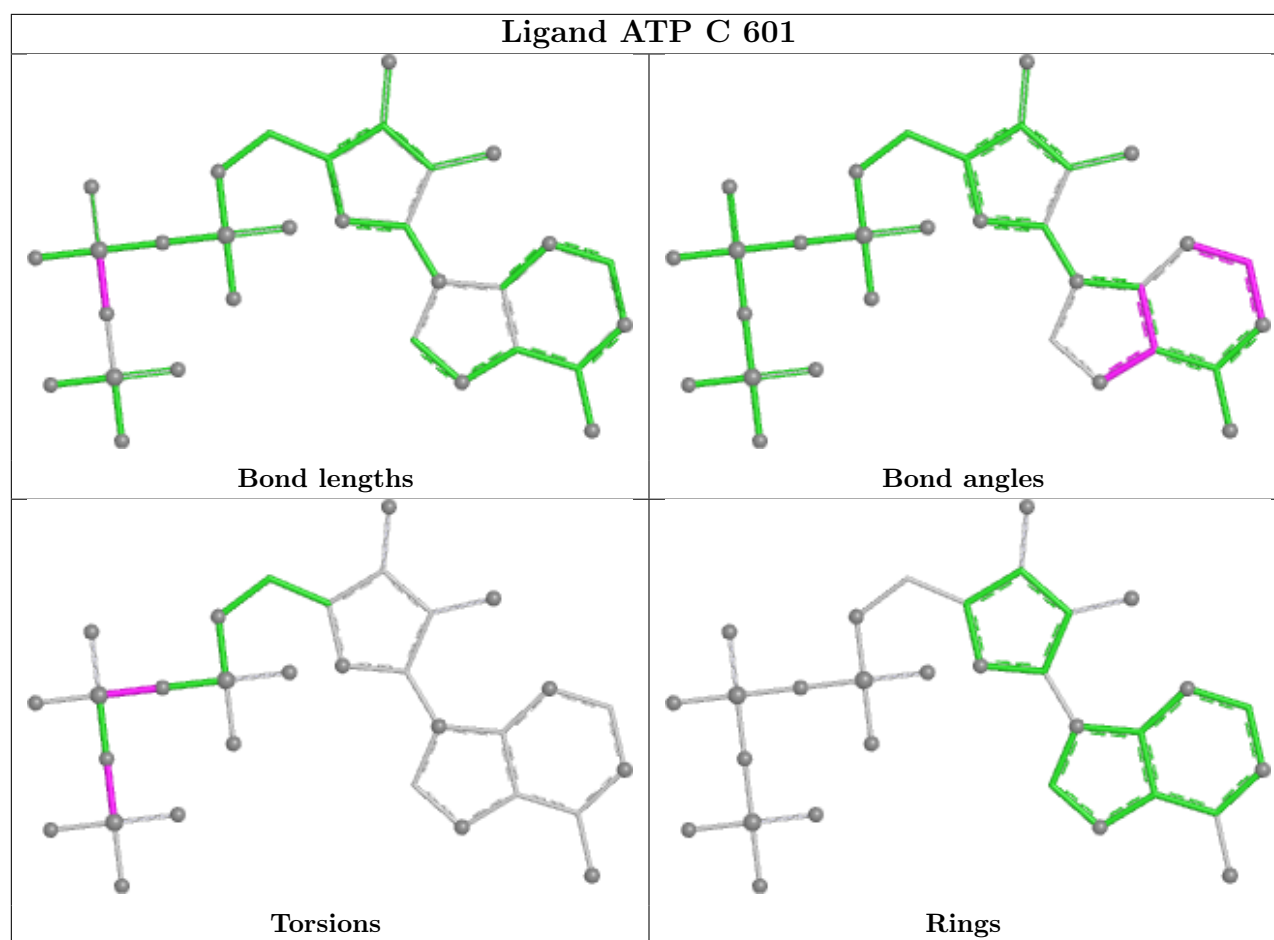
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	507/562 (90%)	0.11	26 (5%)	34	31	15, 40, 73, 95	2 (0%)
1	B	495/562 (88%)	0.36	32 (6%)	26	23	27, 47, 89, 113	0
1	C	512/562 (91%)	0.26	26 (5%)	34	31	26, 46, 77, 115	0
1	D	498/562 (88%)	0.31	33 (6%)	26	23	19, 48, 84, 109	1 (0%)
All	All	2012/2248 (89%)	0.26	117 (5%)	30	27	15, 45, 81, 115	3 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	499	GLY	7.0
1	C	362	ILE	6.9
1	B	52	ASP	5.8
1	B	65	GLY	5.7
1	A	219	VAL	5.3
1	B	547	ASN	5.1
1	D	207	ARG	4.7
1	C	67	SER	4.6
1	C	500	LEU	4.3
1	B	574	ILE	4.2
1	C	25	HIS	4.2
1	D	500	LEU	4.1
1	B	258	ASP	4.0
1	C	216	SER	3.9
1	C	69	GLU	3.9
1	B	72	PHE	3.8
1	B	372	ASN	3.7
1	C	577	THR	3.7
1	A	71	LYS	3.7
1	A	499	GLY	3.7
1	C	372	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	500	LEU	3.5
1	A	362	ILE	3.5
1	A	69	GLU	3.5
1	D	446	PRO	3.5
1	C	495	PRO	3.4
1	C	71	LYS	3.4
1	B	54	ALA	3.4
1	D	222	VAL	3.4
1	D	552	ARG	3.4
1	D	69	GLU	3.3
1	B	446	PRO	3.3
1	B	495	PRO	3.3
1	D	463	LYS	3.3
1	D	419	GLY	3.2
1	A	106	LEU	3.2
1	B	548	GLY	3.1
1	A	25	HIS	3.1
1	B	89	GLU	3.1
1	B	551	GLN	3.1
1	D	563	LEU	3.0
1	C	464	ALA	3.0
1	D	58	ALA	3.0
1	D	68	PRO	3.0
1	B	85	ASP	3.0
1	C	45	LEU	3.0
1	D	64	LEU	2.9
1	B	207	ARG	2.9
1	B	420	ASP	2.9
1	D	104	ASN	2.9
1	C	37	GLU	2.9
1	C	108	LEU	2.8
1	C	215	HIS	2.8
1	C	68	PRO	2.7
1	B	554	LYS	2.6
1	A	45	LEU	2.6
1	C	49	GLU	2.6
1	A	90	THR	2.6
1	A	175	GLN	2.6
1	B	549	GLN	2.5
1	A	578	LEU	2.5
1	D	60	VAL	2.5
1	A	207	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	78[A]	SER	2.5
1	B	463	LYS	2.5
1	A	68	PRO	2.5
1	C	373	ASN	2.5
1	B	418	GLU	2.4
1	A	446	PRO	2.4
1	C	160	ILE	2.4
1	C	552	ARG	2.4
1	D	372	ASN	2.4
1	C	549	GLN	2.4
1	D	67	SER	2.4
1	A	464	ALA	2.4
1	A	85	ASP	2.3
1	D	561	LEU	2.3
1	B	50	ARG	2.3
1	A	49	GLU	2.3
1	C	547	ASN	2.3
1	B	308	HIS	2.3
1	D	99	LEU	2.3
1	A	495	PRO	2.2
1	B	35	GLU	2.2
1	D	89	GLU	2.2
1	B	220	ARG	2.2
1	C	445	PHE	2.2
1	D	160	ILE	2.2
1	A	108	LEU	2.2
1	D	30	LEU	2.2
1	D	40	LEU	2.2
1	C	550	GLU	2.2
1	D	434	TYR	2.2
1	D	258	ASP	2.2
1	B	61	CYS	2.2
1	A	35	GLU	2.2
1	D	36	LYS	2.1
1	C	300	ASN	2.1
1	A	84	CYS	2.1
1	C	208	GLN	2.1
1	B	222	VAL	2.1
1	A	36	LYS	2.1
1	B	56	PHE	2.1
1	D	50	ARG	2.1
1	A	445	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	420	ASP	2.1
1	B	58	ALA	2.1
1	D	49	GLU	2.1
1	A	50	ARG	2.1
1	D	26	ARG	2.1
1	B	64	LEU	2.1
1	B	416	HIS	2.1
1	D	308	HIS	2.1
1	D	35	GLU	2.0
1	D	106	LEU	2.0
1	A	160	ILE	2.0
1	D	84	CYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

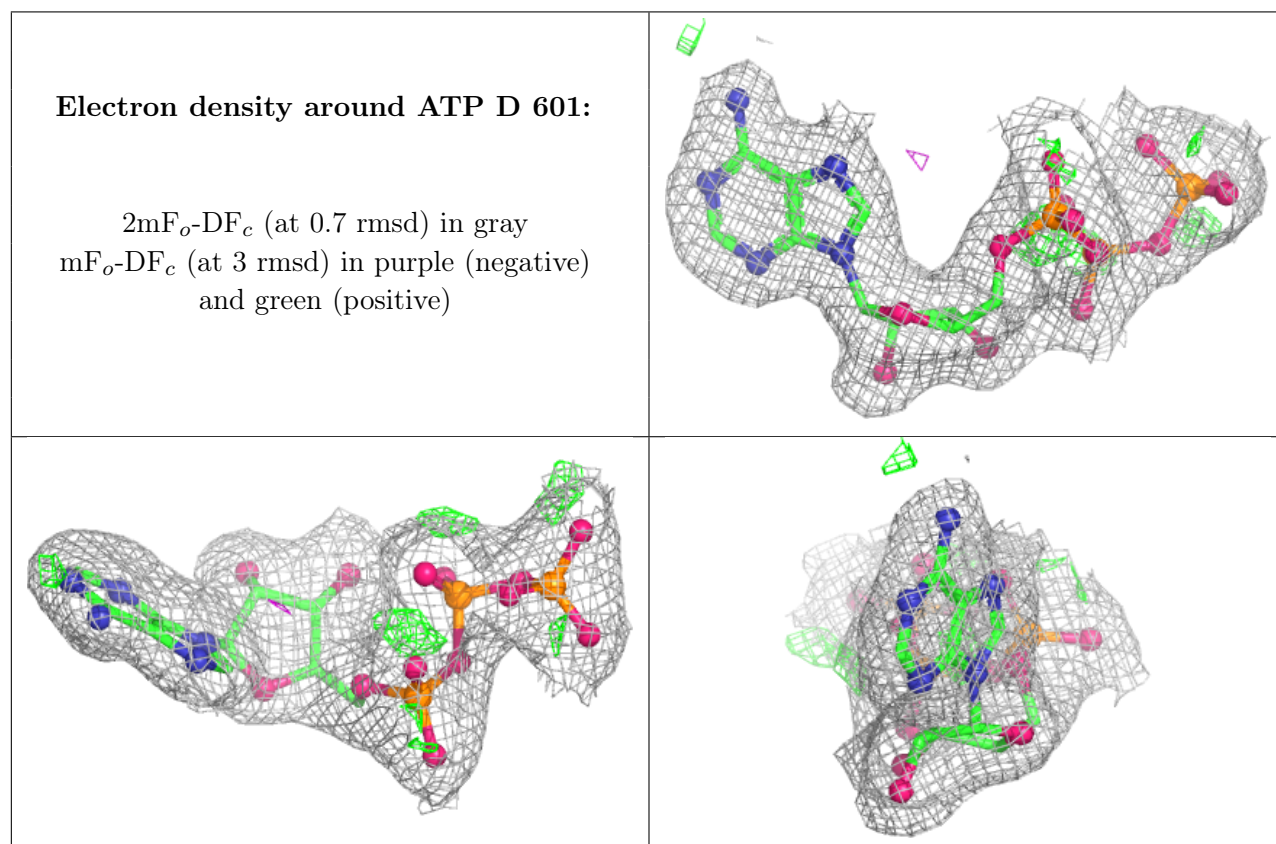
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	C	604	1/1	0.82	0.21	57,57,57,57	0
4	SO4	C	602	5/5	0.97	0.10	45,46,49,50	0
3	MG	A	902	1/1	0.97	0.04	29,29,29,29	0
2	ATP	D	601	31/31	0.98	0.06	22,28,32,35	0
2	ATP	A	901	31/31	0.98	0.06	21,27,31,33	0
3	MG	D	602	1/1	0.98	0.04	25,25,25,25	0
2	ATP	B	601	31/31	0.98	0.06	22,28,34,37	0
2	ATP	C	601	31/31	0.98	0.06	22,27,36,44	0
3	MG	C	603	1/1	0.99	0.04	27,27,27,27	0
3	MG	B	602	1/1	0.99	0.08	23,23,23,23	0

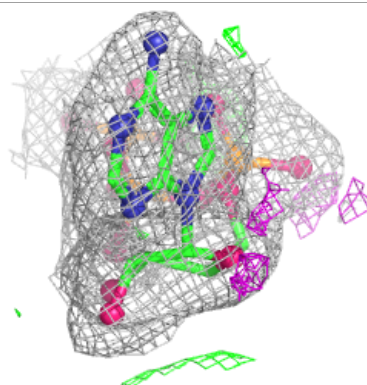
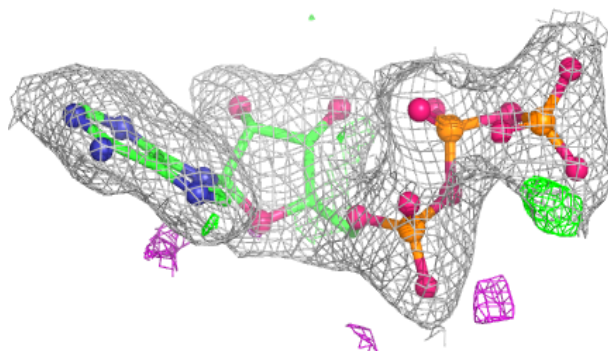
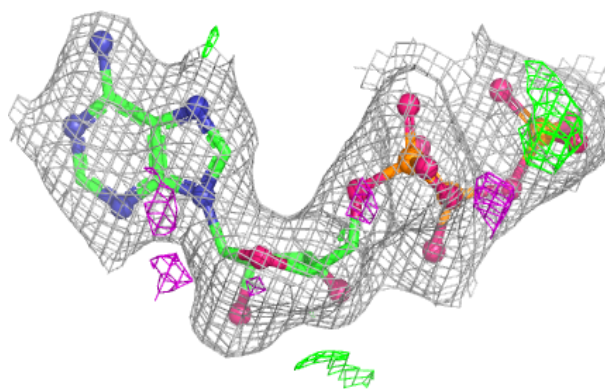
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



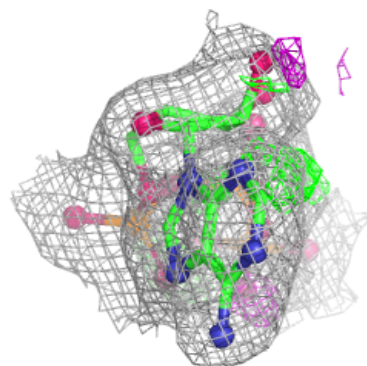
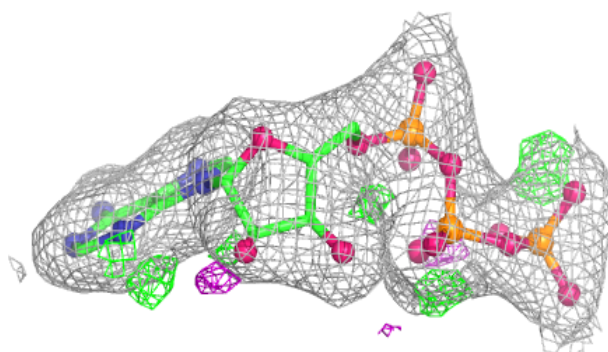
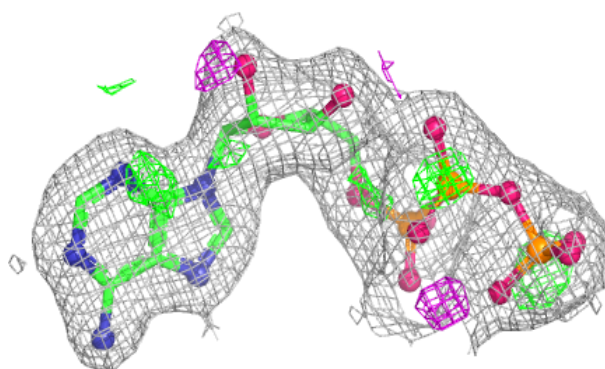


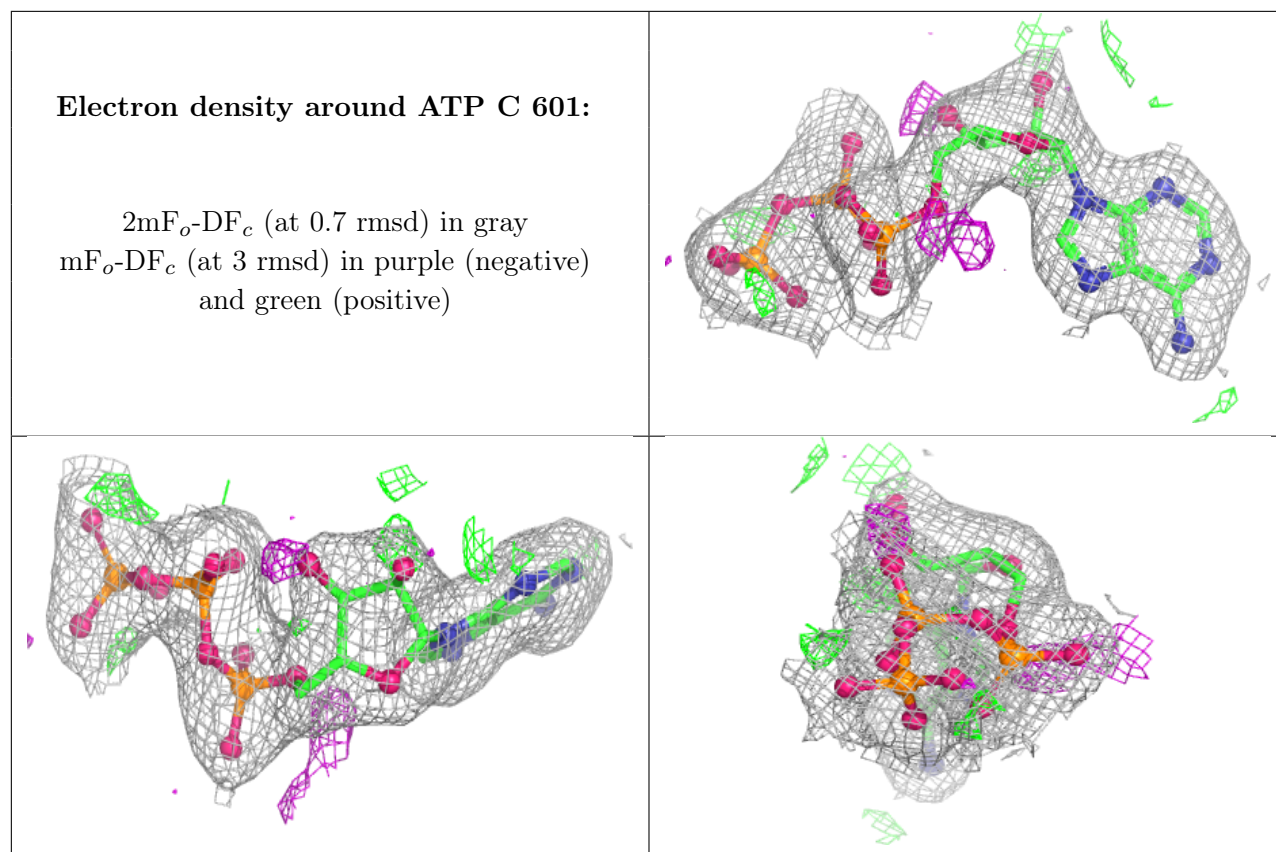
**Electron density around ATP A 901:**

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

**Electron density around ATP B 601:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.