



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:32 am BST

PDB ID : 4M9S  
Title : crystal structure of CED-4 bound CED-3 fragment  
Authors : Huang, W.J.; Jinag, T.Y.; Choi, W.Y.; Wang, J.W.; Shi, Y.G.  
Deposited on : 2013-08-15  
Resolution : 3.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.11  
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

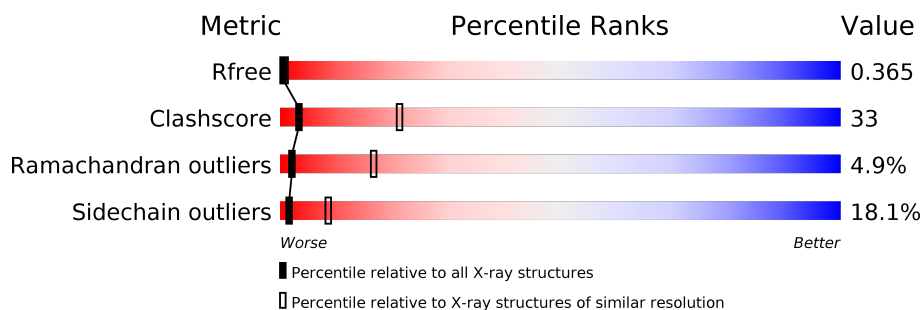
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	
1	C	549	
1	D	549	
2	E	8	
2	F	8	
2	G	8	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	H	8	 A horizontal bar chart showing the quality of chain H. The bar is divided into five segments with the following percentages from left to right: 13% (green), 25% (yellow), 25% (orange), 13% (red), and 25% (grey).

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16687 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 Cell death protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	B	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			
1	C	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	D	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			

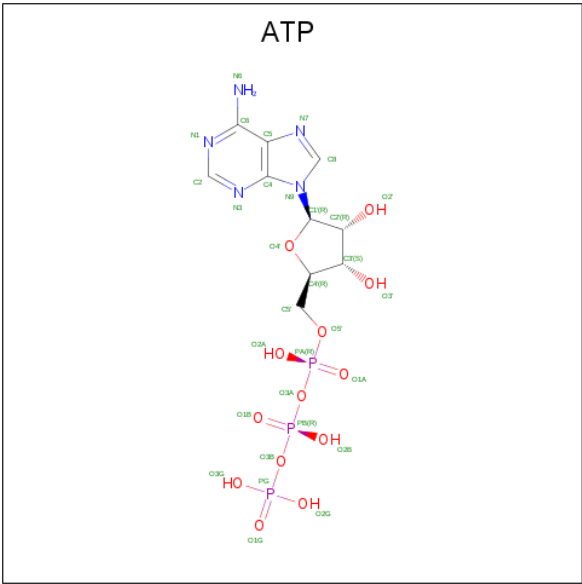
- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	Se	0	0	0
			50	34	7	7	2			
2	F	5	Total	C	N	O	Se	0	0	0
			46	32	6	6	2			
2	G	5	Total	C	N	O	Se	0	0	0
			46	32	6	6	2			
2	H	6	Total	C	N	O	Se	0	0	0
			53	37	7	7	2			

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

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

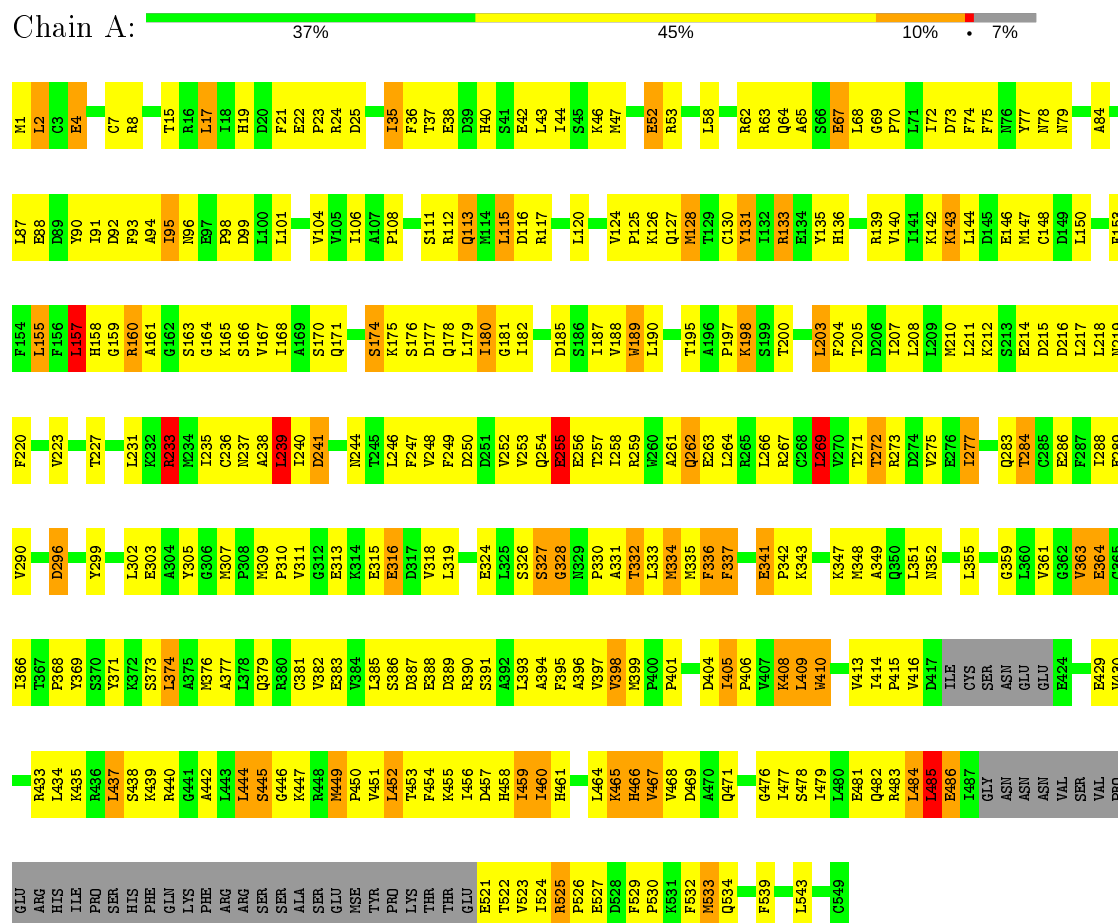
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



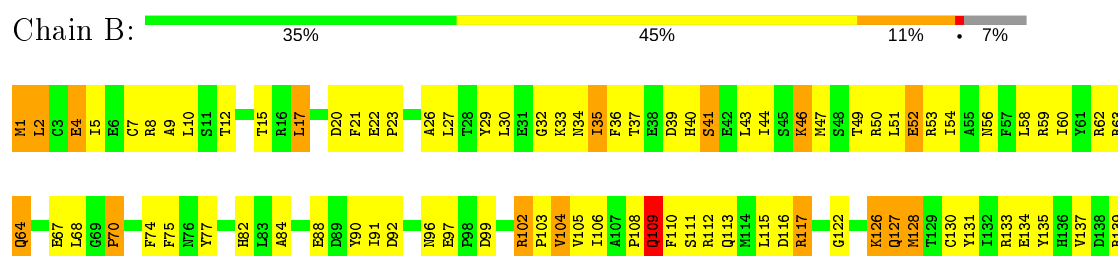
### 3 Residue-property plots

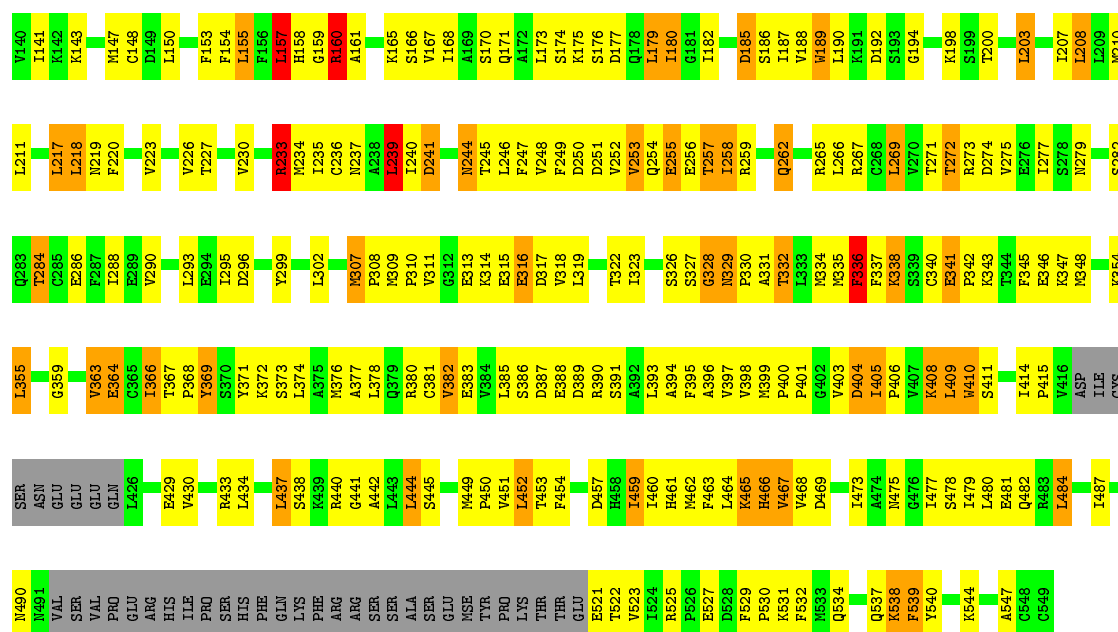
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: Cell death protein 4



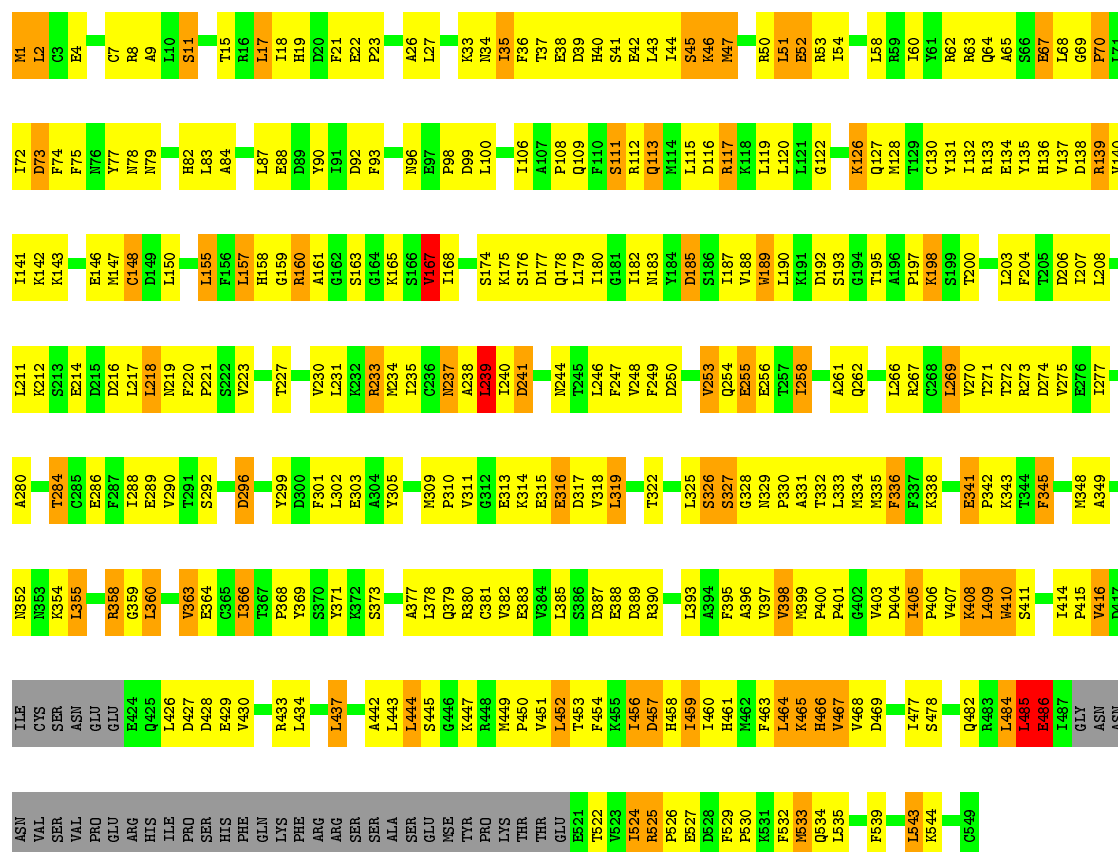
#### • Molecule 1: Cell death protein 4





• Molecule 1: Cell death protein 4

Chain C: 35% 45% 12% 7%



• Molecule 1: Cell death protein 4





F748
M749
F750
M751
F752
M753
GLY
CYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.81Å 178.81Å 201.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.85 – 3.21 40.85 – 3.21	Depositor EDS
% Data completeness (in resolution range)	55.5 (40.85-3.21) 69.2 (40.85-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.283 , 0.334 0.313 , 0.365	Depositor DCC
$R_{free}$ test set	1877 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	16687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	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 40.62 % 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 2.6626e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.82	1/4147 (0.0%)	1.12	14/5577 (0.3%)
1	B	0.80	0/4153	1.13	11/5585 (0.2%)
1	C	0.77	1/4147 (0.0%)	1.05	5/5577 (0.1%)
1	D	0.79	2/4153 (0.0%)	1.08	8/5585 (0.1%)
2	E	1.02	0/50	1.00	0/62
2	F	1.00	0/46	1.11	0/57
2	G	0.87	0/46	1.14	0/57
2	H	1.11	0/53	1.15	0/65
All	All	0.80	4/16795 (0.0%)	1.09	38/22565 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	G	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	381	CYS	CB-SG	6.49	1.93	1.82
1	C	167	VAL	CB-CG2	-6.25	1.39	1.52
1	A	236	CYS	CB-SG	5.96	1.92	1.82
1	D	167	VAL	CB-CG2	-5.10	1.42	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	LEU	CA-CB-CG	7.72	133.06	115.30
1	A	409	LEU	CA-CB-CG	7.60	132.78	115.30
1	D	239	LEU	CA-CB-CG	7.53	132.63	115.30
1	B	239	LEU	CA-CB-CG	6.87	131.10	115.30
1	C	360	LEU	CA-CB-CG	6.84	131.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	346	GLU	Sidechain
2	G	752	PHE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4088	0	4107	277	0
1	B	4094	0	4115	267	0
1	C	4088	0	4108	287	1
1	D	4094	0	4115	274	1
2	E	50	0	44	6	0
2	F	46	0	41	6	0
2	G	46	0	41	6	0
2	H	53	0	49	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	5	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
All	All	16687	0	16668	1091	1

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 33.

The worst 5 of 1091 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:A:63:ARG:HE	1:A:240:ILE:HD11	1.24	1.02
1:D:128:MSE:HG3	1:D:167:VAL:HG22	1.48	0.94
1:D:364:GLU:HB2	1:D:373:SER:HB3	1.54	0.89
1:A:484:LEU:HD11	1:A:533:MSE:HG2	1.52	0.89
1:C:63:ARG:HE	1:C:240:ILE:HD11	1.39	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LEU:O	1:D:113:GLN:NE2[4_555]	2.19	0.01

## 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	504/549 (92%)	404 (80%)	77 (15%)	23 (5%)	2	18
1	B	505/549 (92%)	407 (81%)	73 (14%)	25 (5%)	2	16
1	C	504/549 (92%)	404 (80%)	76 (15%)	24 (5%)	2	17
1	D	505/549 (92%)	405 (80%)	77 (15%)	23 (5%)	2	18
2	E	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
2	F	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	G	3/8 (38%)	1 (33%)	0	2 (67%)	0	0
2	H	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
All	All	2032/2228 (91%)	1624 (80%)	308 (15%)	100 (5%)	2	17

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	341	GLU
1	A	398	VAL
1	A	445	SER
1	A	486	GLU

### 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	462/483 (96%)	386 (84%)	76 (16%)	2	10
1	B	464/483 (96%)	387 (83%)	77 (17%)	2	10
1	C	462/483 (96%)	375 (81%)	87 (19%)	1	8
1	D	464/483 (96%)	372 (80%)	92 (20%)	1	7
2	E	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	F	5/5 (100%)	4 (80%)	1 (20%)	1	6
2	G	5/5 (100%)	4 (80%)	1 (20%)	1	6
2	H	6/5 (120%)	3 (50%)	3 (50%)	0	0
All	All	1873/1952 (96%)	1534 (82%)	339 (18%)	1	8

5 of 339 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	539	PHE
1	C	185	ASP
1	D	381	CYS
1	C	11	SER
1	C	99	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	475	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	64	GLN
1	D	262	GLN
1	A	379	GLN
1	C	80	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
4	ATP	A	602	3	26,33,33	1.26	1 (3%)	31,52,52	1.75	8 (25%)
4	ATP	C	602	3	26,33,33	1.22	2 (7%)	31,52,52	1.54	4 (12%)
4	ATP	B	602	3	26,33,33	1.14	3 (11%)	31,52,52	2.04	8 (25%)
4	ATP	D	602	3	26,33,33	1.63	5 (19%)	31,52,52	1.96	9 (29%)

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
4	ATP	A	602	3	-	1/18/38/38	0/3/3/3
4	ATP	C	602	3	-	1/18/38/38	0/3/3/3
4	ATP	B	602	3	-	2/18/38/38	0/3/3/3
4	ATP	D	602	3	-	1/18/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	ATP	C5-C4	4.28	1.52	1.40
4	C	602	ATP	C5-C4	3.66	1.50	1.40
4	D	602	ATP	C4-N3	3.61	1.40	1.35
4	A	602	ATP	C5-C4	3.13	1.49	1.40
4	D	602	ATP	O4'-C1'	3.05	1.45	1.41

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	N6-C6-N1	5.69	130.38	118.57
4	D	602	ATP	O4'-C1'-C2'	-4.78	99.95	106.93
4	D	602	ATP	N3-C2-N1	-4.20	122.12	128.68
4	C	602	ATP	N3-C2-N1	-4.08	122.31	128.68
4	B	602	ATP	C1'-N9-C4	3.96	133.59	126.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	ATP	PG-O3B-PB-O1B
4	C	602	ATP	PG-O3B-PB-O1B
4	B	602	ATP	PG-O3B-PB-O1B
4	B	602	ATP	PG-O3B-PB-O2B
4	D	602	ATP	C4'-C5'-O5'-PA

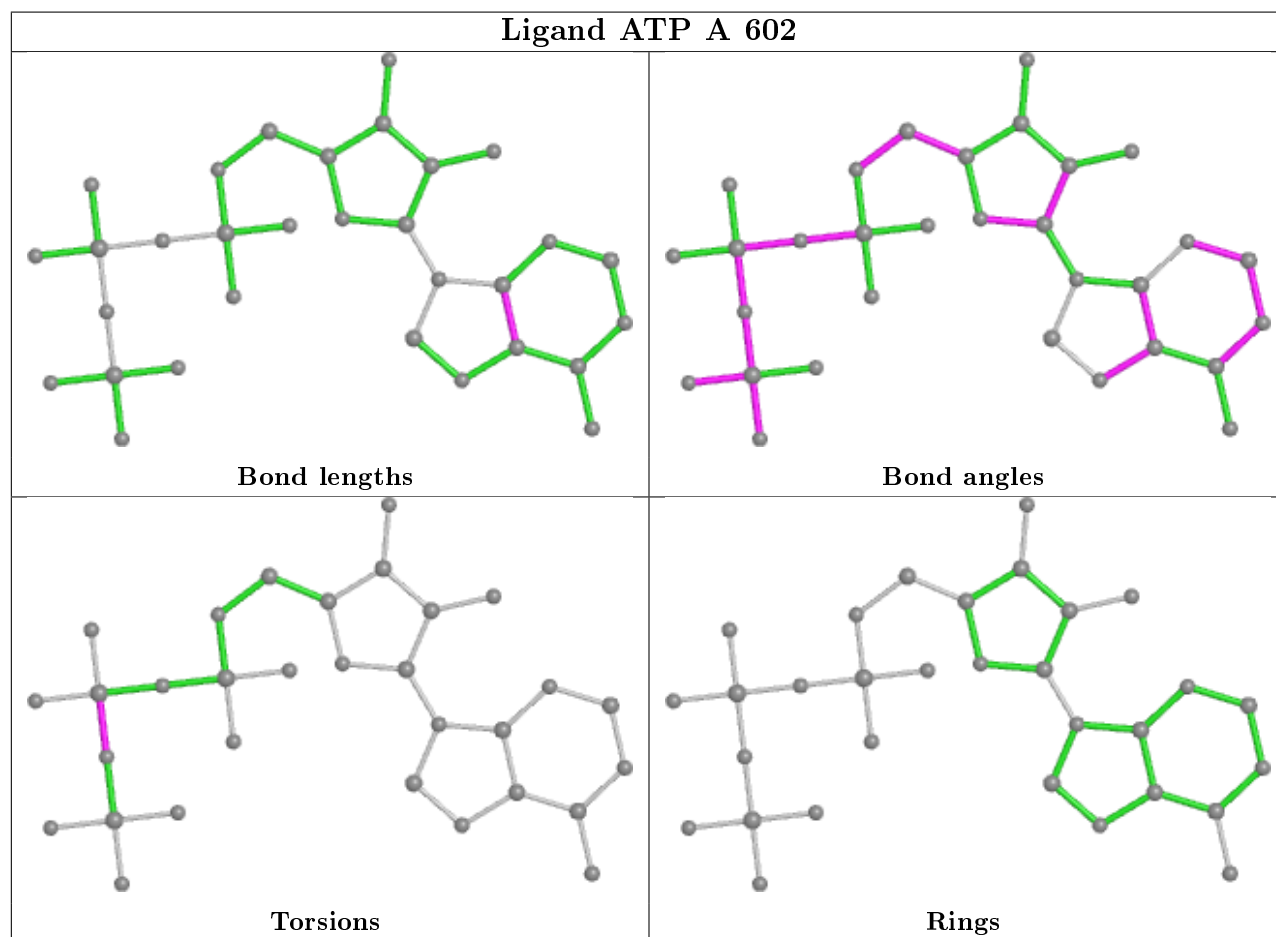
There are no ring outliers.

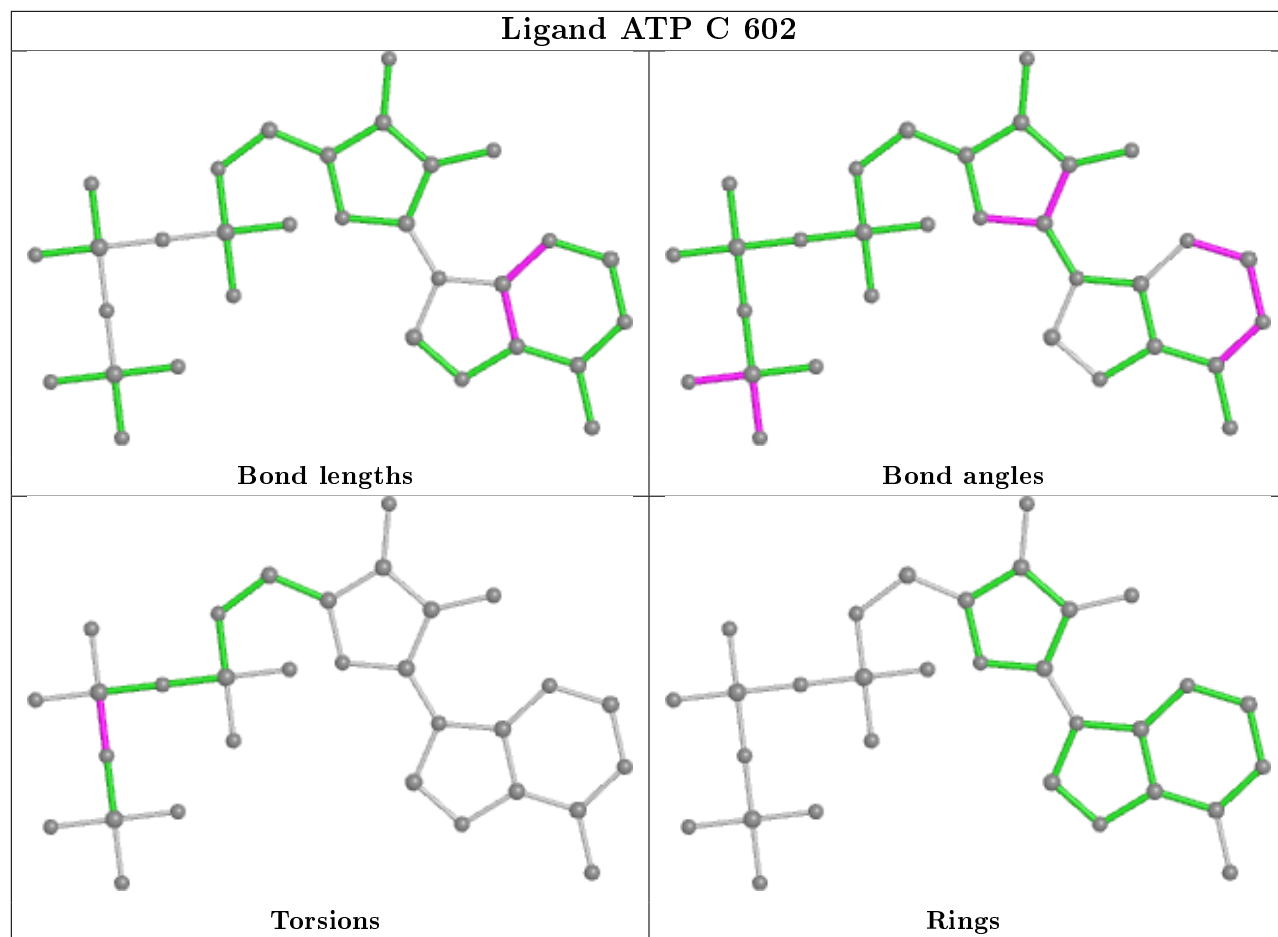
4 monomers are involved in 11 short contacts:

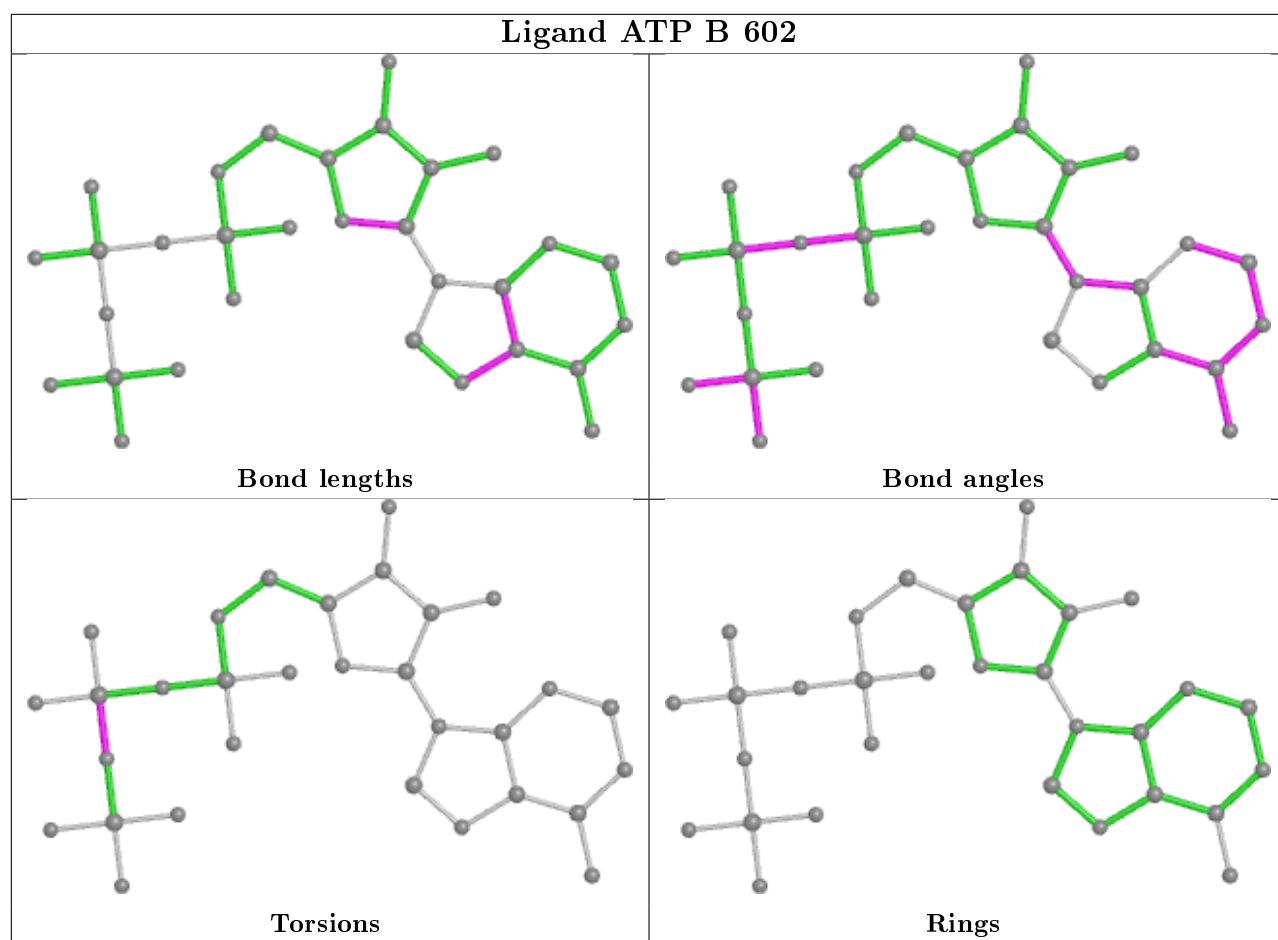
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	4	0
4	C	602	ATP	1	0
4	B	602	ATP	5	0
4	D	602	ATP	1	0

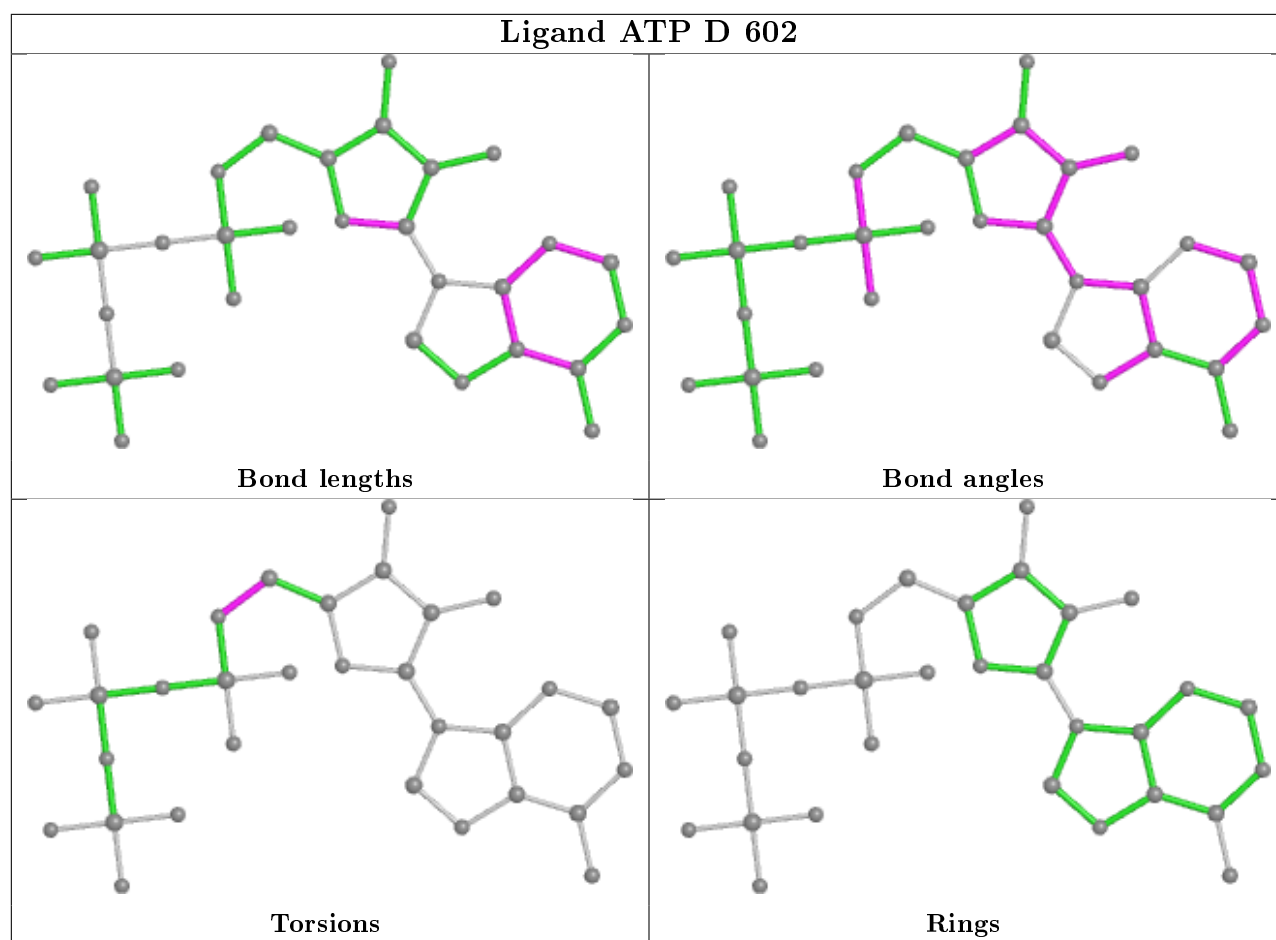


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

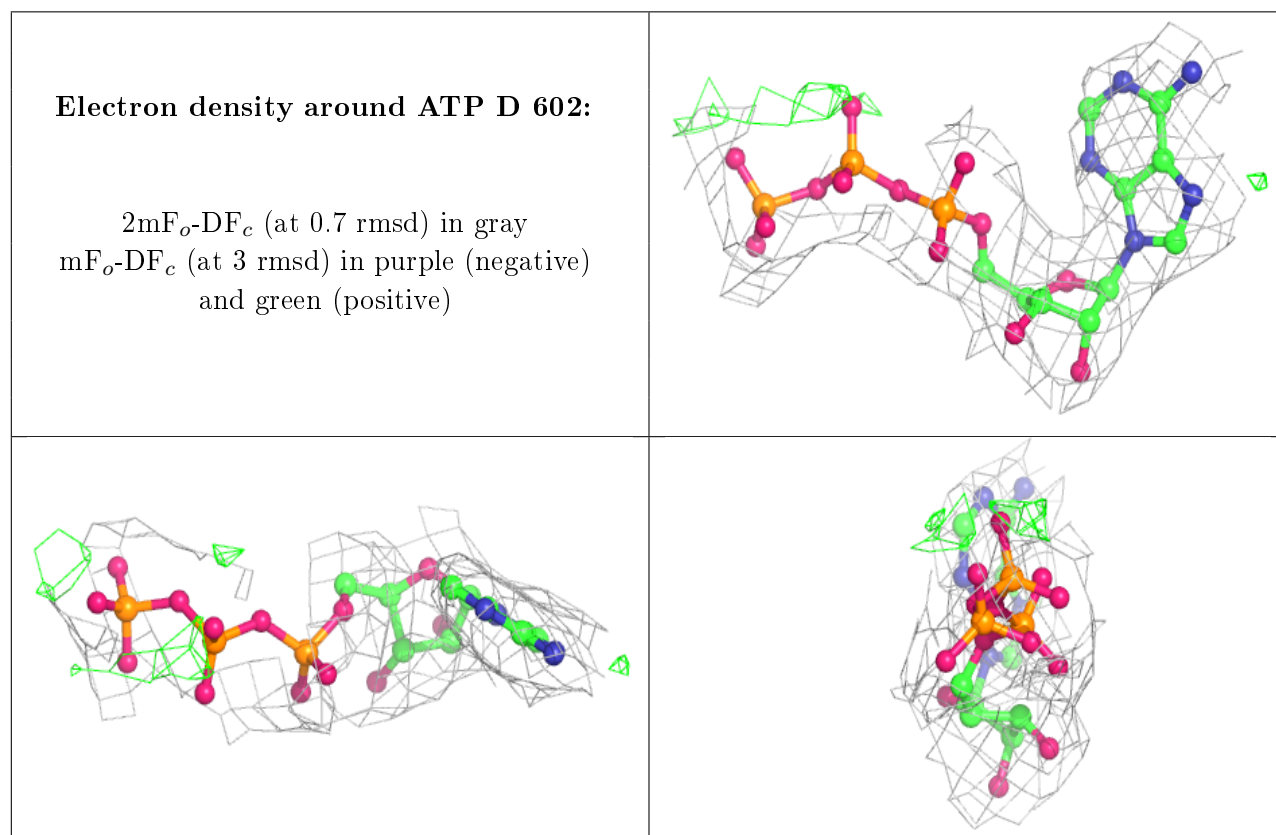
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

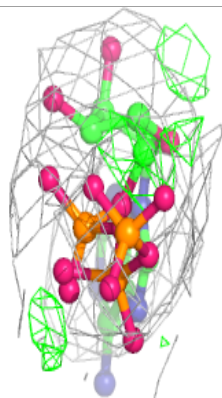
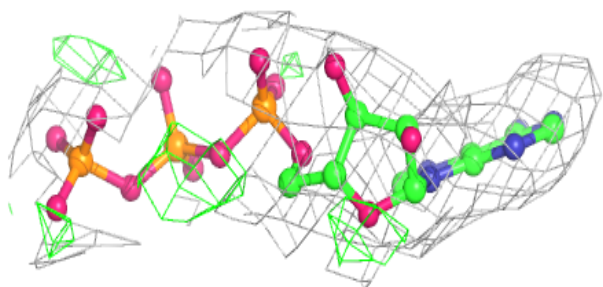
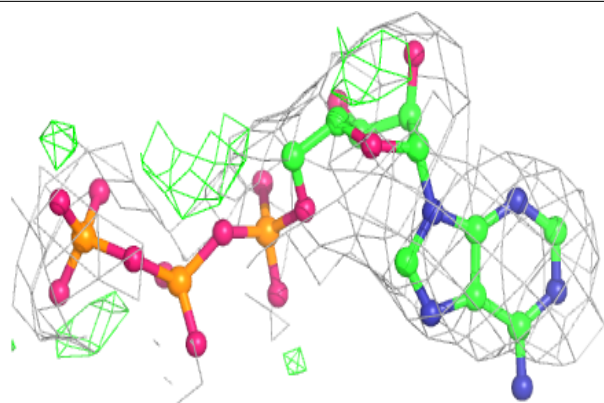
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

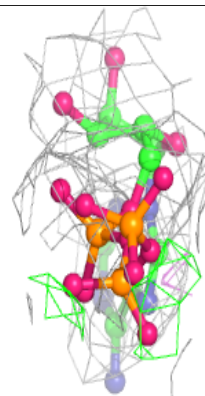
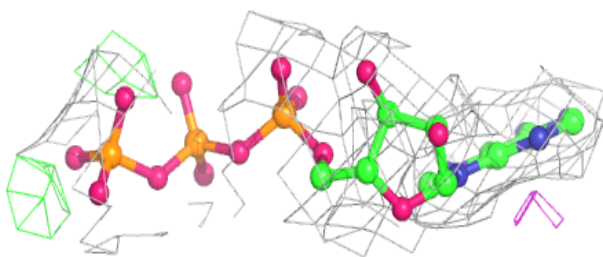
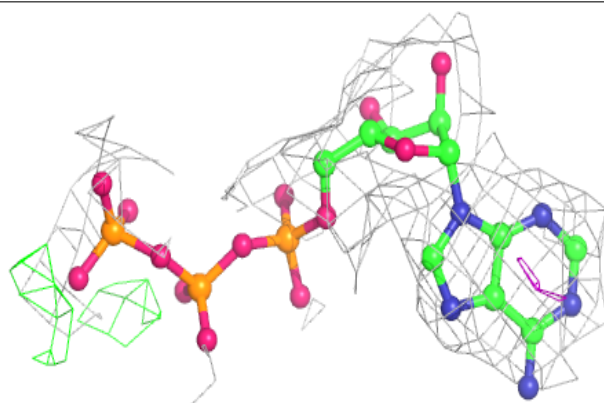


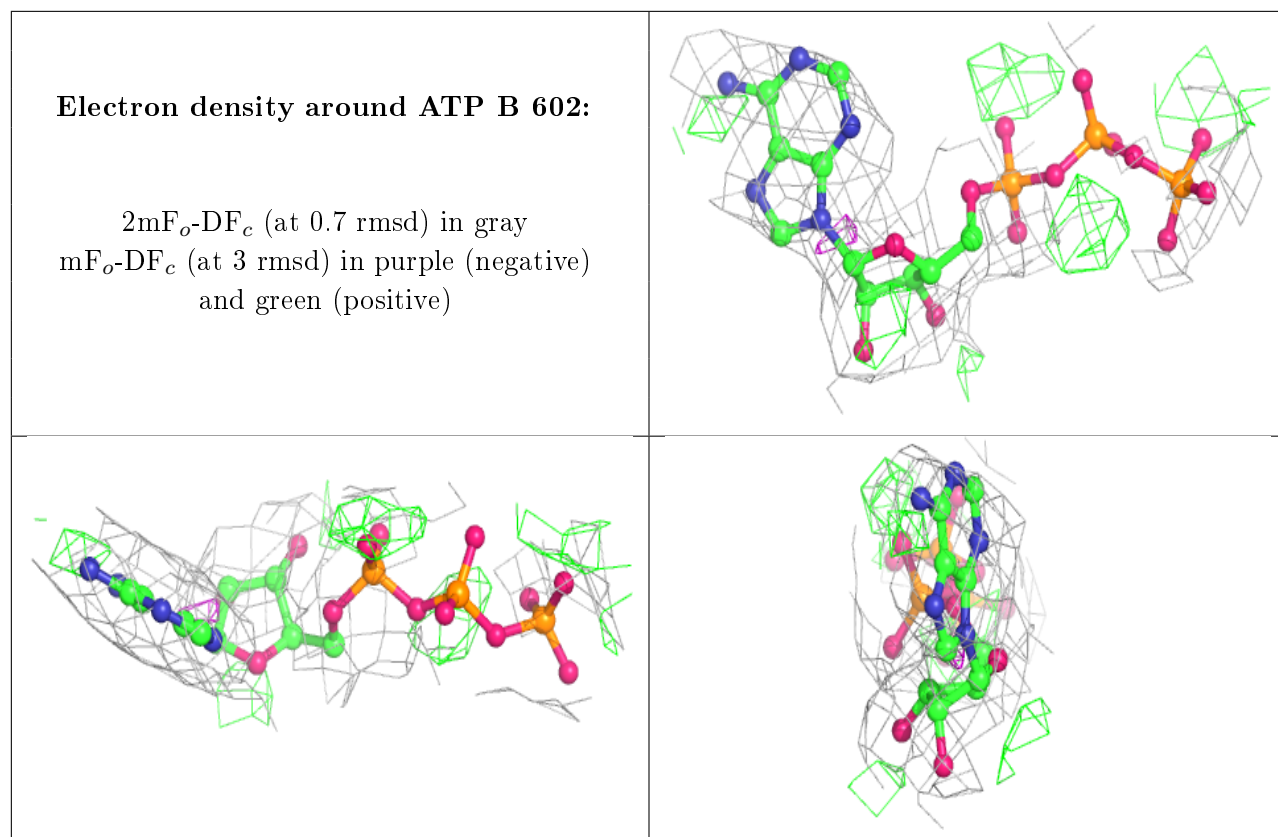
**Electron density around ATP A 602:**

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

**Electron density around ATP C 602:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.