



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:48 pm BST

PDB ID : 6S5O
Title : Non-square conformations of KtrA E125Q mutant rings with bound ADP
Authors : Teixeira-Duarte, C.M.; Fonseca, F.; Morais-Cabral, J.H.
Deposited on : 2019-07-02
Resolution : 3.98 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

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

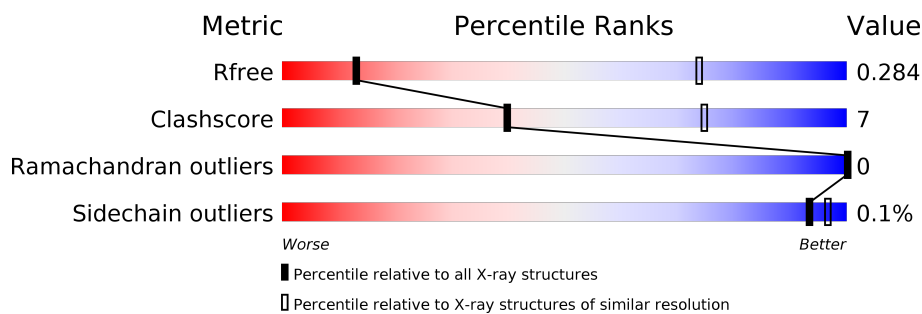
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	222	81% 16% .
1	B	222	81% 16% .
1	C	222	78% 18% .
1	D	222	82% 15% .
1	E	222	84% 13% .
1	F	222	80% 17% .
1	G	222	50% 10% 40%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	222	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment representing 49%, a yellow segment representing 11%, and a grey segment representing 40%. The percentages are labeled below the corresponding segments.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12426 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 Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	24	0	0
			1689	1071	291	319	8			
1	B	215	Total	C	N	O	S	24	0	0
			1689	1071	291	319	8			
1	C	215	Total	C	N	O	S	24	0	0
			1689	1071	291	319	8			
1	D	215	Total	C	N	O	S	24	0	0
			1689	1071	291	319	8			
1	E	215	Total	C	N	O	S	24	0	0
			1689	1071	291	319	8			
1	F	215	Total	C	N	O	S	31	0	0
			1689	1071	291	319	8			
1	G	133	Total	C	N	O	S	0	0	0
			1038	660	180	195	3			
1	H	133	Total	C	N	O	S	0	0	0
			1038	660	180	195	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLN	GLU	engineered mutation	UNP O32080
B	125	GLN	GLU	engineered mutation	UNP O32080
C	125	GLN	GLU	engineered mutation	UNP O32080
D	125	GLN	GLU	engineered mutation	UNP O32080
E	125	GLN	GLU	engineered mutation	UNP O32080
F	125	GLN	GLU	engineered mutation	UNP O32080
G	125	GLN	GLU	engineered mutation	UNP O32080
H	125	GLN	GLU	engineered mutation	UNP O32080

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



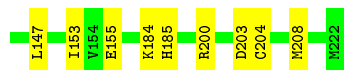
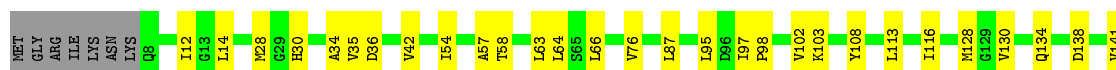
- Molecule 1: Ktr system potassium uptake protein A

Chain E: 84% 13%



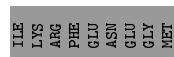
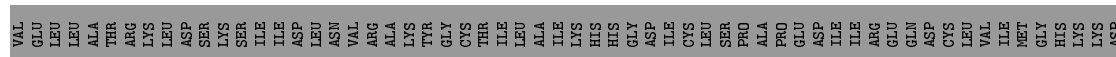
- Molecule 1: Ktr system potassium uptake protein A

Chain F: 80% 17%



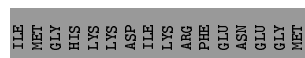
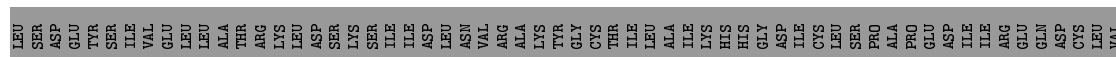
- Molecule 1: Ktr system potassium uptake protein A

Chain G: 50% 10% 40%



- Molecule 1: Ktr system potassium uptake protein A

Chain H: 49% 11% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.20Å 155.22Å 285.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 3.98 47.66 – 3.98	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.66-3.98) 99.5 (47.66-3.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.250 , 0.286 0.255 , 0.284	Depositor DCC
R_{free} test set	2128 reflections (10.18%)	wwPDB-VP
Wilson B-factor (Å ²)	201.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12426	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.22	0/1715	0.41	0/2317
1	B	0.23	0/1715	0.42	0/2317
1	C	0.23	0/1715	0.44	0/2317
1	D	0.22	0/1715	0.42	0/2317
1	E	0.23	0/1715	0.42	0/2317
1	F	0.25	0/1715	0.45	0/2317
1	G	0.22	0/1055	0.39	0/1428
1	H	0.22	0/1055	0.39	0/1428
All	All	0.23	0/12400	0.42	0/16758

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	1689	0	1713	32	0
1	B	1689	0	1713	34	0
1	C	1689	0	1713	34	0
1	D	1689	0	1713	29	0
1	E	1689	0	1713	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1689	0	1713	26	1
1	G	1038	0	1045	16	1
1	H	1038	0	1045	18	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	1	0
All	All	12426	0	12464	179	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 7.

The worst 5 of 179 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:140:ASN:HA	1:C:157:LEU:HG	1.54	0.90
1:C:184:LYS:HB3	1:C:204:CYS:HB2	1.57	0.87
1:B:69:ARG:HH12	1:C:200:ARG:HG2	1.40	0.86
1:E:184:LYS:HB3	1:E:204:CYS:HB2	1.59	0.83
1:B:184:LYS:HB3	1:B:204:CYS:HB2	1.61	0.82

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:F:200:ARG:NH1	1:G:96:ASP:OD2[5_445]	2.17	0.03

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	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	B	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	C	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	D	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	E	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	F	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
1	G	131/222 (59%)	126 (96%)	5 (4%)	0	100	100
1	H	131/222 (59%)	126 (96%)	5 (4%)	0	100	100
All	All	1540/1776 (87%)	1500 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	184/190 (97%)	184 (100%)	0	100	100
1	B	184/190 (97%)	184 (100%)	0	100	100
1	C	184/190 (97%)	184 (100%)	0	100	100
1	D	184/190 (97%)	184 (100%)	0	100	100
1	E	184/190 (97%)	184 (100%)	0	100	100
1	F	184/190 (97%)	183 (100%)	1 (0%)	88	93
1	G	110/190 (58%)	110 (100%)	0	100	100
1	H	110/190 (58%)	110 (100%)	0	100	100
All	All	1324/1520 (87%)	1323 (100%)	1 (0%)	93	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	108	TYR

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

Mol	Chain	Res	Type
1	E	134	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	B	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	H	601	-	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	F	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.43	4 (13%)
2	ADP	G	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	E	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.40	4 (13%)
2	ADP	C	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	D	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	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
2	ADP	B	601	-	-	3/12/32/32	0/3/3/3
2	ADP	H	601	-	-	3/12/32/32	0/3/3/3
2	ADP	F	601	-	-	3/12/32/32	0/3/3/3
2	ADP	G	601	-	-	2/12/32/32	0/3/3/3
2	ADP	E	601	-	-	2/12/32/32	0/3/3/3
2	ADP	C	601	-	-	3/12/32/32	0/3/3/3
2	ADP	A	601	-	-	4/12/32/32	0/3/3/3
2	ADP	D	601	-	-	3/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	2.48	1.47	1.40
2	D	601	ADP	C5-C4	2.45	1.47	1.40
2	G	601	ADP	C5-C4	2.45	1.47	1.40
2	F	601	ADP	C5-C4	2.45	1.47	1.40
2	A	601	ADP	C5-C4	2.44	1.47	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	ADP	PA-O3A-PB	-3.51	120.77	132.83
2	D	601	ADP	PA-O3A-PB	-3.48	120.89	132.83
2	G	601	ADP	PA-O3A-PB	-3.42	121.10	132.83
2	C	601	ADP	PA-O3A-PB	-3.32	121.43	132.83
2	B	601	ADP	N3-C2-N1	-3.27	123.57	128.68

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

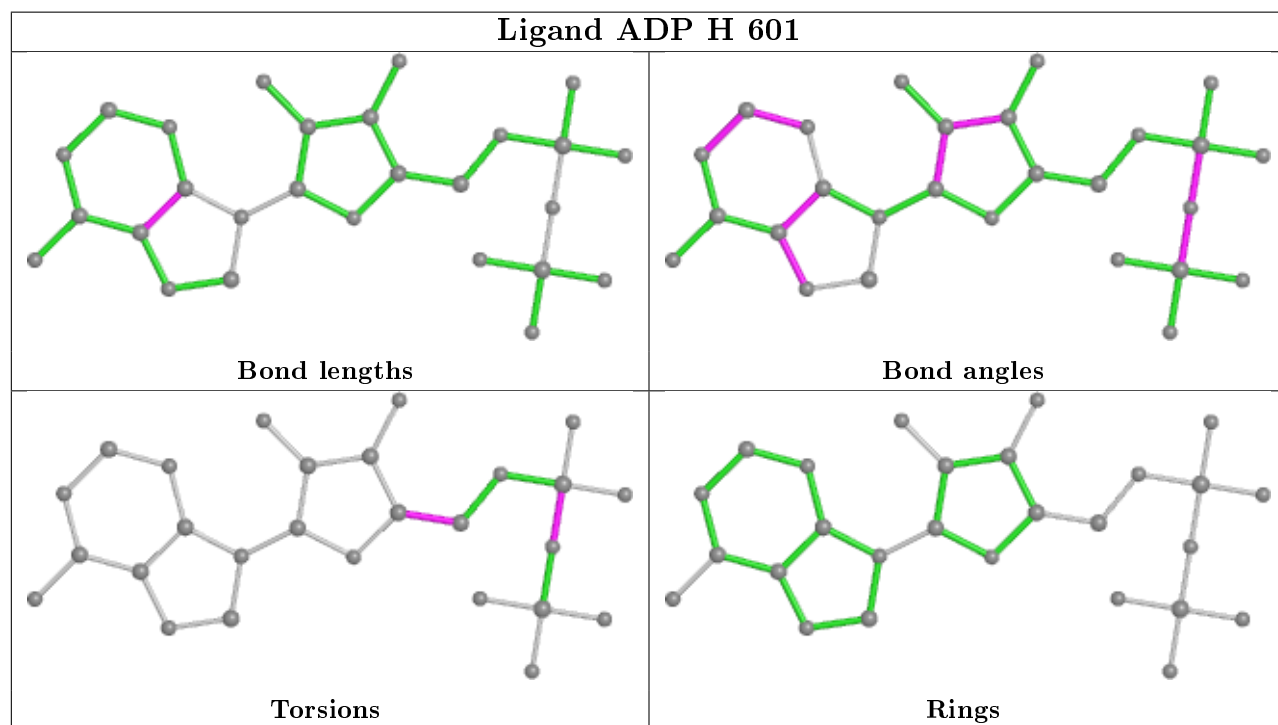
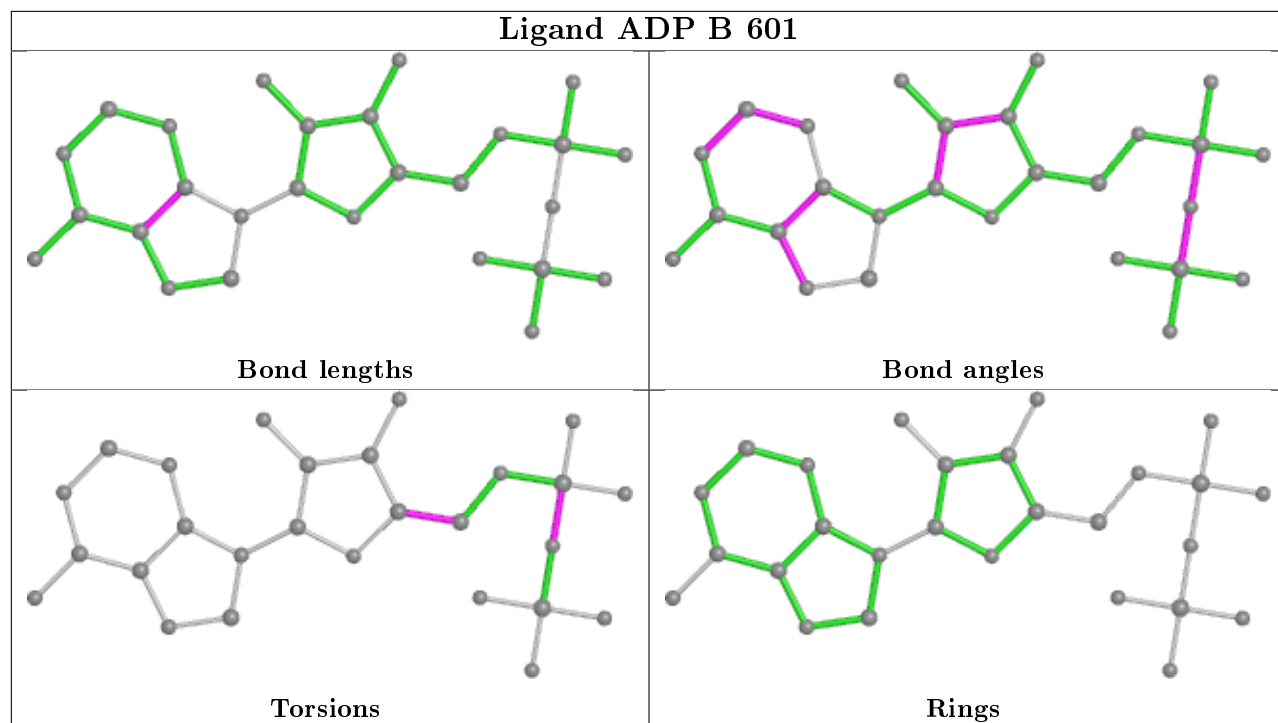
Mol	Chain	Res	Type	Atoms
2	A	601	ADP	O4'-C4'-C5'-O5'
2	H	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	C3'-C4'-C5'-O5'
2	H	601	ADP	C3'-C4'-C5'-O5'
2	D	601	ADP	PB-O3A-PA-O1A

There are no ring outliers.

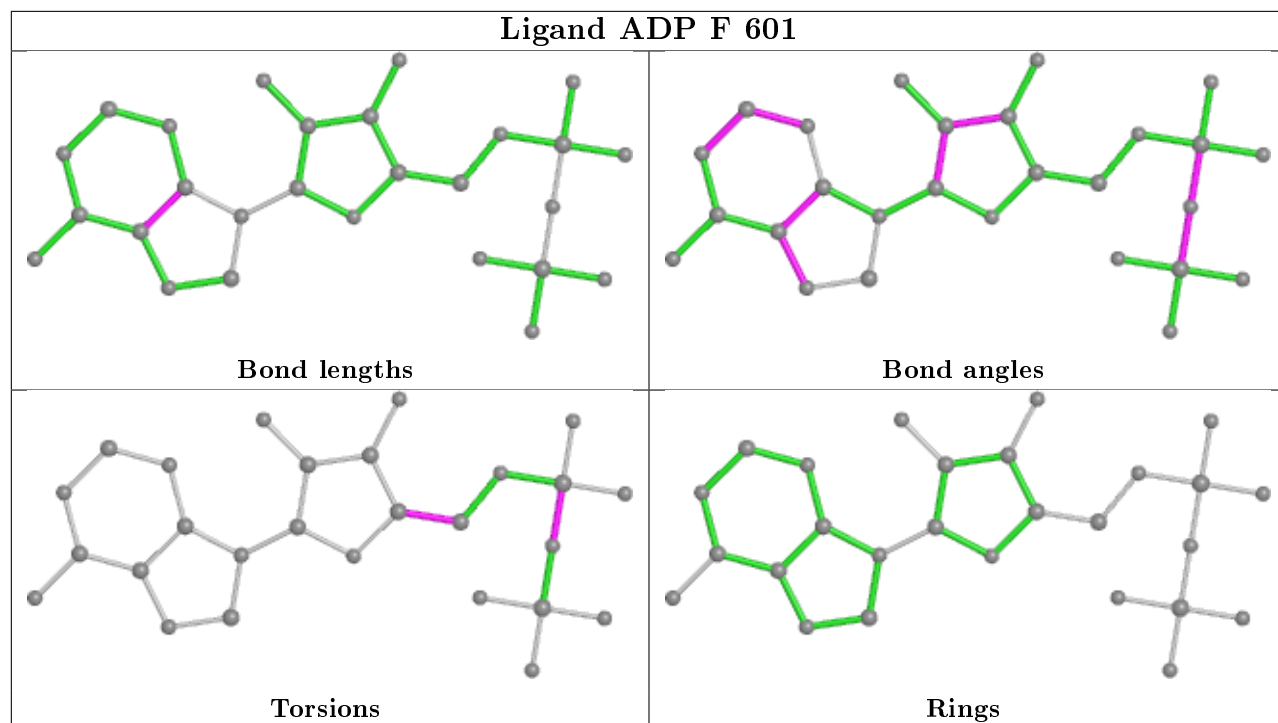
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADP	1	0
2	H	601	ADP	1	0
2	F	601	ADP	1	0
2	G	601	ADP	1	0
2	E	601	ADP	1	0
2	C	601	ADP	1	0
2	A	601	ADP	2	0
2	D	601	ADP	1	0

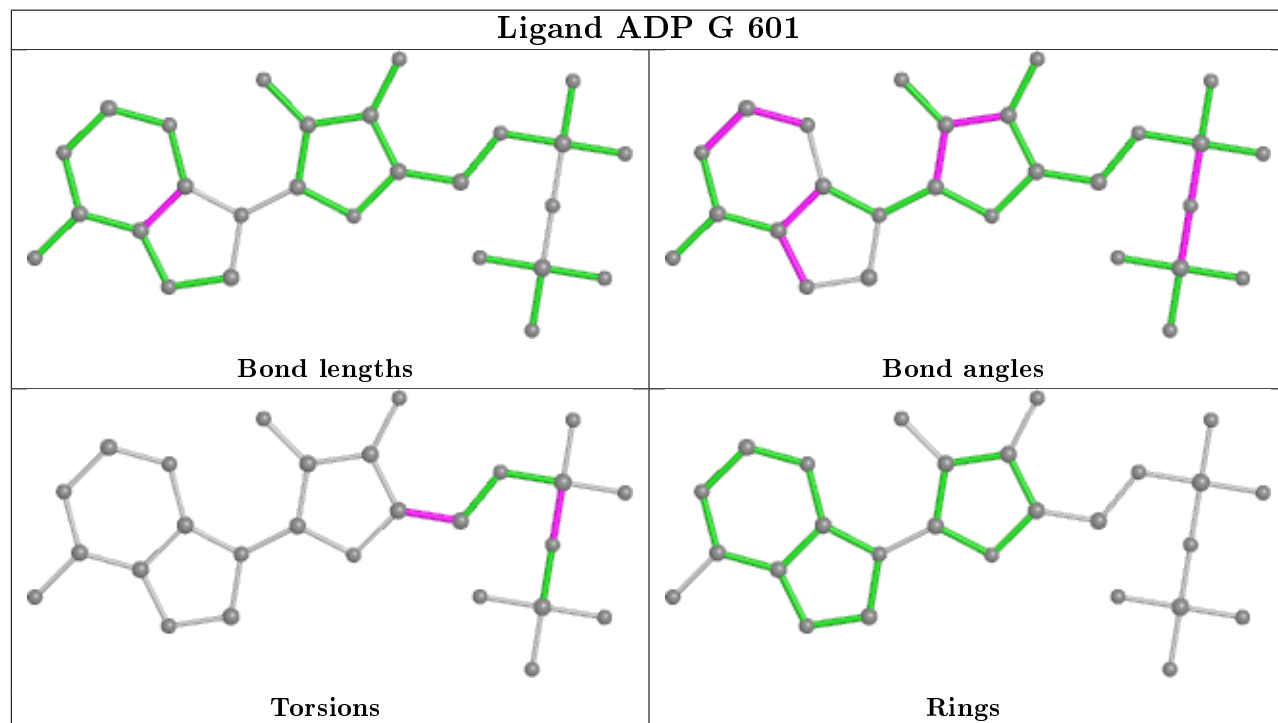
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



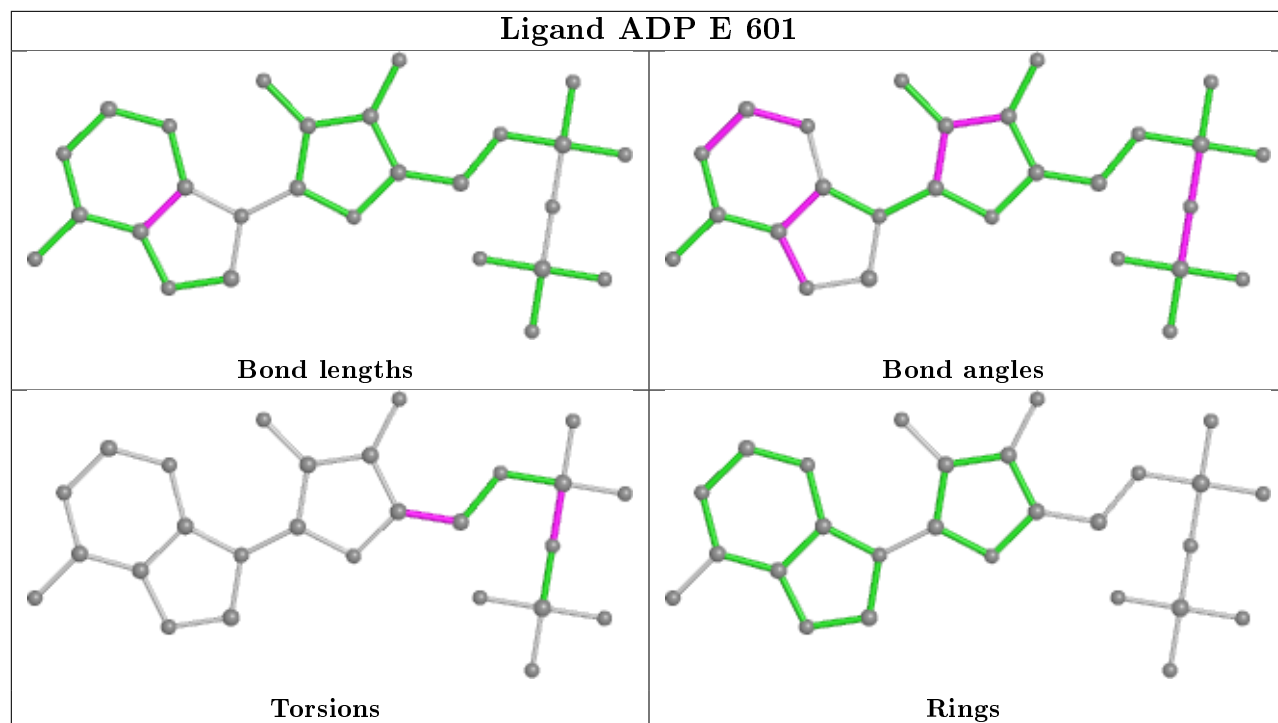
Ligand ADP F 601



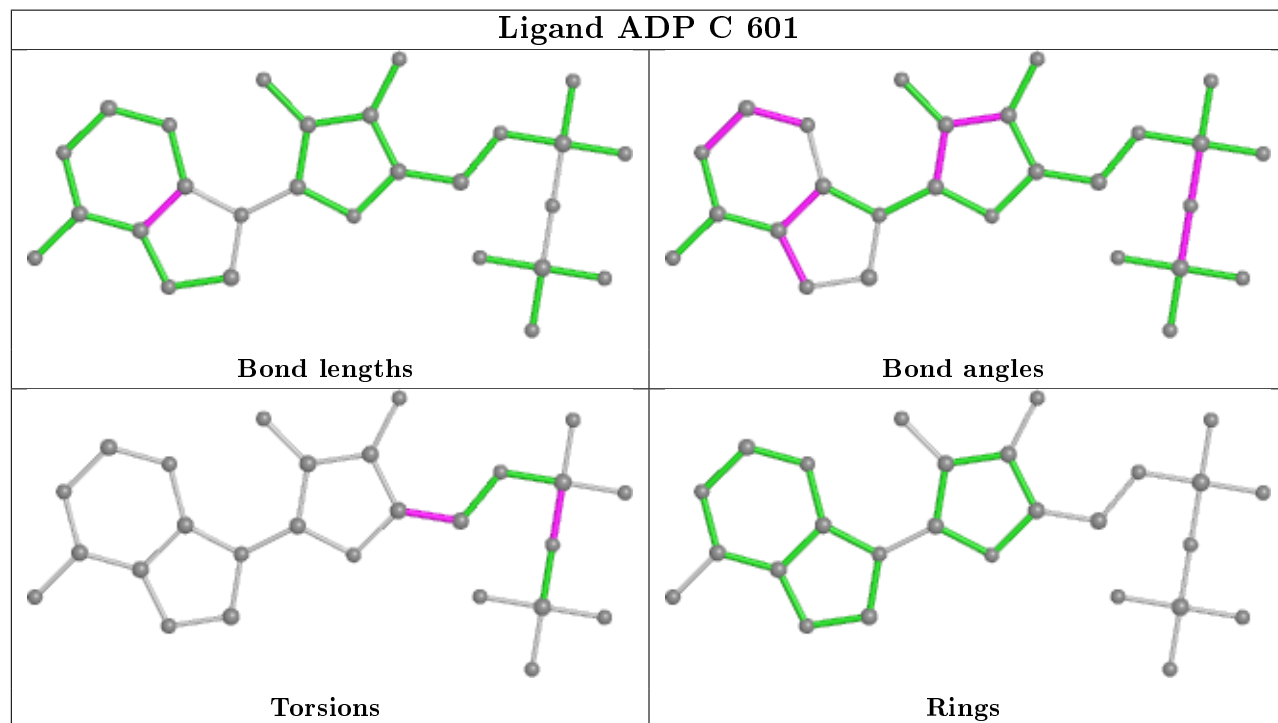
Ligand ADP G 601

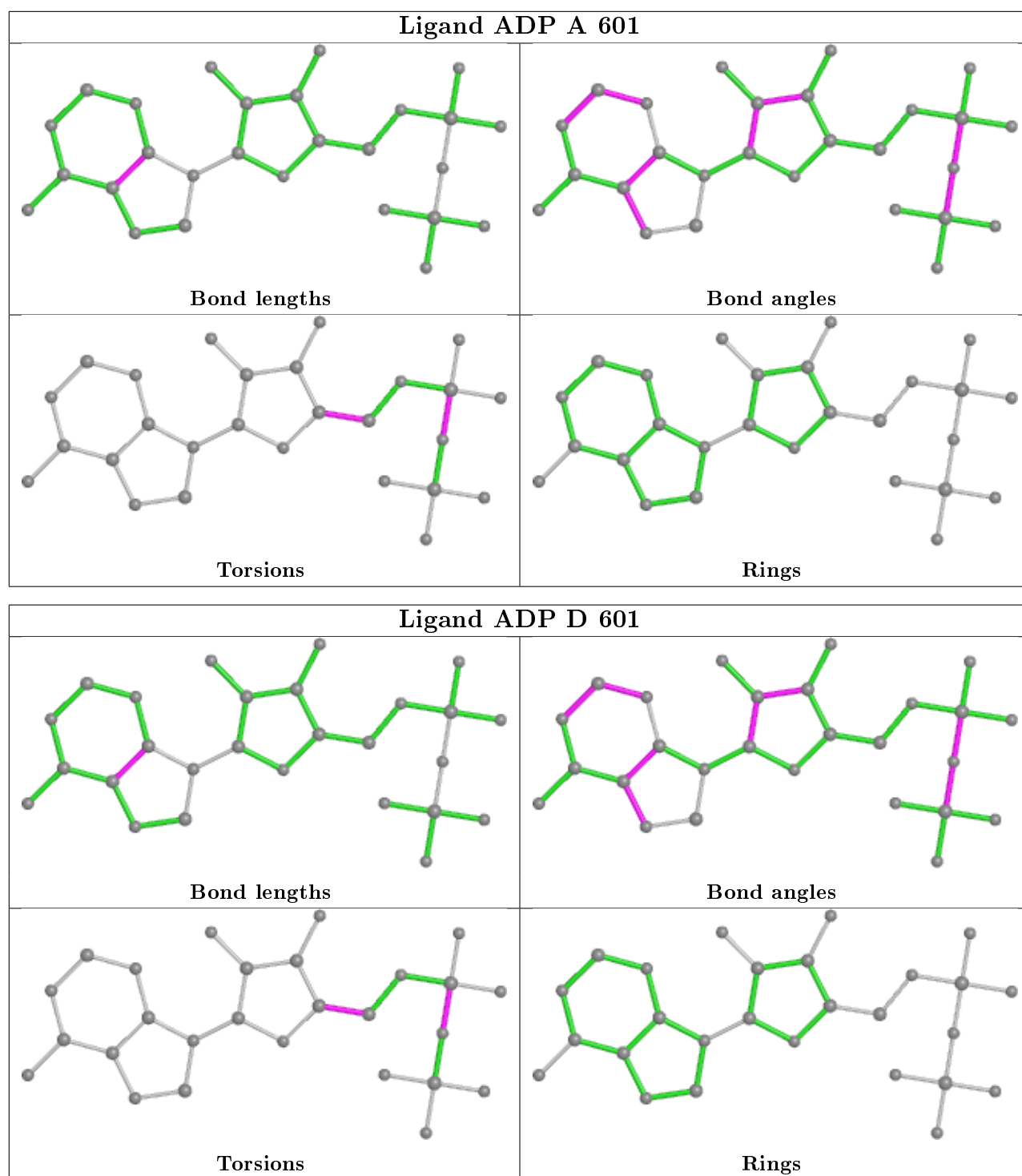


Ligand ADP E 601



Ligand ADP C 601





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

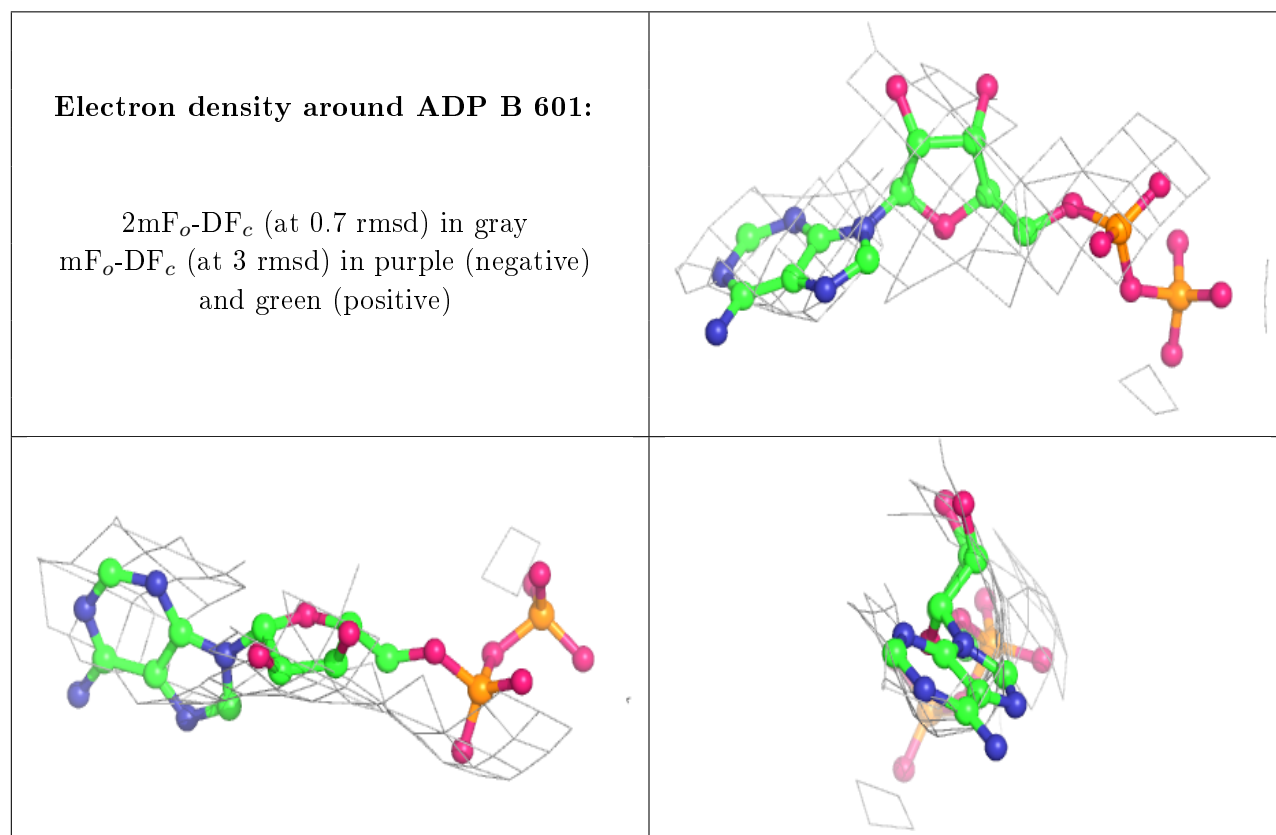
6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

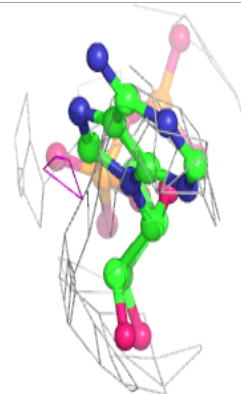
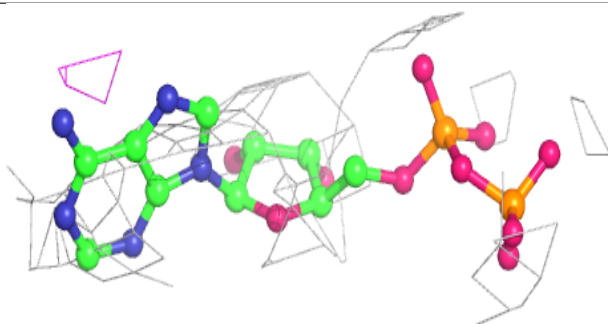
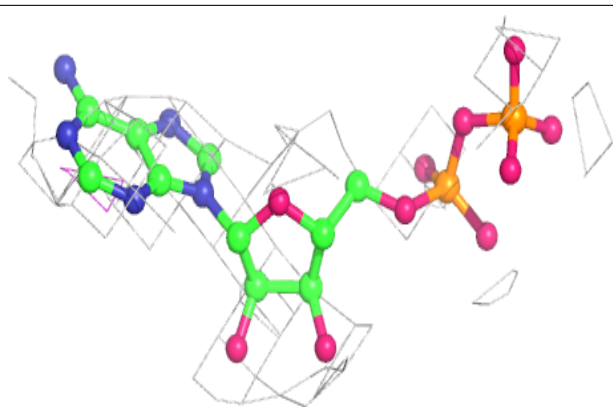
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

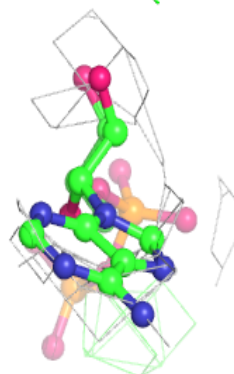
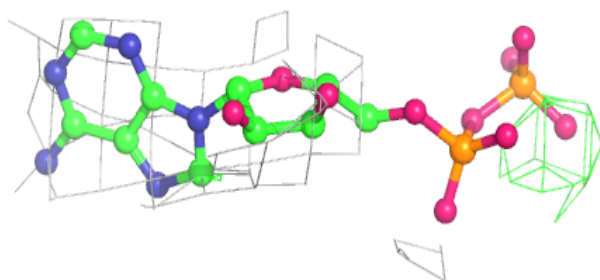
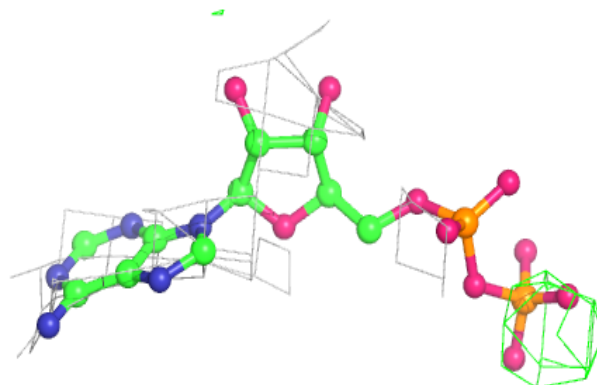


Electron density around ADP H 601:

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

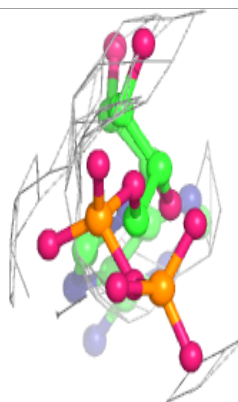
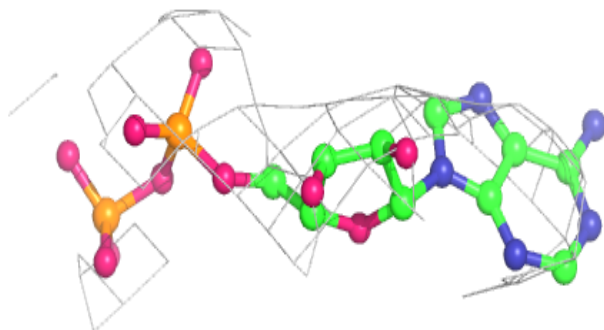
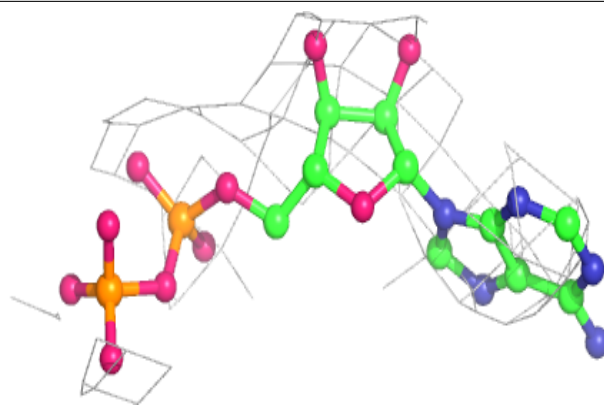
**Electron density around ADP F 601:**

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

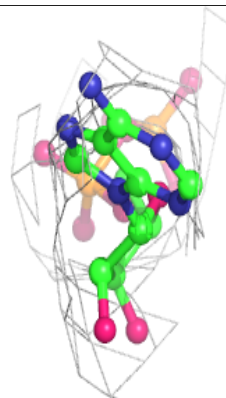
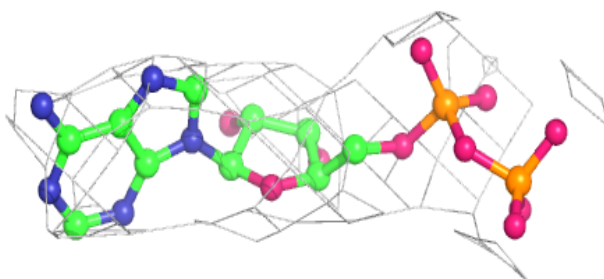
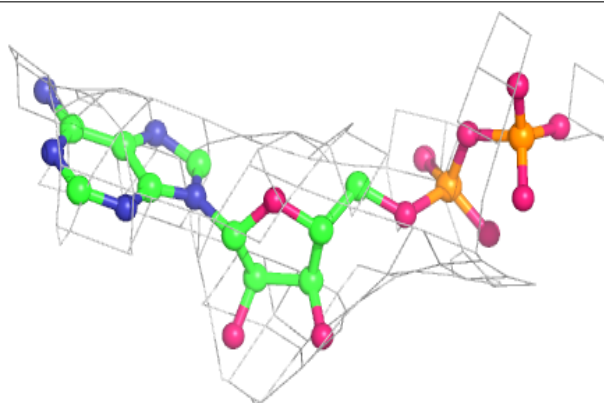


Electron density around ADP G 601:

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

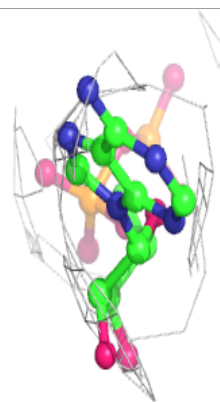
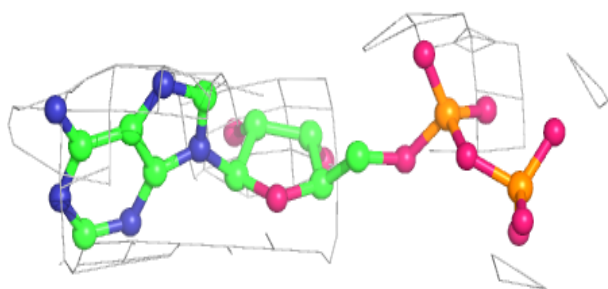
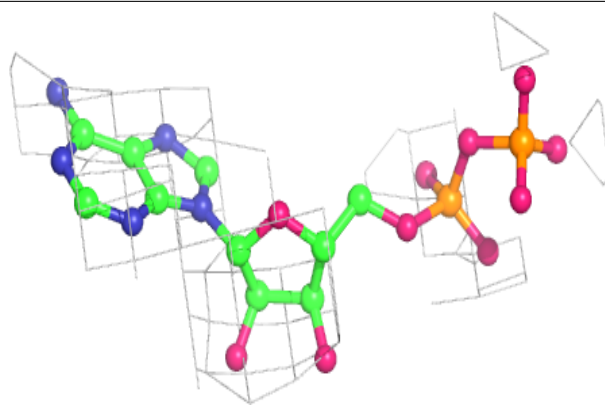
**Electron density around ADP E 601:**

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

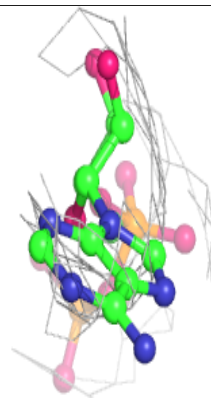
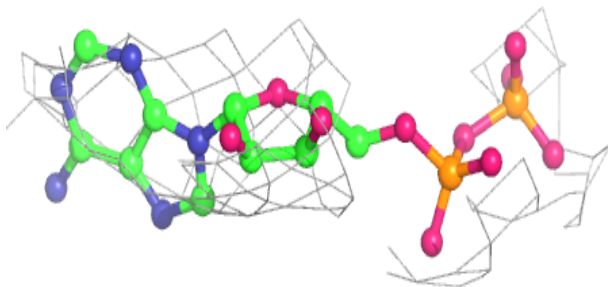
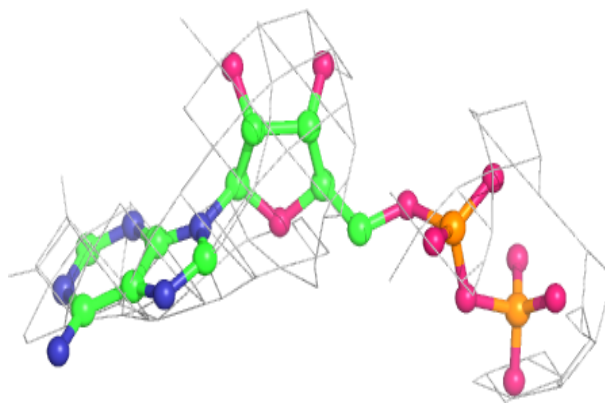


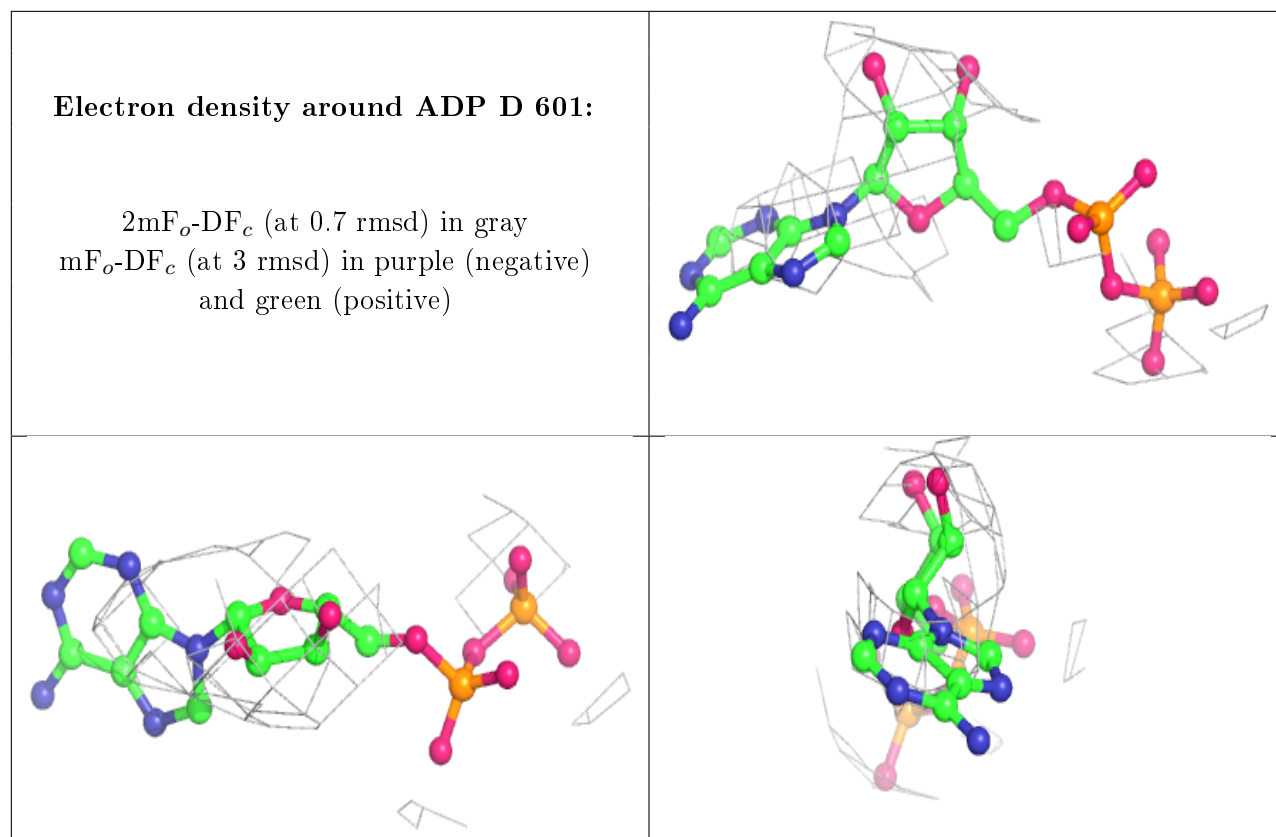
Electron density around ADP C 601:

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

**Electron density around ADP 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)





6.5 Other polymers [i](#)

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