wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 12:36 pm BST

PDB ID	:	1Z6T
Title	:	Structure of the apoptotic protease-activating factor 1 bound to ADP
Authors	:	Riedl, S.J.; Li, W.; Chao, Y.; Schwarzenbacher, R.; Shi, Y.
Deposited on	:	2005-03-23
Resolution	:	2.21 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

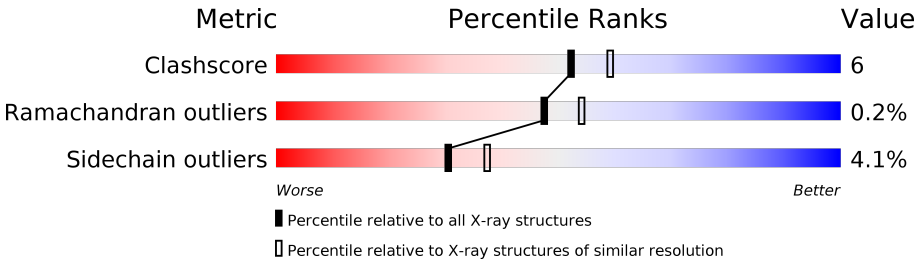
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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))
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	591	83% 13%
1	B	591	85% 12%
1	C	591	84% 14%
1	D	591	84% 12%

2 Entry composition

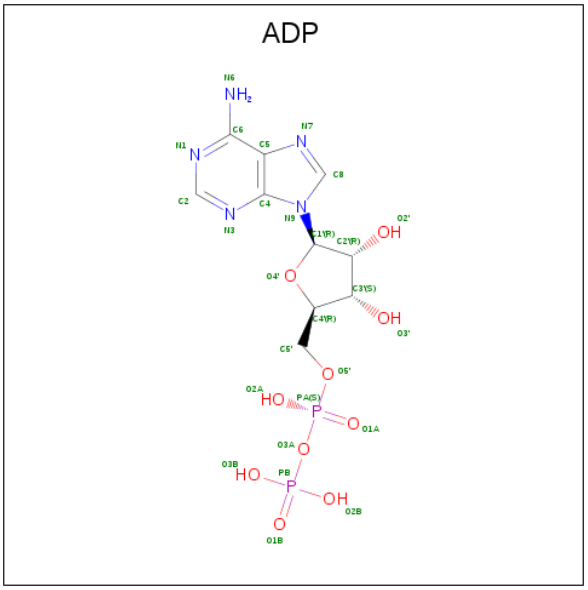
There are 3 unique types of molecules in this entry. The entry contains 19663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Apoptotic protease activating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4656	2968	795	862	31			
1	B	586	Total	C	N	O	S	0	0	0
			4720	3003	806	880	31			
1	C	586	Total	C	N	O	S	0	0	0
			4720	3003	806	880	31			
1	D	576	Total	C	N	O	S	0	0	0
			4656	2968	795	862	31			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	204	Total	O	0	0
			204	204		
3	B	220	Total	O	0	0
			220	220		
3	C	193	Total	O	0	0
			193	193		
3	D	186	Total	O	0	0
			186	186		

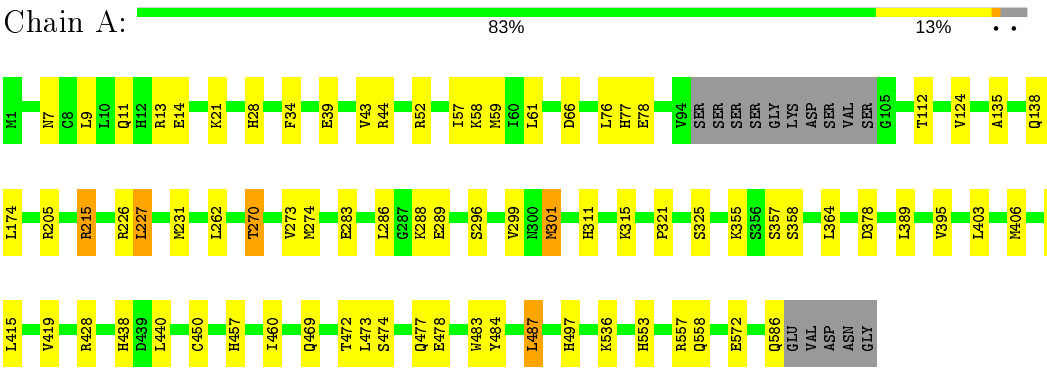
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

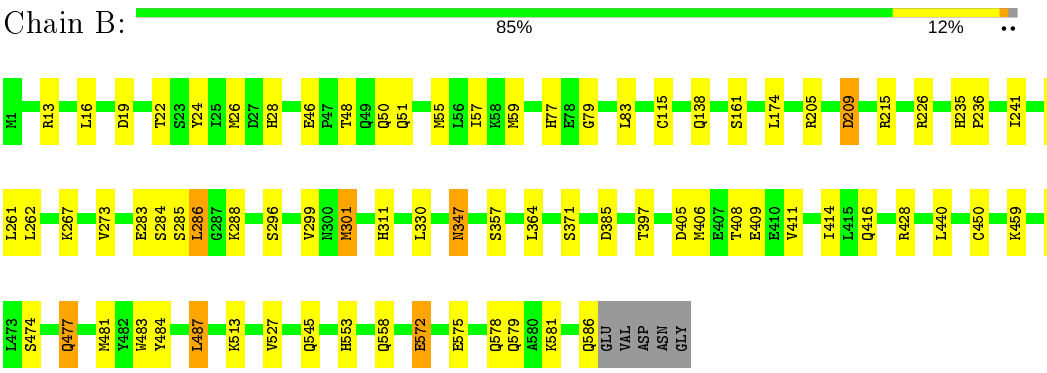
- Molecule 1: Apoptotic protease activating factor 1

Chain A:



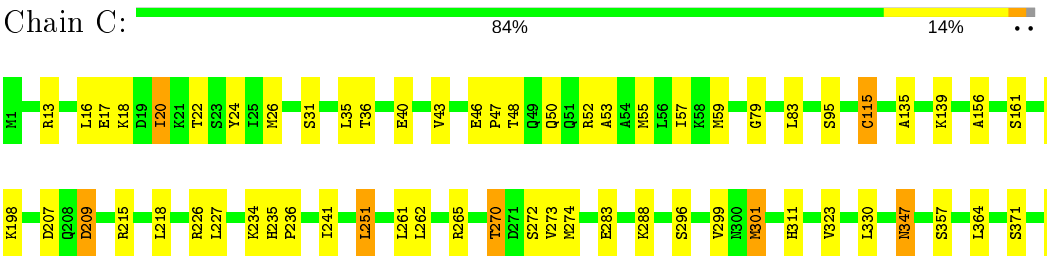
- Molecule 1: Apoptotic protease activating factor 1

Chain B:



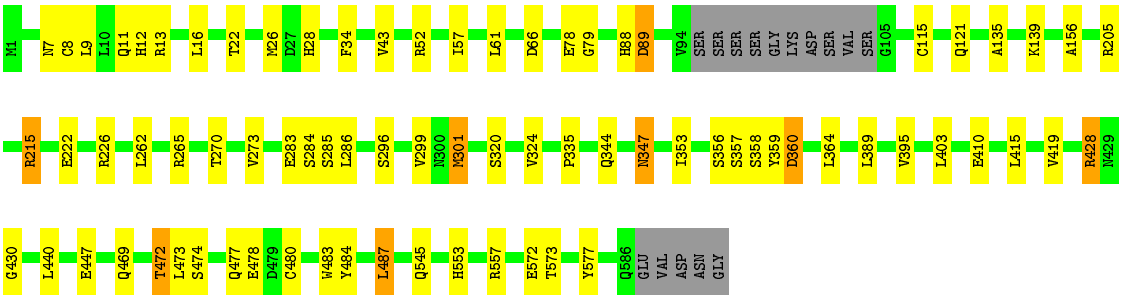
- Molecule 1: Apoptotic protease activating factor 1

Chain C:



- Molecule 1: Apoptotic protease activating factor 1

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.95Å 92.88Å 94.99Å 62.96° 89.99° 90.05°	Depositor
Resolution (Å)	15.00 – 2.21	Depositor
% Data completeness (in resolution range)	89.2 (15.00-2.21)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.189 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19663	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.63	0/4749	0.71	2/6405 (0.0%)
1	B	0.65	1/4814 (0.0%)	0.71	1/6493 (0.0%)
1	C	0.66	2/4814 (0.0%)	0.72	0/6493
1	D	0.65	0/4749	0.71	2/6405 (0.0%)
All	All	0.65	3/19126 (0.0%)	0.71	5/25796 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	450	CYS	CB-SG	8.88	1.97	1.82
1	B	450	CYS	CB-SG	6.25	1.92	1.82
1	C	569	CYS	CB-SG	-5.42	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	D	205	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	205	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	205	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	205	ARG	NE-CZ-NH2	-5.50	117.55	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4656	0	4696	54	1
1	B	4720	0	4756	51	1
1	C	4720	0	4756	59	0
1	D	4656	0	4696	51	2
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
3	A	204	0	0	13	0
3	B	220	0	0	11	0
3	C	193	0	0	8	2
3	D	186	0	0	10	0
All	All	19663	0	18952	208	3

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 6.

The worst 5 of 208 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:26:MET:SD	1:C:35:LEU:HD21	1.72	1.29
1:A:157:GLY:HA2	3:A:1076:HOH:O	1.33	1.22
1:B:55:MET:HB2	3:B:1008:HOH:O	1.40	1.16
1:D:335:PRO:O	3:D:1050:HOH:O	1.82	0.96
1:D:121:GLN:OE1	3:D:912:HOH:O	1.84	0.94

All (3) 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:D:360:ASP:OD1	3:C:1047:HOH:O[1_546]	1.97	0.23
1:D:360:ASP:OD2	3:C:1061:HOH:O[1_546]	2.10	0.10
1:A:469:GLN:NE2	1:B:357:SER:O[1_546]	2.17	0.03

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	572/591 (97%)	560 (98%)	11 (2%)	1 (0%)	47	54
1	B	584/591 (99%)	576 (99%)	8 (1%)	0	100	100
1	C	584/591 (99%)	571 (98%)	12 (2%)	1 (0%)	47	54
1	D	572/591 (97%)	558 (98%)	12 (2%)	2 (0%)	41	45
All	All	2312/2364 (98%)	2265 (98%)	43 (2%)	4 (0%)	47	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	LYS
1	D	358	SER
1	D	89	ASP
1	C	18	LYS

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	521/534 (98%)	498 (96%)	23 (4%)	28	34
1	B	530/534 (99%)	509 (96%)	21 (4%)	31	38
1	C	530/534 (99%)	506 (96%)	24 (4%)	27	33
1	D	521/534 (98%)	503 (96%)	18 (4%)	36	44
All	All	2102/2136 (98%)	2016 (96%)	86 (4%)	30	37

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	487	LEU
1	C	161	SER
1	D	403	LEU
1	B	572	GLU
1	B	586	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	521	HIS
1	B	553	HIS
1	D	153	HIS
1	B	543	ASN
1	B	586	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)

4 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	D	903	-	24,29,29	1.00	1 (4%)	29,45,45	1.29	4 (13%)
2	ADP	B	901	-	24,29,29	0.98	0	29,45,45	1.37	4 (13%)
2	ADP	C	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.27	2 (6%)
2	ADP	A	900	-	24,29,29	1.08	2 (8%)	29,45,45	1.55	5 (17%)

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	D	903	-	-	1/12/32/32	0/3/3/3
2	ADP	B	901	-	-	1/12/32/32	0/3/3/3
2	ADP	C	902	-	-	1/12/32/32	0/3/3/3
2	ADP	A	900	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	903	ADP	C5-C4	2.44	1.47	1.40
2	A	900	ADP	C5-C4	2.20	1.46	1.40
2	C	902	ADP	C5-C4	2.19	1.46	1.40
2	A	900	ADP	O4'-C1'	2.12	1.44	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	902	ADP	N3-C2-N1	-4.02	122.39	128.68
2	B	901	ADP	N3-C2-N1	-3.84	122.67	128.68
2	A	900	ADP	N3-C2-N1	-3.72	122.87	128.68
2	D	903	ADP	N3-C2-N1	-3.24	123.61	128.68
2	A	900	ADP	O3B-PB-O2B	3.22	119.93	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	ADP	PA-O3A-PB-O2B
2	C	902	ADP	PA-O3A-PB-O2B
2	D	903	ADP	PA-O3A-PB-O2B

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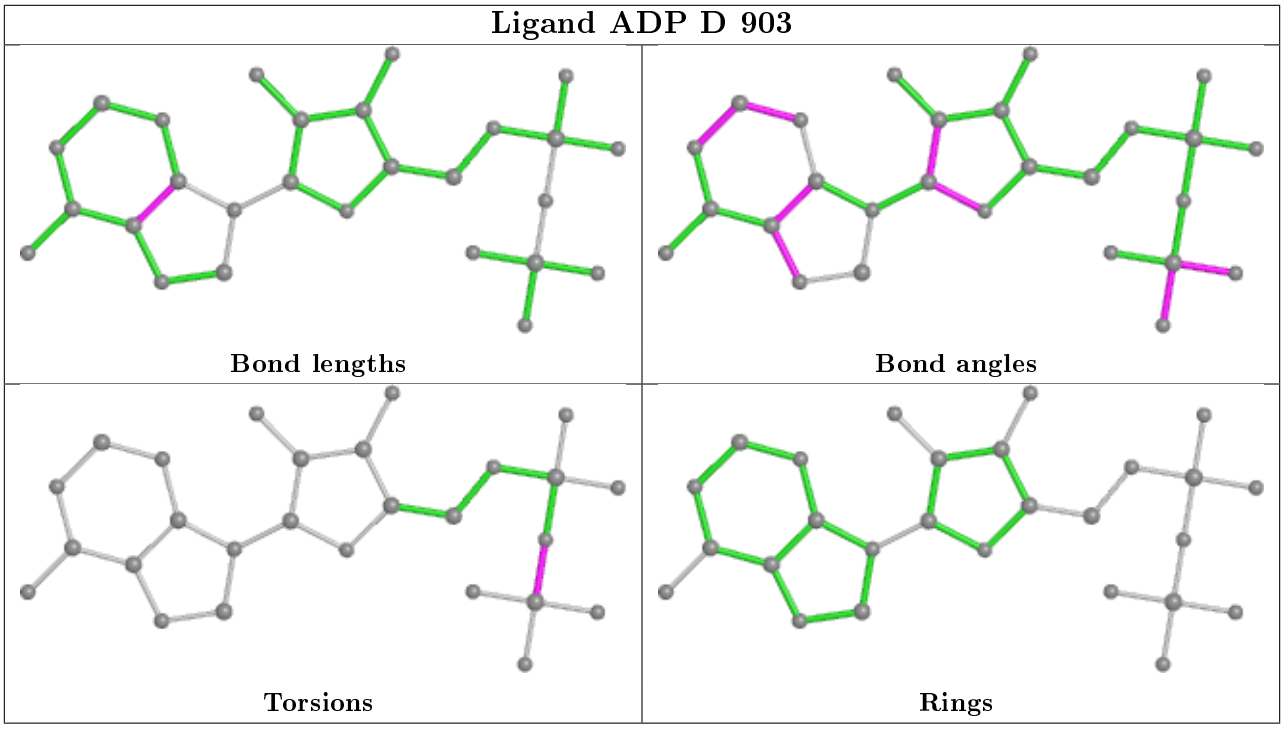
Mol	Chain	Res	Type	Atoms
2	B	901	ADP	PA-O3A-PB-O2B

There are no ring outliers.

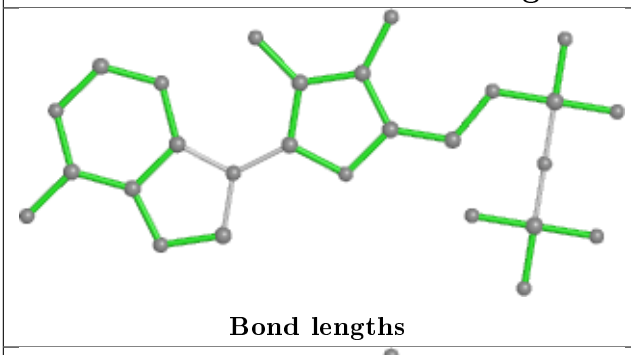
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	ADP	1	0

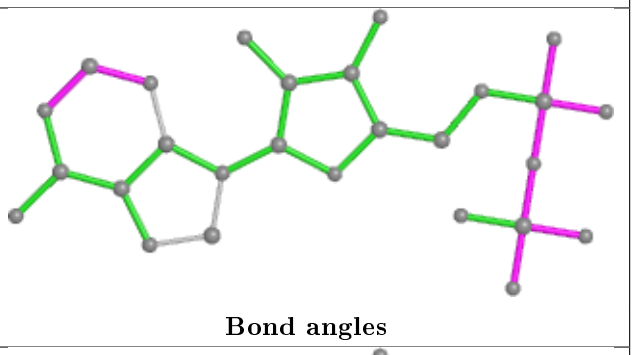
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



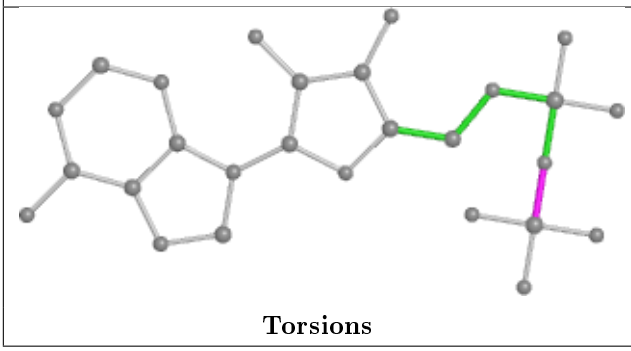
Ligand ADP B 901



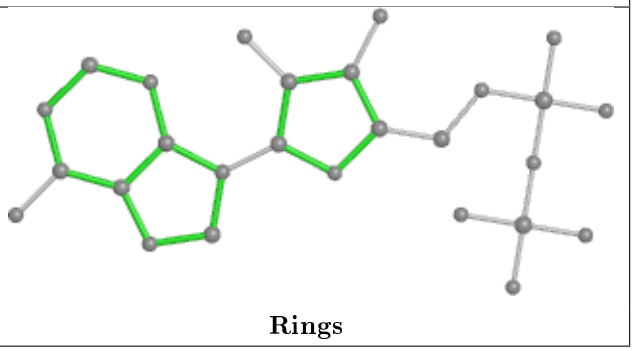
Bond lengths



Bond angles

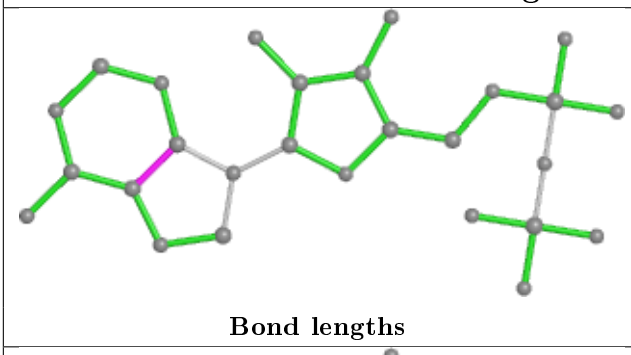


Torsions

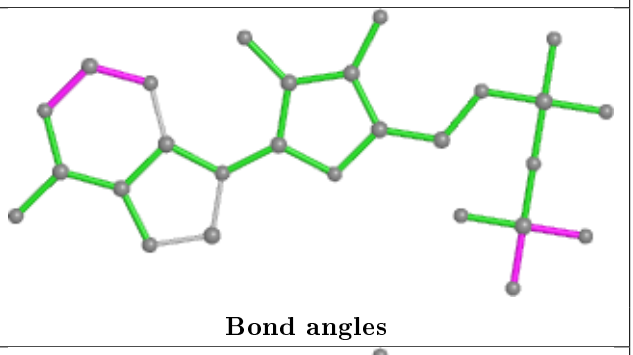


Rings

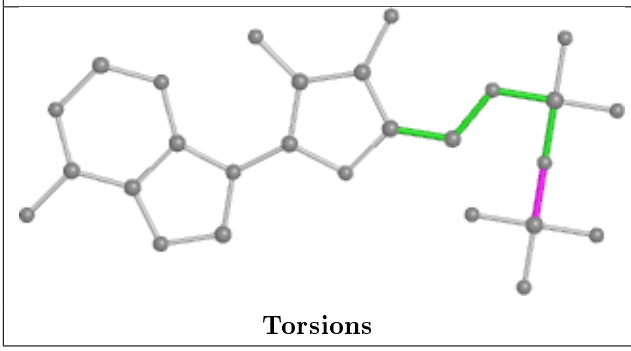
Ligand ADP C 902



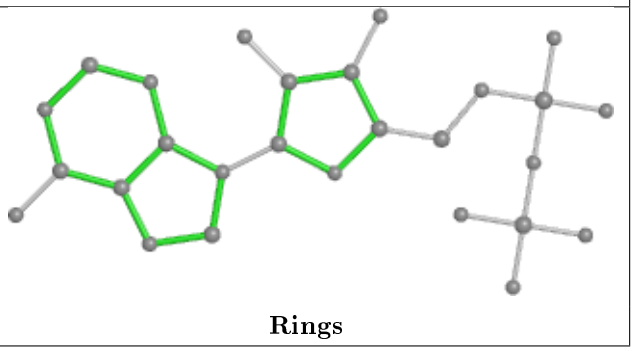
Bond lengths



Bond angles

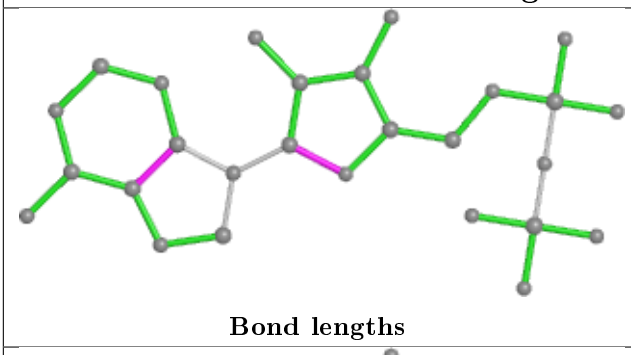


Torsions

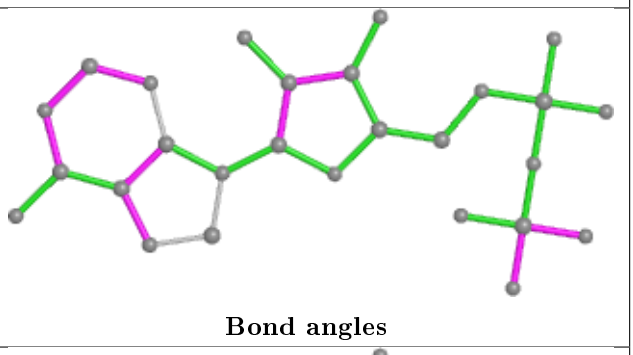


Rings

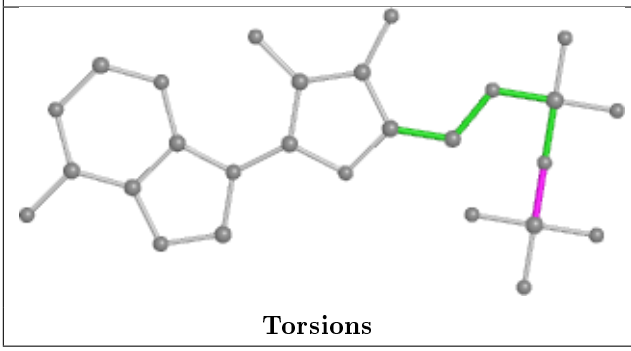
Ligand ADP A 900



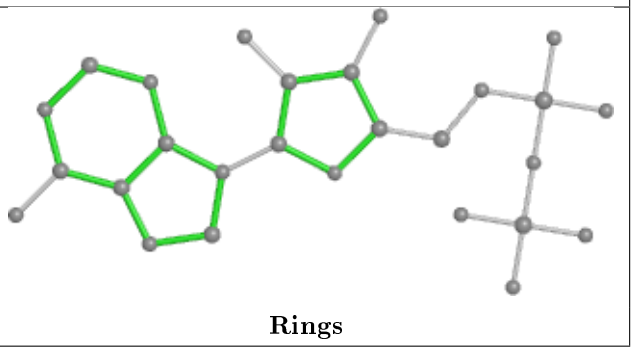
Bond lengths



Bond angles



Torsions



Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.