



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 05:01 PM EDT

PDB ID : 1AD5
Title : SRC FAMILY KINASE HCK-AMP-PNP COMPLEX
Authors : Sicheri, F.; Moarefi, I.; Kuriyan, J.
Deposited on : 1997-02-20
Resolution : 2.60 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 types of validation reports are described at

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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

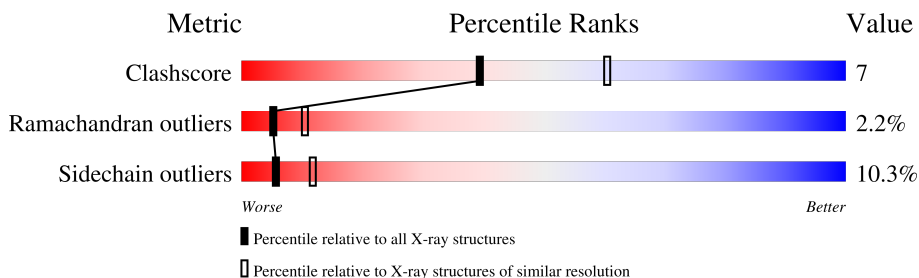
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)

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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	438	 72% 23% . .
1	B	438	 69% 26% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8572 atoms, of which 1536 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 HAEMATOPHOETIC CELL KINASE HCK.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	P	S		0	0	0
			4253	2232	768	585	647	1	20				
1	B	438	Total	C	H	N	O	P	S		0	0	0
			4253	2232	768	585	647	1	20				

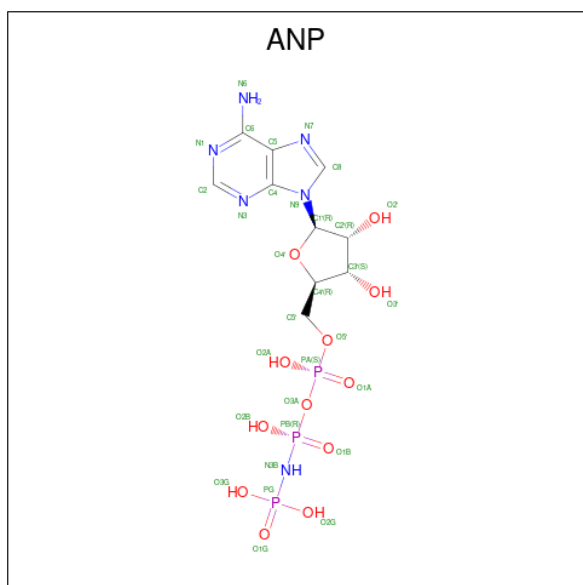
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	?	-	ASP	deletion	UNP P08631
A	?	-	ASN	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	?	-	TYR	deletion	UNP P08631
A	?	-	THR	deletion	UNP P08631
A	?	-	ALA	deletion	UNP P08631
A	?	-	ARG	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	527	PTR	TYR	modified residue	UNP P08631
B	?	-	ILE	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	?	-	ASP	deletion	UNP P08631
B	?	-	ASN	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	?	-	TYR	deletion	UNP P08631
B	?	-	THR	deletion	UNP P08631
B	?	-	ALA	deletion	UNP P08631
B	?	-	ARG	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	527	PTR	TYR	modified residue	UNP P08631

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



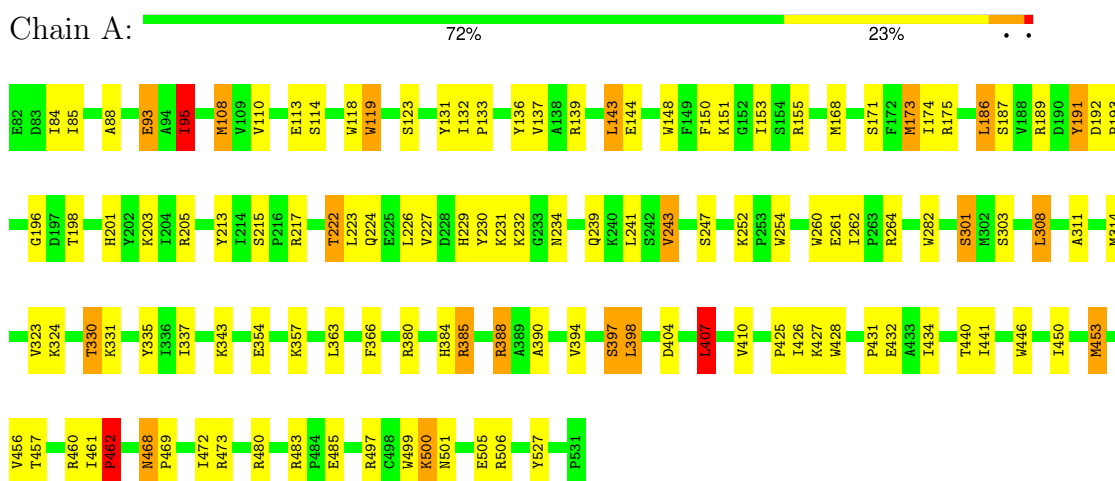
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 10 6 12 3	0	0
3	B	1	Total C N O P 31 10 6 12 3	0	0

3 Residue-property plots

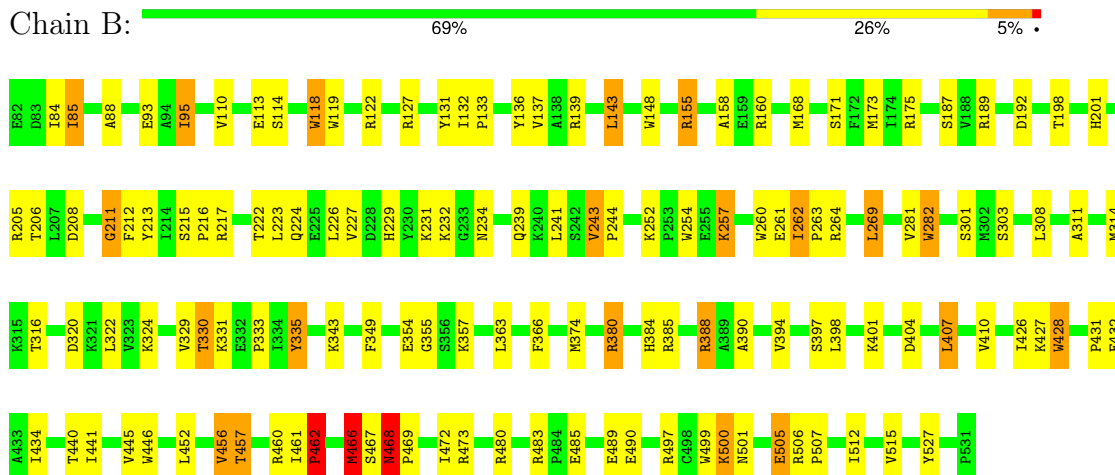
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: HAEMATOPHOETIC CELL KINASE HCK



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.77Å 92.36Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60	Depositor
% Data completeness (in resolution range)	79.4 (18.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.239 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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: CA, PTR, ANP

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	0.92	0/3552	1.62	61/4799 (1.3%)
1	B	0.93	0/3552	1.64	68/4799 (1.4%)
All	All	0.93	0/7104	1.63	129/9598 (1.3%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	TYR	CB-CG-CD2	-9.32	115.41	121.00
1	A	118	TRP	CD1-CG-CD2	9.27	113.72	106.30
1	B	260	TRP	CD1-CG-CD2	9.19	113.65	106.30
1	B	499	TRP	CD1-CG-CD2	9.08	113.57	106.30
1	B	282	TRP	CD1-CG-CD2	9.02	113.52	106.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	192	ASP	Peptide

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	3485	768	3422	45	0
1	B	3485	768	3421	49	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	2	0
All	All	7036	1536	6869	92	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 7.

The worst 5 of 92 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:203:LYS:HD3	1:B:489:GLU:HG3	1.62	0.82
1:B:427:LYS:HD3	1:B:462:PRO:HB2	1.60	0.82
1:A:427:LYS:HD3	1:A:462:PRO:HB2	1.64	0.78
1:B:457:THR:HB	1:B:460:ARG:HB3	1.78	0.64
1:A:457:THR:HB	1:A:460:ARG:HB3	1.80	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/438 (99%)	392 (90%)	32 (7%)	9 (2%)	5	11
1	B	433/438 (99%)	390 (90%)	33 (8%)	10 (2%)	5	10
All	All	866/876 (99%)	782 (90%)	65 (8%)	19 (2%)	5	10

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	PRO
1	A	468	ASN
1	A	501	ASN
1	B	208	ASP
1	B	462	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	369/382 (97%)	331 (90%)	38 (10%)	6	12
1	B	369/382 (97%)	331 (90%)	38 (10%)	6	12
All	All	738/764 (97%)	662 (90%)	76 (10%)	6	12

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	262	ILE
1	B	466	MET
1	B	308	LEU
1	B	431	PRO
1	B	505	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	201	HIS
1	A	391	ASN
1	B	201	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	PTR	B	527	2,1	15,16,17	0.95	1 (6%)	17,22,24	1.22	2 (11%)
1	PTR	A	527	2,1	15,16,17	1.06	1 (6%)	17,22,24	1.11	0

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
1	PTR	B	527	2,1	-	2/10/11/13	0/1/1/1
1	PTR	A	527	2,1	-	2/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	OH-CZ	2.48	1.46	1.40
1	B	527	PTR	P-O3P	-2.20	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	PTR	CE2-CZ-CE1	2.44	123.72	120.16
1	B	527	PTR	CD2-CG-CD1	2.08	121.33	118.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	PTR	CZ-OH-P-O1P
1	B	527	PTR	CZ-OH-P-O1P
1	A	527	PTR	N-CA-CB-CG
1	B	527	PTR	CZ-OH-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
3	ANP	B	532	2	29,33,33	1.40	6 (20%)	31,52,52	1.82	6 (19%)
3	ANP	A	1	2	29,33,33	1.42	6 (20%)	31,52,52	1.79	7 (22%)

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
3	ANP	B	532	2	-	2/14/38/38	0/3/3/3
3	ANP	A	1	2	-	1/14/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	ANP	PB-O3A	-3.32	1.54	1.59
3	B	532	ANP	PB-O2B	-2.96	1.48	1.56
3	A	1	ANP	PG-O3G	-2.90	1.49	1.56
3	B	532	ANP	PG-O2G	-2.83	1.49	1.56
3	A	1	ANP	PG-O2G	-2.77	1.49	1.56

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	532	ANP	O1G-PG-N3B	-5.72	103.35	111.77
3	A	1	ANP	O1G-PG-N3B	-5.71	103.36	111.77
3	B	532	ANP	O2B-PB-O1B	4.28	119.05	109.87
3	A	1	ANP	O2B-PB-O1B	4.04	118.53	109.87
3	B	532	ANP	O3A-PB-N3B	-2.89	98.57	106.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	ANP	PB-N3B-PG-O1G
3	B	532	ANP	PB-N3B-PG-O1G
3	B	532	ANP	PG-N3B-PB-O1B

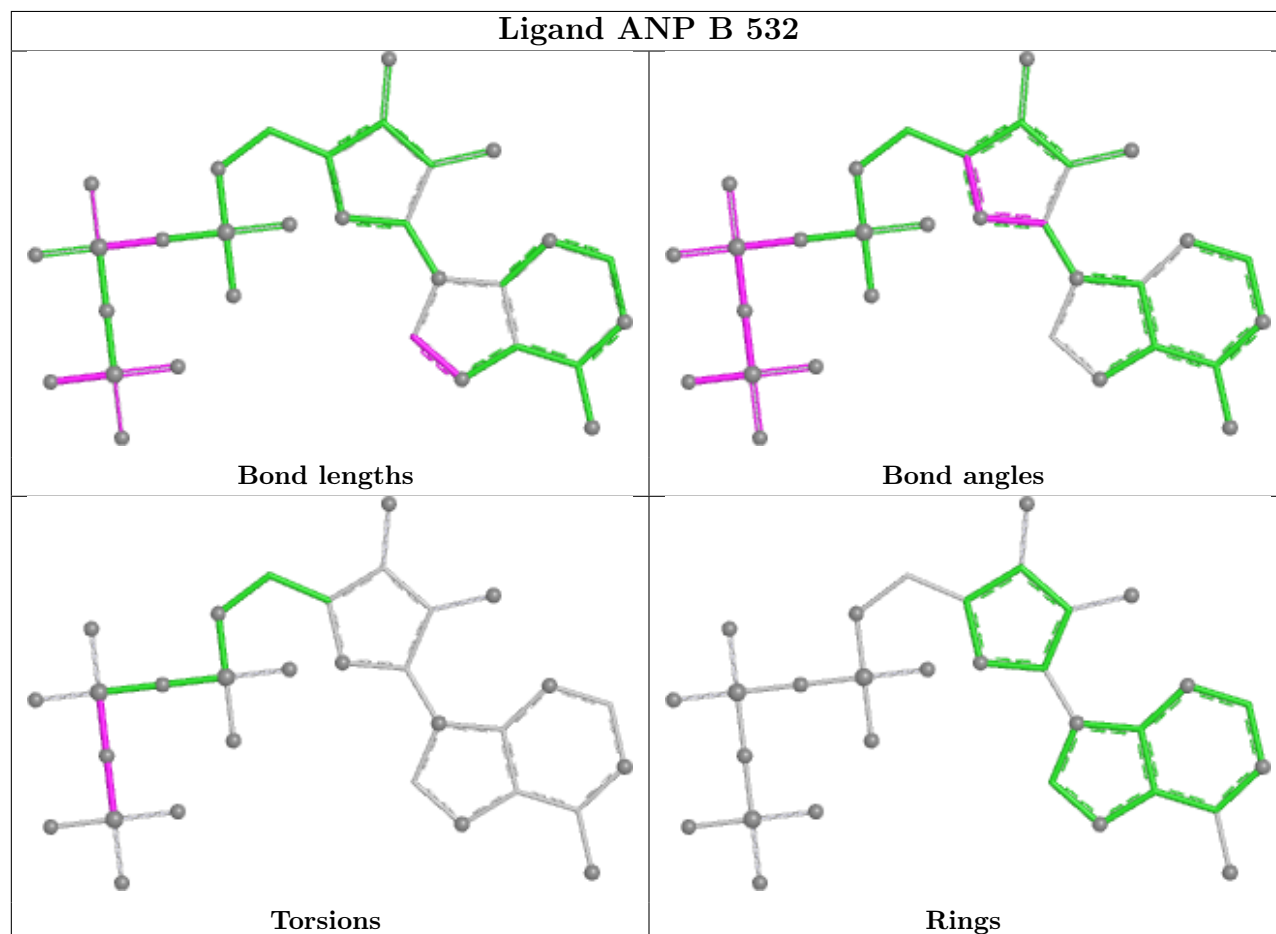
There are no ring outliers.

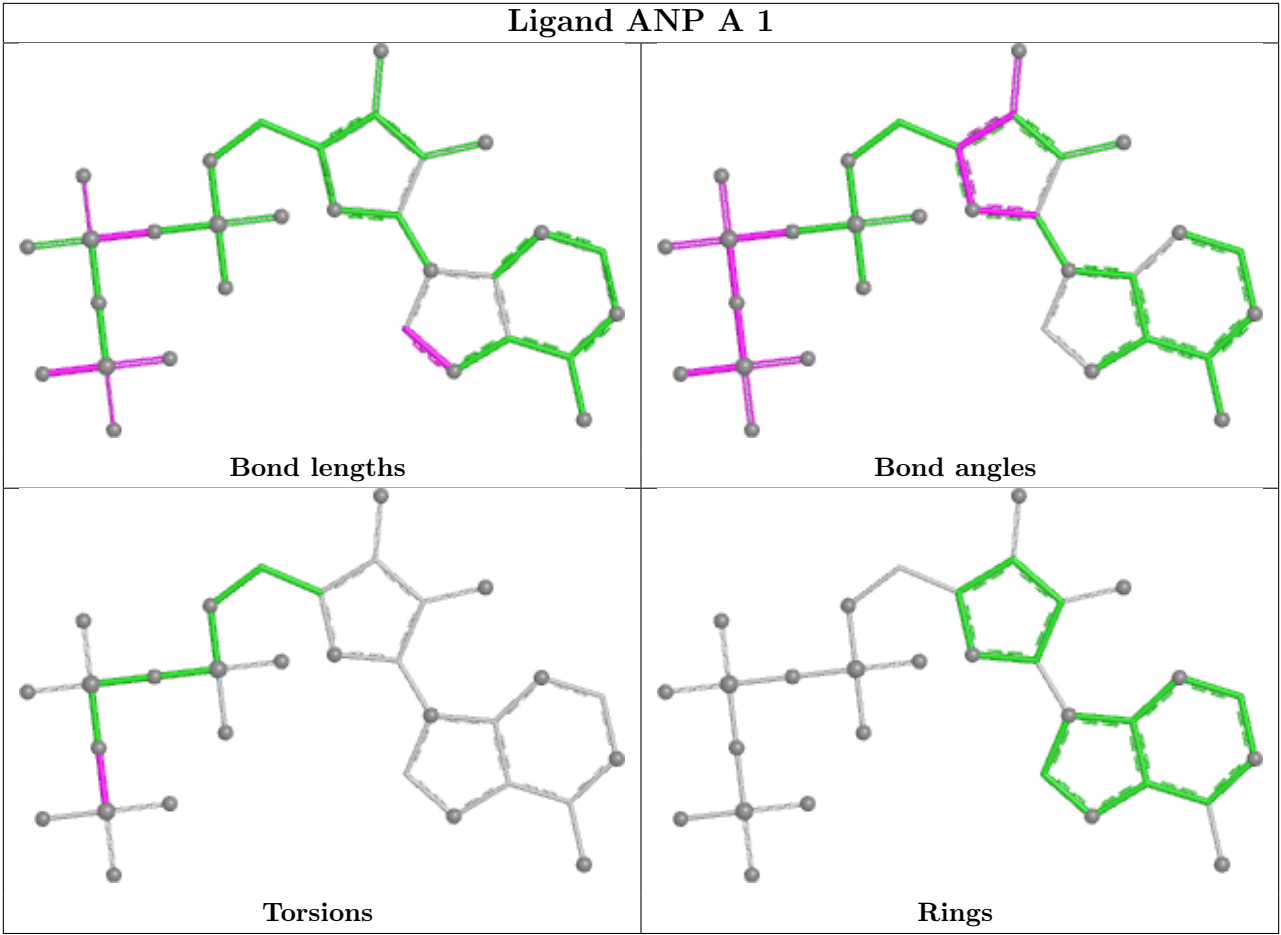
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	532	ANP	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	411:GLY	C	422:ALA	N	8.62
1	B	411:GLY	C	422:ALA	N	8.58

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.