



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 1UN9 / pdb_00001un9
Title : Crystal structure of the dihydroxyacetone kinase from *C. freundii* in complex with AMP-PNP and Mg²⁺
Authors : Siebold, C.; Arnold, I.; Garcia-Alles, L.F.; Baumann, U.; Erni, B.
Deposited on : 2003-09-08
Resolution : 3.10 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

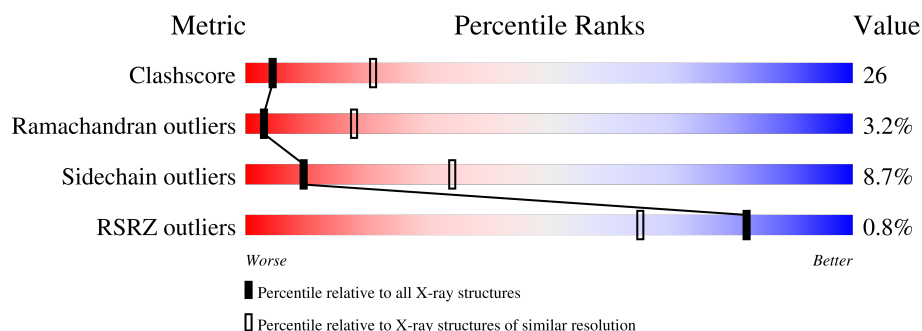
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	552	% 53% 39% 5% .
1	B	552	% 52% 40% . . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7982 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.

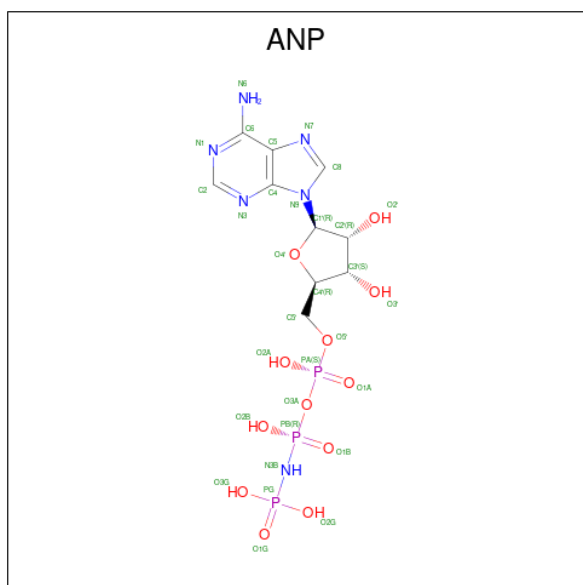
- Molecule 1 is a protein called DIHYDROXYACETONE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			3952	2481	692	761	18			
1	B	537	Total	C	N	O	S	0	0	0
			3952	2481	692	761	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	MET	conflict	UNP P45510
A	538	ALA	ARG	conflict	UNP P45510
B	1	ALA	MET	conflict	UNP P45510
B	538	ALA	ARG	conflict	UNP P45510

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

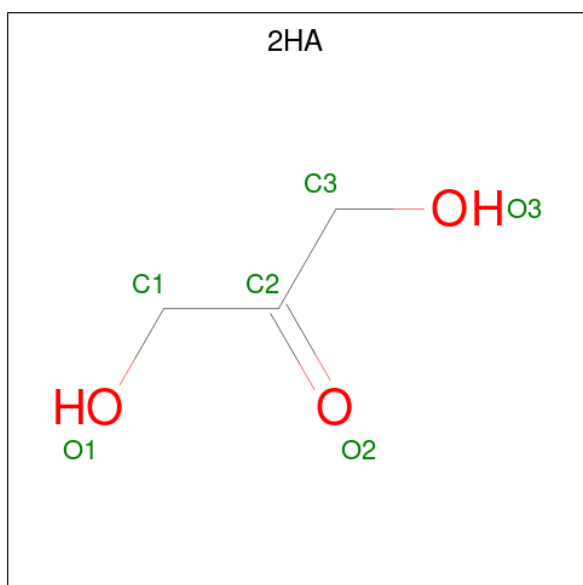


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is Dihydroxyacetone (CCD ID: 2HA) (formula: C₃H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

TVR	LEU	G433	S341	A192
	SER	V434	S342	E268
	SER	L435	R343	S194
	GLU	M436	A344	S195
	SER	S437	S345	C196
	LEU	I438	R347	P199
	L529	Q445	V348	Q200
	GE30	K446	E349	E275
	N531	L447	S353	L276
	M532	E448	L357	S279
A536	Q449	F358	P280	A204
	Q537	G450	L281	A205
	A538	V453	R282	P206
	L539	V454	A359	R207
	V542	G460	S283	P210
	F543	L461	R284	L215
	K544	M464	V362	M217
	E548	Y467	T366	G218
	S549	G468	L372	I219
	E550	M477	E373	H220
GLY	LEU	T475	L376	G221
	GLY	T476	L377	G221
		M478	A393	E222
		T479	A394	P223
		I477	A395	G224
		L481	A396	A225
		Q482	R397	S226
		P483	E398	V227
		L489	I399	I228
		A490	S401	L310
Q491	Q491	L402	K316	T230
	P492	L403	A317	Q231
	R493	H404	L318	A234
	N494	K405	L319	Q235
		Q406	E321	V236
		Q407	V322	V237
		L408	E323	R238
		A497	T324	L239
		A498	L410	M240
		F499	N411	V241
A506		N412	L244	
		L413	L245	
		C510		
		S513		
		K514		
		A515		
	ASN			
	ALA			
	GLY			
	ARG			
SER	ALA	M428	L264	
	SER	G429	V266	
		I420		
		G421		
		E422		
		R423		
		L424		
		T425		
		V426		
		V427		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.79Å 124.87Å 236.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.10 25.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.1 (25.00-3.10) 93.5 (25.00-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , (Not available) 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7982	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 2HA

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	0.59	1/4015 (0.0%)	1.11	15/5459 (0.3%)
1	B	0.58	1/4015 (0.0%)	1.10	18/5459 (0.3%)
All	All	0.58	2/8030 (0.0%)	1.10	33/10918 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	GLY	N-CA	5.22	1.51	1.45
1	B	210	PRO	N-CD	5.17	1.54	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLU	CA-C-N	-20.09	94.73	119.84
1	A	62	GLU	C-N-CA	-20.09	94.73	119.84
1	B	62	GLU	CA-C-N	-18.78	96.37	119.84
1	B	62	GLU	C-N-CA	-18.78	96.37	119.84
1	B	62	GLU	N-CA-C	18.42	150.52	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	GLU	Peptide
1	B	62	GLU	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	3952	0	3978	227	1
1	B	3952	0	3978	219	0
2	A	31	0	13	5	0
2	B	31	0	13	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	6	0	6	1	0
4	B	6	0	6	1	0
All	All	7982	0	7994	422	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 26.

The worst 5 of 422 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:B:133:GLU:HA	1:B:133:GLU:OE1	1.29	1.08
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.13	1.07
1:B:133:GLU:HG3	1:B:176:LEU:HD22	1.35	1.03
1:A:127:ARG:HH11	1:A:127:ARG:CG	1.74	0.99
1:A:348:VAL:HG23	1:B:127:ARG:HH22	1.30	0.96

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:A:342:SER:CB	1:A:342:SER:CB[3_656]	2.08	0.12

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	533/552 (97%)	459 (86%)	56 (10%)	18 (3%)	3	16
1	B	533/552 (97%)	461 (86%)	56 (10%)	16 (3%)	3	19
All	All	1066/1104 (97%)	920 (86%)	112 (10%)	34 (3%)	3	18

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	153	ALA
1	B	62	GLU
1	B	153	ALA
1	A	48	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	414/425 (97%)	378 (91%)	36 (9%)	9	34
1	B	414/425 (97%)	378 (91%)	36 (9%)	9	34
All	All	828/850 (97%)	756 (91%)	72 (9%)	9	34

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	402	LEU

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Mol	Chain	Res	Type
1	B	539	LEU
1	B	422	GLU
1	B	445	GLN
1	A	425	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	ASN
1	B	343	HIS
1	B	180	GLN
1	B	375	HIS
1	A	208	HIS

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 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
2	ANP	A	1551	3	33,33,33	2.91	11 (33%)	45,52,52	1.68	9 (20%)
4	2HA	B	1554	-	5,5,5	5.55	1 (20%)	4,5,5	4.97	2 (50%)
4	2HA	A	1554	-	5,5,5	5.35	1 (20%)	4,5,5	5.35	2 (50%)
2	ANP	B	1551	3	33,33,33	2.88	11 (33%)	45,52,52	1.83	11 (24%)

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	ANP	A	1551	3	-	5/18/38/38	0/3/3/3
4	2HA	B	1554	-	-	2/4/4/4	-
4	2HA	A	1554	-	-	2/4/4/4	-
2	ANP	B	1551	3	-	3/18/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1554	2HA	O2-C2	12.28	1.43	1.21
4	A	1554	2HA	O2-C2	11.91	1.42	1.21
2	B	1551	ANP	PB-O1B	8.69	1.59	1.46
2	B	1551	ANP	PG-O1G	8.65	1.59	1.46
2	A	1551	ANP	PG-O1G	8.56	1.59	1.46

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1554	2HA	O2-C2-C3	-8.27	107.70	120.91
4	A	1554	2HA	O2-C2-C3	-7.78	108.48	120.91
4	A	1554	2HA	O2-C2-C1	-7.24	109.34	120.91
4	B	1554	2HA	O2-C2-C1	-5.44	112.22	120.91
2	B	1551	ANP	C5-C4-N9	4.57	110.79	105.81

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1551	ANP	PG-N3B-PB-O1B
2	A	1551	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	B	1551	ANP	PB-N3B-PG-O1G
4	A	1554	2HA	O1-C1-C2-O2
4	A	1554	2HA	O2-C2-C3-O3

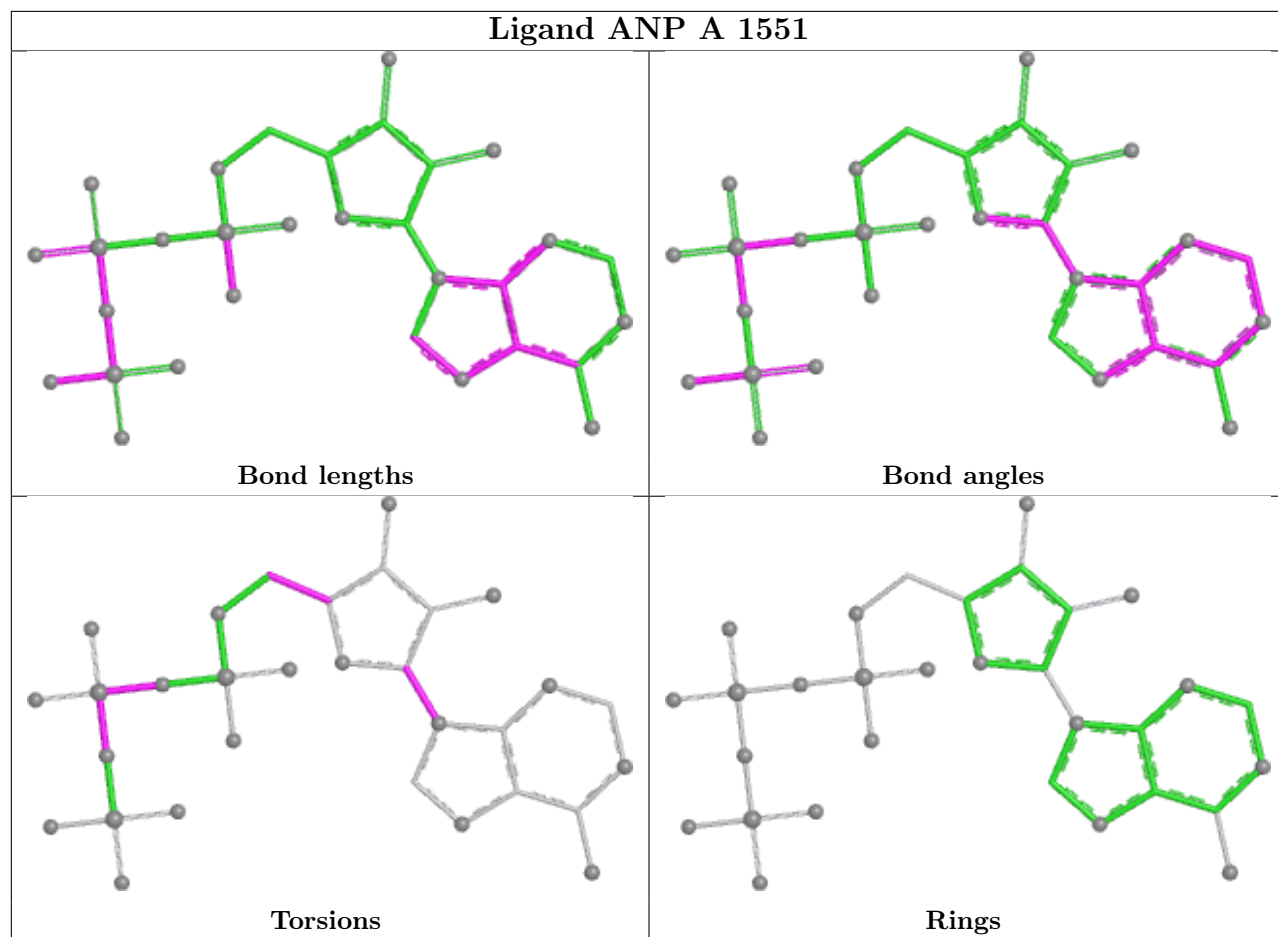
There are no ring outliers.

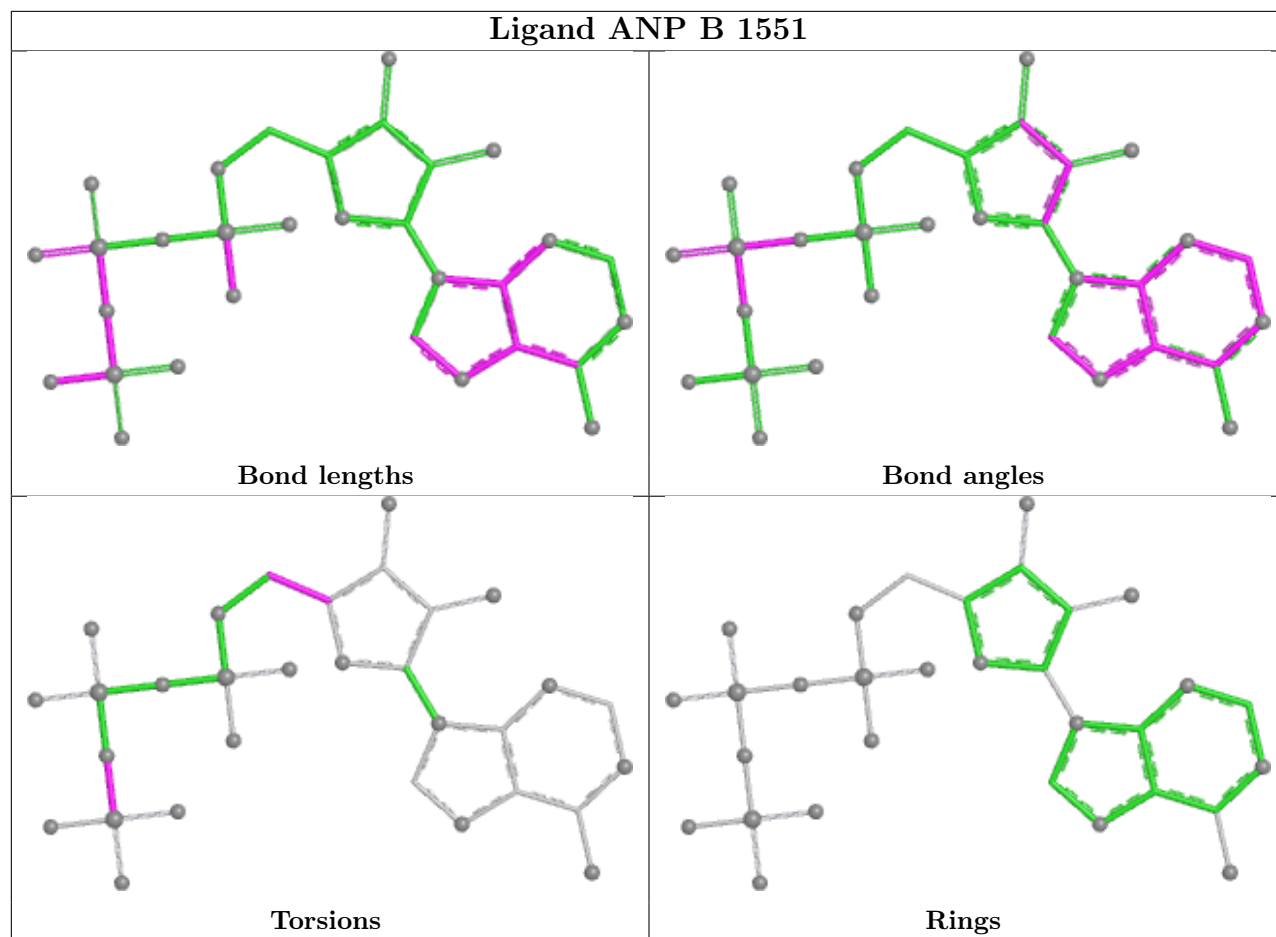
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1551	ANP	5	0
4	B	1554	2HA	1	0
4	A	1554	2HA	1	0
2	B	1551	ANP	3	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 ANP A 1551





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, 95th 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 ²)	Q<0.9
1	A	537/552 (97%)	0.09	5 (0%)	81 63	14, 86, 114, 146	0
1	B	537/552 (97%)	0.17	4 (0%)	84 68	14, 90, 113, 139	0
All	All	1074/1104 (97%)	0.13	9 (0%)	82 65	14, 88, 114, 146	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	GLY	3.3
1	B	70	GLY	3.2
1	A	70	GLY	2.6
1	A	529	LEU	2.6
1	A	62	GLU	2.5

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](#)

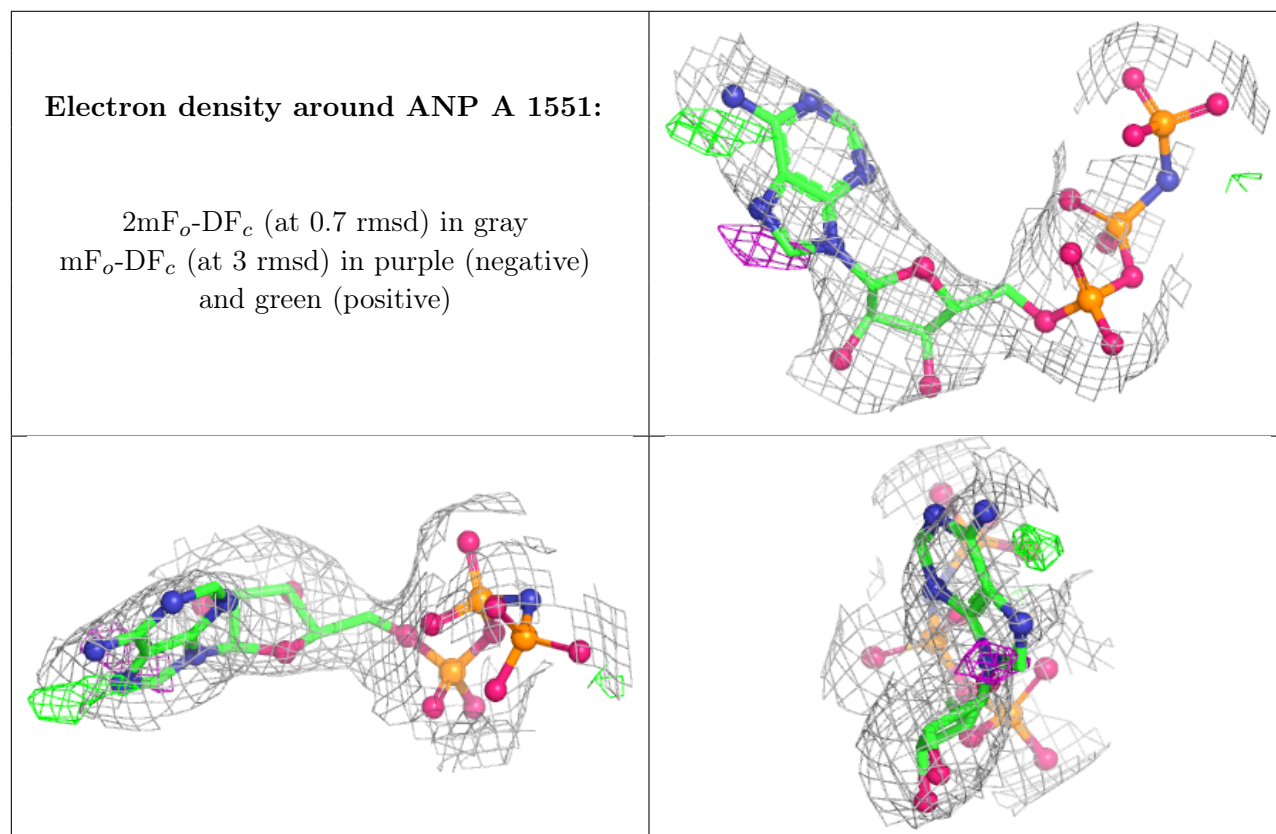
There are no oligosaccharides in this entry.

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, 95th 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.

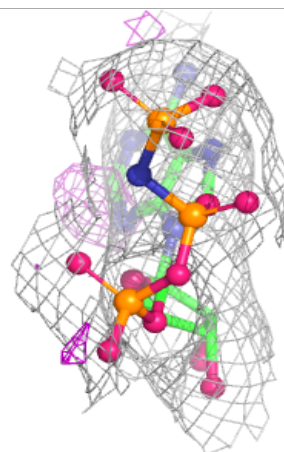
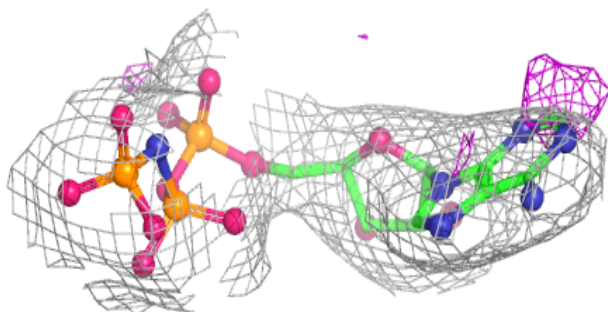
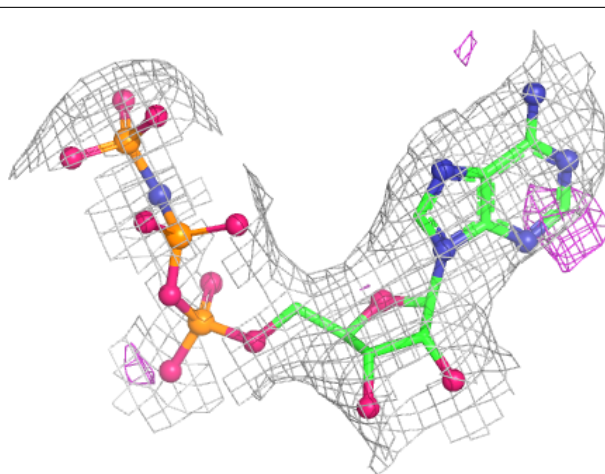
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1553	1/1	0.77	0.09	76,76,76,76	0
3	MG	B	1553	1/1	0.89	0.10	100,100,100,100	0
4	2HA	B	1554	6/6	0.90	0.13	12,16,16,17	0
2	ANP	A	1551	31/31	0.92	0.09	59,64,77,79	0
4	2HA	A	1554	6/6	0.93	0.12	12,15,17,17	0
3	MG	A	1552	1/1	0.93	0.05	90,90,90,90	0
2	ANP	B	1551	31/31	0.94	0.07	50,57,70,72	0
3	MG	B	1552	1/1	0.99	0.05	65,65,65,65	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 ANP B 1551:

$2mF_o-DF_c$ (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.