



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:39 pm BST

PDB ID : 2J9G
Title : Crystal structure of Biotin carboxylase from E. coli in complex with AMPPNP and ADP
Authors : Mochalkin, I.
Deposited on : 2008-03-21
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

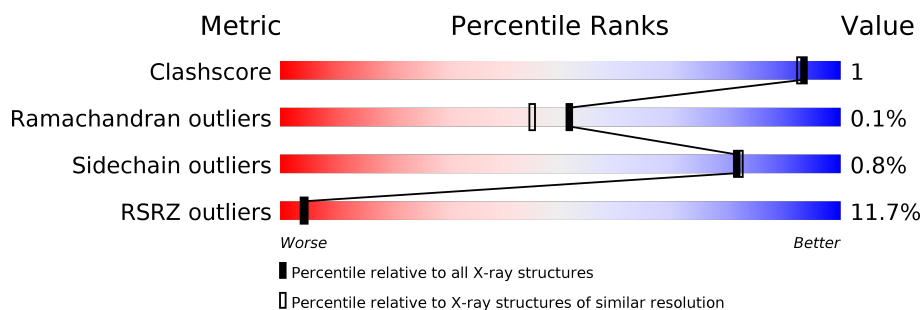
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 $\leq 5\%$. 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	449	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>
1	B	449	<div> <div>17%</div> <div>94%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7604 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 BIOTIN CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	3	0
			3441	2166	616	637	22			
1	B	442	Total	C	N	O	S	8	3	1
			3424	2156	612	634	22			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

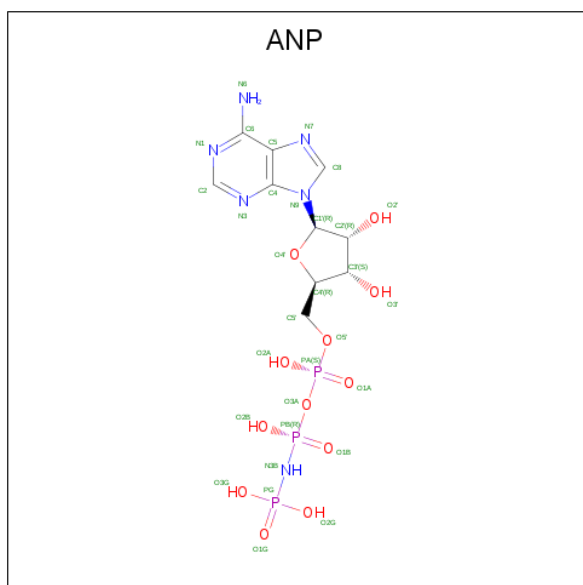
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

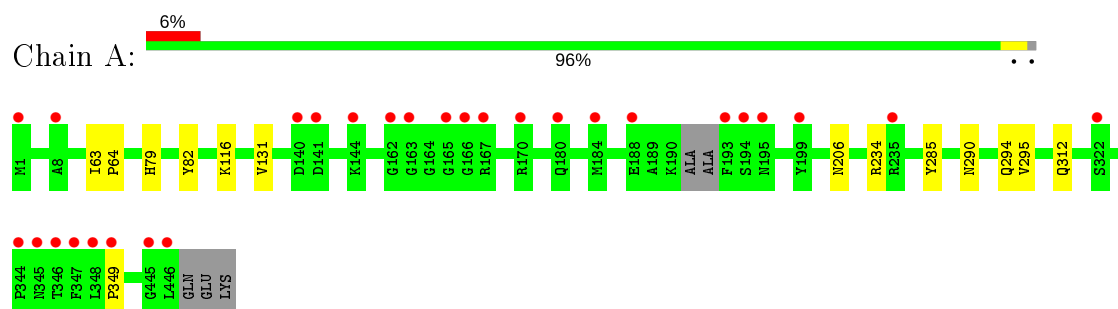
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	367	Total	O	0	0
			367	367		
6	B	302	Total	O	0	0
			302	302		

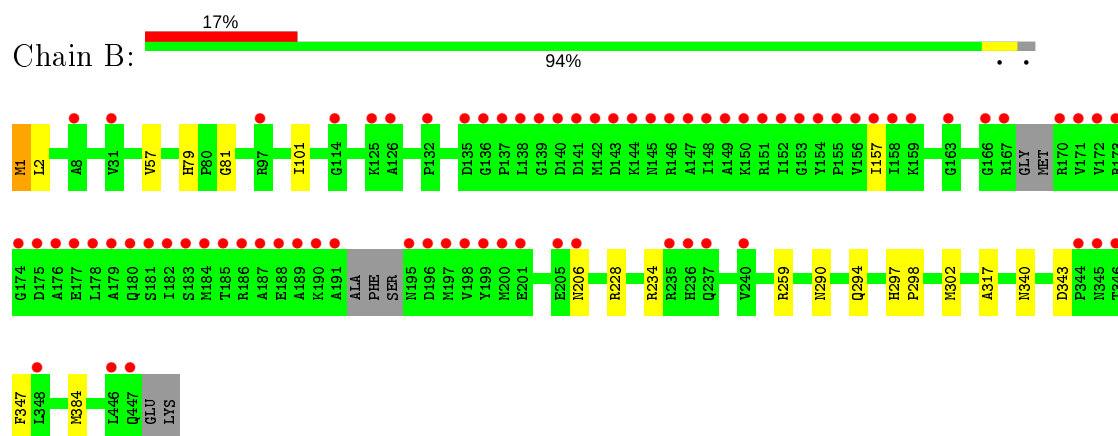
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: BIOTIN CARBOXYLASE



• Molecule 1: BIOTIN CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.70Å 112.25Å 121.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.48 – 2.05 22.19 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (82.48-2.05) 97.2 (22.19-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.236 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	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	0.94	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, SO4, 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	0.36	0/3513	0.54	0/4738
1	B	0.37	0/3484	0.54	0/4700
All	All	0.36	0/6997	0.54	0/9438

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

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	3441	0	3464	8	0
1	B	3424	0	3449	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	31	0	13	3	0
5	B	27	0	12	0	0
6	A	367	0	0	0	0
6	B	302	0	0	3	0
All	All	7604	0	6938	20	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 1.

All (20) 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:79:HIS:HD1	1:B:81:GLY:H	1.44	0.63
1:A:116:LYS:HZ1	4:A:1449:ANP:PB	2.28	0.56
1:B:228:ARG:HH21	1:B:294:GLN:NE2	2.03	0.56
1:A:116:LYS:NZ	4:A:1449:ANP:PB	2.78	0.56
1:A:79:HIS:HE2	1:A:312:GLN:NE2	2.05	0.55
1:B:157:ILE:N	6:B:2122:HOH:O	2.41	0.51
1:A:116:LYS:HZ3	4:A:1449:ANP:PG	2.35	0.50
1:B:340:ASN:HD22	1:B:384:MET:HA	1.76	0.49
1:A:131:VAL:HG22	1:A:285:TYR:HB3	1.96	0.48
1:B:57[A]:VAL:HG23	6:B:2050:HOH:O	2.16	0.46
1:A:290:ASN:ND2	1:A:294:GLN:OE1	2.37	0.45
1:B:343:ASP:O	1:B:347:PHE:HA	2.18	0.44
1:B:298:PRO:O	1:B:302:MET:HG2	2.18	0.43
1:A:82:TYR:CZ	1:A:295:VAL:HG22	2.53	0.43
1:B:1[B]:MET:HE1	1:B:317:ALA:CB	2.49	0.42
1:B:157:ILE:HG22	6:B:2122:HOH:O	2.19	0.42
1:B:2:LEU:HD21	1:B:101:ILE:HD12	2.02	0.42
1:B:290:ASN:ND2	1:B:294:GLN:OE1	2.49	0.41
1:A:63:ILE:HB	1:A:64:PRO:HD3	2.02	0.41
1:B:297:HIS:N	1:B:298:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

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	443/449 (99%)	426 (96%)	16 (4%)	1 (0%)	47 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/449 (98%)	424 (97%)	14 (3%)	0	100	100
All	All	881/898 (98%)	850 (96%)	30 (3%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	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	361/361 (100%)	359 (99%)	2 (1%)	86	87
1	B	358/361 (99%)	353 (99%)	5 (1%)	67	65
All	All	719/722 (100%)	712 (99%)	7 (1%)	81	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	234	ARG
1	B	1[A]	MET
1	B	1[B]	MET
1	B	206	ASN
1	B	234	ARG
1	B	259	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	237	GLN
1	A	312	GLN

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Mol	Chain	Res	Type
1	A	319	GLN
1	A	404	ASN
1	B	145	ASN
1	B	180	GLN
1	B	206	ASN
1	B	290	ASN
1	B	294	GLN
1	B	312	GLN
1	B	340	ASN
1	B	404	ASN

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 ⓘ

Of 6 ligands modelled in this entry, 2 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$
3	SO4	A	1448	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	B	1448	-	4,4,4	0.19	0	6,6,6	0.17	0
4	ANP	A	1449	-	29,33,33	1.95	7 (24%)	31,52,52	1.81	6 (19%)
5	ADP	B	1449	2	24,29,29	1.00	1 (4%)	29,45,45	1.28	3 (10%)

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
5	ADP	B	1449	2	-	0/12/32/32	0/3/3/3
4	ANP	A	1449	-	-	5/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1449	ANP	PB-N3B	5.05	1.76	1.63
4	A	1449	ANP	PG-N3B	4.96	1.76	1.63
4	A	1449	ANP	PB-O1B	3.58	1.51	1.46
4	A	1449	ANP	PG-O1G	2.99	1.50	1.46
5	B	1449	ADP	C5-C4	2.59	1.47	1.40
4	A	1449	ANP	O4'-C1'	2.44	1.44	1.41
4	A	1449	ANP	PB-O3A	2.40	1.62	1.59
4	A	1449	ANP	C5-C4	2.36	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1449	ANP	O1G-PG-N3B	-5.32	103.93	111.77
4	A	1449	ANP	O2B-PB-O1B	3.99	118.28	109.92
4	A	1449	ANP	N3-C2-N1	-3.59	123.07	128.68
5	B	1449	ADP	N3-C2-N1	-3.52	123.18	128.68
4	A	1449	ANP	PA-O3A-PB	-3.34	120.86	132.62
4	A	1449	ANP	O3G-PG-O2G	2.66	114.72	107.64
5	B	1449	ADP	C4-C5-N7	-2.63	106.66	109.40
4	A	1449	ANP	C4-C5-N7	-2.55	106.74	109.40
5	B	1449	ADP	C3'-C2'-C1'	2.27	104.40	100.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

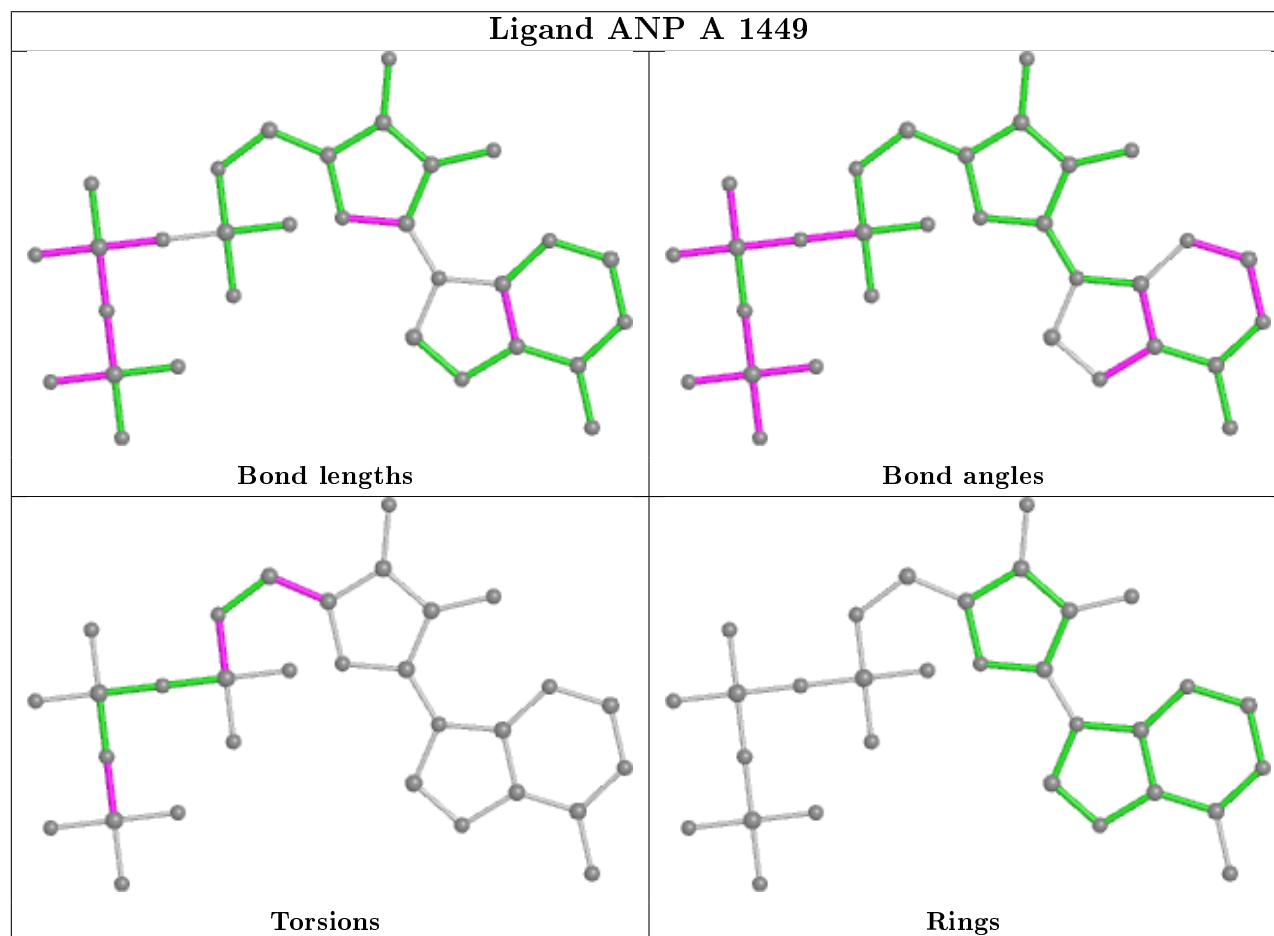
Mol	Chain	Res	Type	Atoms
4	A	1449	ANP	C5'-O5'-PA-O1A
4	A	1449	ANP	C5'-O5'-PA-O3A
4	A	1449	ANP	C3'-C4'-C5'-O5'
4	A	1449	ANP	O4'-C4'-C5'-O5'
4	A	1449	ANP	PB-N3B-PG-O1G

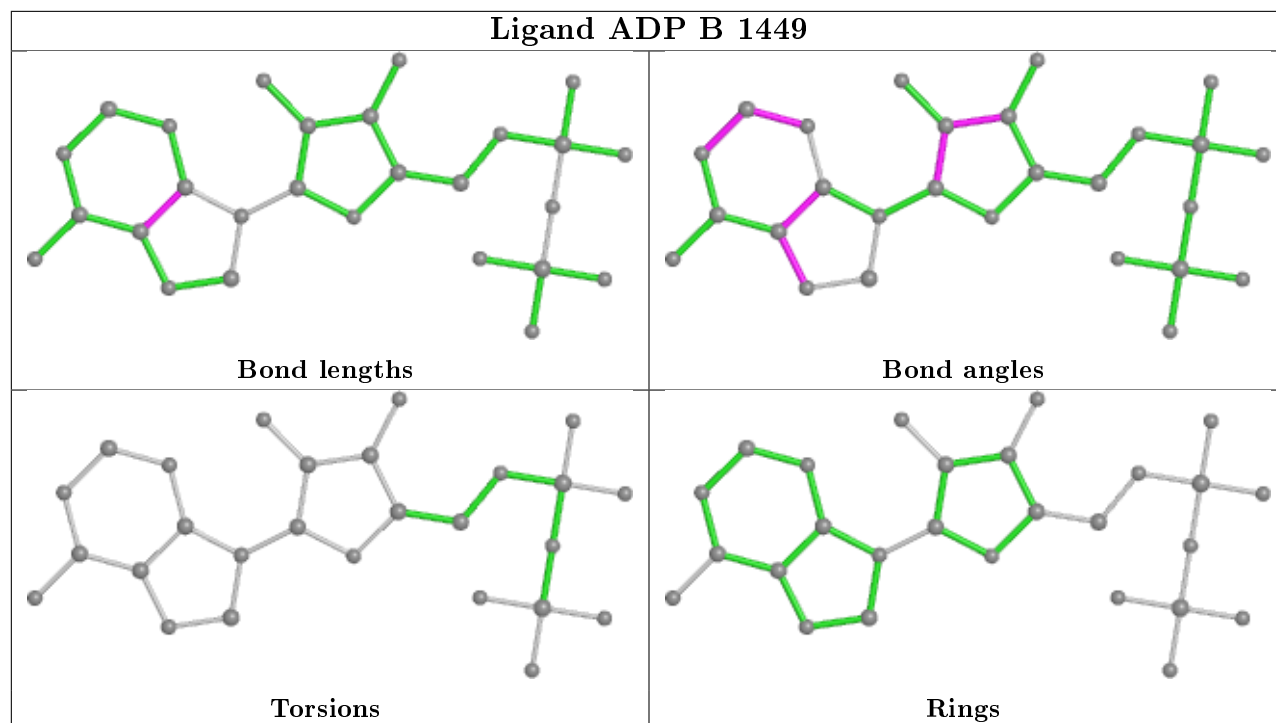
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1449	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.





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

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	444/449 (98%)	0.30	28 (6%) 20 21	18, 24, 43, 56	2 (0%)
1	B	442/449 (98%)	1.14	76 (17%) 1 1	19, 24, 69, 127	2 (0%)
All	All	886/898 (98%)	0.72	104 (11%) 4 4	18, 24, 64, 127	4 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ALA	30.8
1	B	183	SER	24.0
1	B	182	ILE	17.7
1	B	178	LEU	17.5
1	B	187	ALA	17.4
1	B	176	ALA	17.2
1	B	184	MET	11.6
1	B	172	VAL	10.7
1	B	186	ARG	10.7
1	B	170	ARG	10.6
1	B	180	GLN	10.3
1	B	139	GLY	9.4
1	B	152	ILE	8.8
1	B	140	ASP	8.7
1	B	147	ALA	7.7
1	B	196	ASP	7.6
1	B	188	GLU	7.6
1	B	148	ILE	7.3
1	B	181	SER	7.2
1	B	167	ARG	7.1
1	B	150	LYS	6.8
1	B	197	MET	6.5
1	A	446	LEU	6.5
1	B	144	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	137	PRO	5.8
1	B	348	LEU	5.7
1	A	165	GLY	5.4
1	B	190	LYS	5.4
1	B	138	LEU	5.3
1	B	200	MET	5.3
1	B	206	ASN	5.2
1	B	141	ASP	5.2
1	B	175	ASP	5.2
1	A	163	GLY	5.1
1	B	158	ILE	5.1
1	B	154	TYR	5.0
1	B	198	VAL	4.9
1	B	346	THR	4.7
1	A	445	GLY	4.7
1	B	151	ARG	4.6
1	B	156	VAL	4.5
1	B	143	ASP	4.5
1	B	171	VAL	4.4
1	B	446	LEU	4.4
1	A	140	ASP	4.2
1	A	347	PHE	4.1
1	A	194	SER	4.0
1	B	157	ILE	4.0
1	B	135	ASP	4.0
1	B	185	THR	3.9
1	B	189	ALA	3.9
1	A	193	PHE	3.8
1	A	1	MET	3.8
1	B	166	GLY	3.7
1	A	349	PRO	3.7
1	B	145	ASN	3.7
1	B	345	ASN	3.7
1	A	188	GLU	3.7
1	A	348	LEU	3.6
1	A	167	ARG	3.6
1	B	174	GLY	3.6
1	A	346	THR	3.5
1	B	126	ALA	3.2
1	B	155	PRO	3.2
1	B	195	ASN	3.2
1	B	142	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	177	GLU	3.1
1	A	184	MET	3.1
1	B	149	ALA	3.1
1	A	345	ASN	3.1
1	A	180	GLN	3.0
1	B	447	GLN	3.0
1	B	97	ARG	3.0
1	A	166	GLY	2.9
1	B	136	GLY	2.9
1	B	125	LYS	2.9
1	A	141	ASP	2.9
1	B	235	ARG	2.8
1	B	132	PRO	2.8
1	B	201	GLU	2.7
1	B	153	GLY	2.7
1	A	235	ARG	2.7
1	B	191	ALA	2.6
1	A	344	PRO	2.6
1	B	199	TYR	2.6
1	A	195	ASN	2.5
1	B	173	ARG	2.5
1	B	31	VAL	2.4
1	B	114	GLY	2.4
1	B	205	GLU	2.4
1	A	322	SER	2.4
1	A	199	TYR	2.4
1	A	144	LYS	2.3
1	B	344	PRO	2.3
1	B	8	ALA	2.2
1	B	146	ARG	2.2
1	B	237	GLN	2.2
1	B	159	LYS	2.2
1	B	163	GLY	2.2
1	A	170	ARG	2.2
1	A	8	ALA	2.1
1	B	240	VAL	2.1
1	A	162	GLY	2.0
1	B	236	HIS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

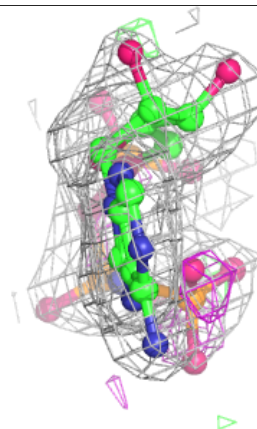
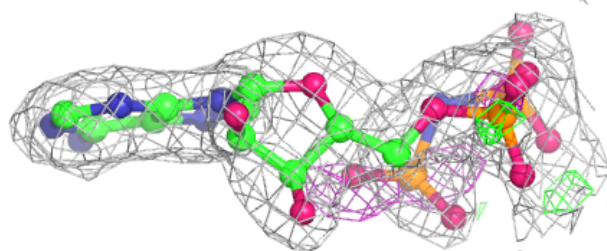
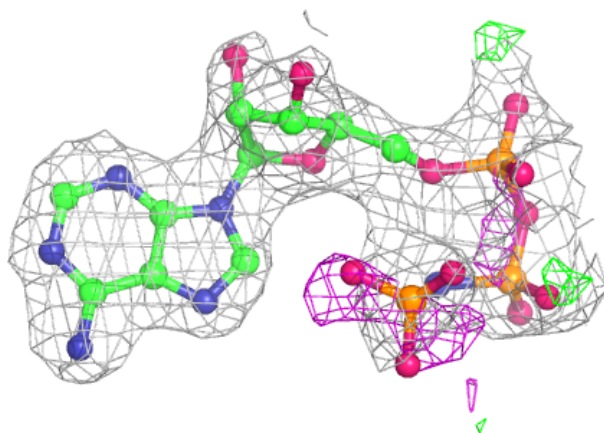
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ANP	A	1449	31/31	0.81	0.19	34,40,62,62	0
3	SO4	A	1448	5/5	0.82	0.30	47,48,48,49	0
3	SO4	B	1448	5/5	0.86	0.19	51,52,53,53	0
5	ADP	B	1449	27/27	0.91	0.13	37,38,40,40	0
2	MG	B	1447	1/1	0.92	0.06	35,35,35,35	0
2	MG	A	1447	1/1	0.94	0.05	42,42,42,42	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.

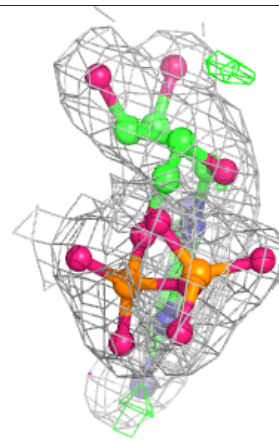
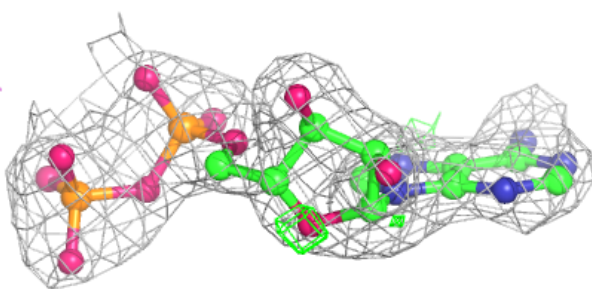
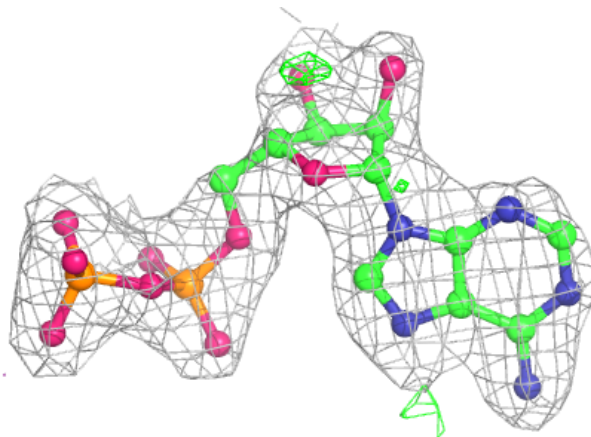
Electron density around ANP A 1449:

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



Electron density around ADP B 1449:

$2mF_o-DF_c$ (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.