



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:22 PM EDT

PDB ID : 9O56 / pdb\_00009o56  
Title : Caldalkalibacillus thermarum Acyl-CoA dehydrogenase member 10 bound to ANP and magnesium  
Authors : Tomchick, D.R.; Ye, J.S.; Tagliabracci, V.S.  
Deposited on : 2025-04-09  
Resolution : 2.15 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](mailto: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

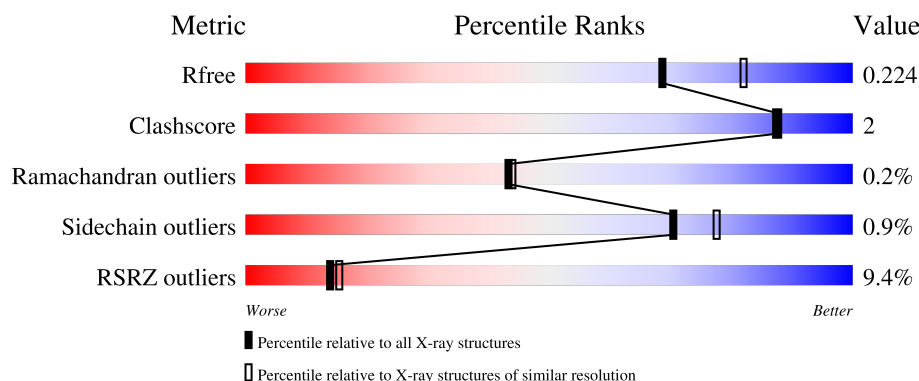
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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  $\geq 3$ , 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	355	<div> <div>7%</div> <div>90%</div> <div>6%</div> </div>
1	B	355	<div> <div>10%</div> <div>88%</div> <div>8%</div> </div>
1	C	355	<div> <div>7%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	D	355	<div> <div>12%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

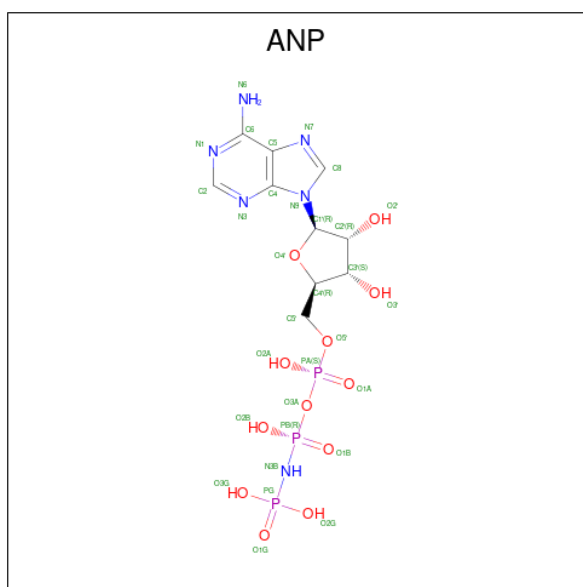
There are 3 unique types of molecules in this entry. The entry contains 22126 atoms, of which 10738 are hydrogens and 0 are deuteriums.

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 Aminoglycoside phosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	H	N	O	S	0	0	0
			5519	1800	2744	474	490	11			
1	B	327	Total	C	H	N	O	S	0	0	0
			5253	1718	2604	448	473	10			
1	C	338	Total	C	H	N	O	S	0	0	0
			5431	1771	2692	469	488	11			
1	D	333	Total	C	H	N	O	S	0	0	0
			5334	1740	2646	458	479	11			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
2	B	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	
			44	10	13	6	12	3	
2	D	1	Total	C	H	N	O	P	
			44	10	13	6	12	3	

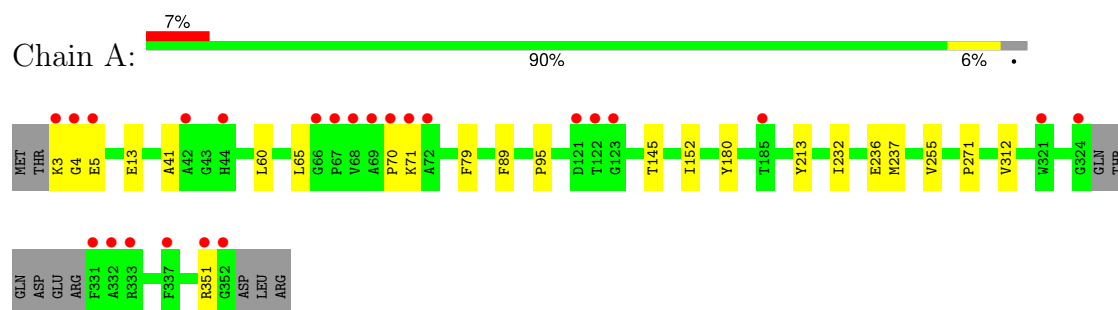
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O		
			158	158	0	0
3	B	69	Total	O		
			69	69	0	0
3	C	120	Total	O		
			120	120	0	0
3	D	66	Total	O		
			66	66	0	0

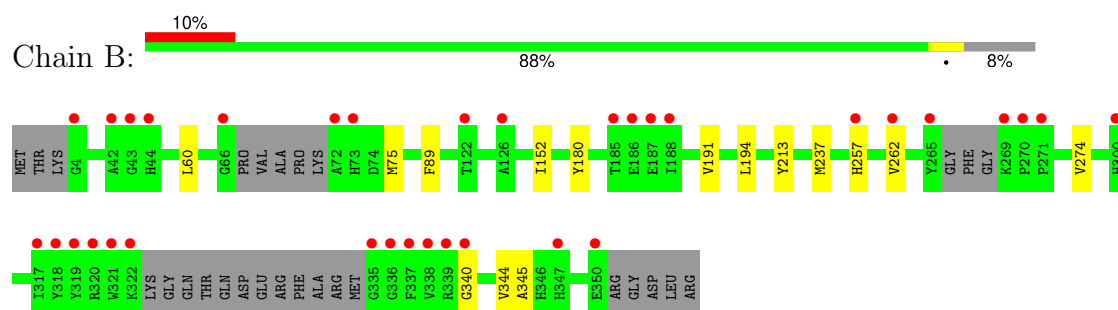
### 3 Residue-property plots [i](#)

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 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.

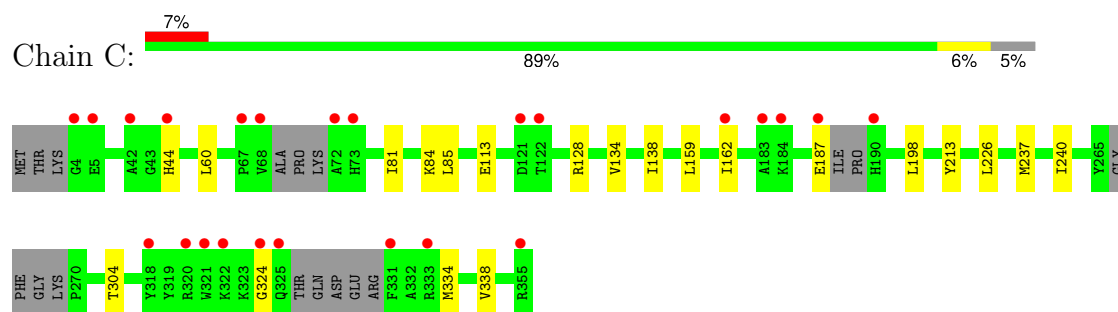
- Molecule 1: Aminoglycoside phosphotransferase



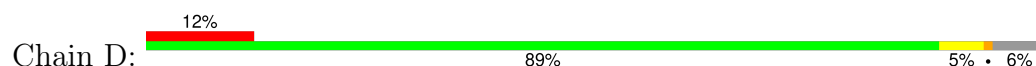
- Molecule 1: Aminoglycoside phosphotransferase

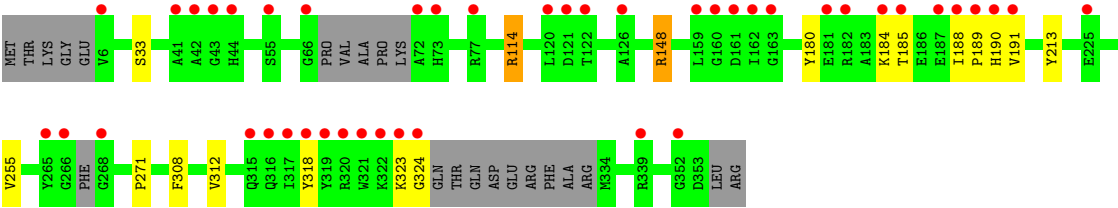


- Molecule 1: Aminoglycoside phosphotransferase



- Molecule 1: Aminoglycoside phosphotransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.97Å 95.89Å 95.54Å 90.00° 114.09° 90.00°	Depositor
Resolution (Å)	36.89 – 2.15 36.89 – 2.15	Depositor EDS
% Data completeness (in resolution range)	93.2 (36.89-2.15) 93.2 (36.89-2.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.185 , 0.225 0.185 , 0.224	Depositor DCC
$R_{free}$ test set	2002 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.12	0/2858	0.29	0/3879
1	B	0.11	0/2726	0.27	0/3702
1	C	0.12	0/2816	0.28	0/3816
1	D	0.11	0/2765	0.29	0/3751
All	All	0.11	0/11165	0.28	0/15148

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	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	114	ARG	Sidechain
1	D	148	ARG	Sidechain

### 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	2775	2744	2742	13	0
1	B	2649	2604	2603	10	0
1	C	2739	2692	2692	11	0
1	D	2688	2646	2645	8	0
2	A	31	13	13	0	0
2	B	31	13	13	0	0
2	C	31	13	13	1	0
2	D	31	13	13	0	0
3	A	158	0	0	0	0
3	B	69	0	0	0	0
3	C	120	0	0	0	0
3	D	66	0	0	0	0
All	All	11388	10738	10734	43	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 2.

All (43) 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:334:MET:O	1:C:338:VAL:HG23	1.96	0.64
1:D:148:ARG:HG3	1:D:148:ARG:HH11	1.64	0.62
2:C:401:ANP:H5'1	2:C:401:ANP:H8	1.80	0.62
1:D:180:TYR:HB2	1:D:312:VAL:HG22	1.85	0.57
1:D:255:VAL:HG21	1:D:271:PRO:HG2	1.87	0.56
1:B:257:HIS:HA	1:B:274:VAL:HG23	1.87	0.56
1:A:3:LYS:CD	1:A:41:ALA:HB1	2.37	0.54
1:C:128:ARG:HG3	1:C:226:LEU:HD12	1.89	0.54
1:B:237:MET:HA	1:B:237:MET:HE2	1.88	0.54
1:B:75:MET:HA	1:B:75:MET:HE2	1.91	0.51
1:A:180:TYR:HB2	1:A:312:VAL:HG22	1.93	0.50
1:D:308:PHE:O	1:D:312:VAL:HG23	2.12	0.49
1:B:340:GLY:O	1:B:344:VAL:HG23	2.12	0.49
1:B:180:TYR:CE2	1:B:191:VAL:HG11	2.48	0.49
1:A:89:PHE:HB2	1:A:152:ILE:HD11	1.95	0.48
1:C:237:MET:HE2	1:C:237:MET:HA	1.95	0.48
1:D:188:ILE:O	1:D:191:VAL:HG12	2.13	0.48
1:A:13:GLU:HG2	1:A:65:LEU:HD11	1.96	0.48
1:A:145:THR:HG21	1:A:232:ILE:HD11	1.96	0.48
1:A:3:LYS:HD2	1:A:41:ALA:HB1	1.96	0.47
1:A:3:LYS:HD3	1:A:41:ALA:HB1	1.97	0.47
1:A:70:PRO:O	1:A:71:LYS:HB3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:THR:HG21	1:D:318:TYR:CE2	2.51	0.45
1:C:134:VAL:O	1:C:138:ILE:HD13	2.18	0.44
1:C:128:ARG:CG	1:C:226:LEU:HD12	2.48	0.44
1:C:81:ILE:HD11	1:C:162:ILE:HD12	2.00	0.43
1:B:60:LEU:C	1:B:60:LEU:HD23	2.43	0.43
1:C:84:LYS:HB2	1:C:159:LEU:HD21	2.00	0.43
1:A:60:LEU:C	1:A:60:LEU:HD23	2.44	0.42
1:B:194:LEU:HD11	1:B:345:ALA:HB3	2.01	0.42
1:D:323:LYS:O	1:D:324:GLY:C	2.62	0.42
1:C:198:LEU:HD21	1:C:304:THR:HG22	2.02	0.42
1:A:255:VAL:HB	1:A:271:PRO:HG2	2.02	0.41
1:B:262:VAL:HG21	1:B:340:GLY:HA3	2.00	0.41
1:C:81:ILE:O	1:C:85:LEU:HB2	2.20	0.41
1:A:4:GLY:O	1:A:5:GLU:HB2	2.21	0.41
1:A:79:PHE:CE1	1:A:95:PRO:HB2	2.55	0.41
1:C:162:ILE:CG1	1:C:240:ILE:HG12	2.51	0.41
1:C:60:LEU:C	1:C:60:LEU:HD23	2.45	0.41
1:B:274:VAL:O	1:B:274:VAL:HG22	2.20	0.41
1:B:89:PHE:CD1	1:B:152:ILE:HD11	2.55	0.41
1:A:236:GLU:HG3	1:A:237:MET:SD	2.61	0.40
1:D:189:PRO:O	1:D:190:HIS:HB2	2.20	0.40

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	340/355 (96%)	329 (97%)	11 (3%)	0	100	100
1	B	319/355 (90%)	307 (96%)	12 (4%)	0	100	100
1	C	328/355 (92%)	318 (97%)	9 (3%)	1 (0%)	36	34
1	D	325/355 (92%)	309 (95%)	15 (5%)	1 (0%)	36	34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1312/1420 (92%)	1263 (96%)	47 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	184	LYS
1	C	324	GLY

### 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	294/305 (96%)	292 (99%)	2 (1%)	76	82
1	B	283/305 (93%)	282 (100%)	1 (0%)	84	89
1	C	291/305 (95%)	287 (99%)	4 (1%)	59	66
1	D	286/305 (94%)	283 (99%)	3 (1%)	68	75
All	All	1154/1220 (95%)	1144 (99%)	10 (1%)	70	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	TYR
1	A	351	ARG
1	B	213	TYR
1	C	44	HIS
1	C	113	GLU
1	C	187	GLU
1	C	213	TYR
1	D	33	SER
1	D	114	ARG
1	D	213	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	B	190	HIS
1	C	347	HIS
1	D	94	GLN
1	D	346	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](#)

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	ANP	B	401	-	33,33,33	2.27	5 (15%)	45,52,52	1.21	3 (6%)
2	ANP	D	401	-	33,33,33	2.28	5 (15%)	45,52,52	1.23	3 (6%)
2	ANP	C	401	-	33,33,33	2.19	5 (15%)	45,52,52	1.33	5 (11%)
2	ANP	A	401	-	33,33,33	2.27	5 (15%)	45,52,52	1.28	3 (6%)

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	B	401	-	-	5/18/38/38	0/3/3/3
2	ANP	D	401	-	-	7/18/38/38	0/3/3/3
2	ANP	C	401	-	-	6/18/38/38	0/3/3/3
2	ANP	A	401	-	-	1/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ANP	PB-O3A	8.81	1.70	1.59
2	B	401	ANP	PB-O3A	8.74	1.69	1.59
2	A	401	ANP	PB-O3A	8.66	1.69	1.59
2	C	401	ANP	PB-O3A	7.98	1.69	1.59
2	D	401	ANP	PG-N3B	6.34	1.79	1.63
2	B	401	ANP	PG-N3B	6.26	1.79	1.63
2	C	401	ANP	PG-N3B	6.21	1.79	1.63
2	A	401	ANP	PG-N3B	6.17	1.79	1.63
2	A	401	ANP	PG-O1G	4.74	1.53	1.46
2	D	401	ANP	PG-O1G	4.64	1.53	1.46
2	B	401	ANP	PG-O1G	4.58	1.53	1.46
2	C	401	ANP	PG-O1G	4.55	1.53	1.46
2	C	401	ANP	PB-O1B	2.71	1.50	1.46
2	D	401	ANP	PB-O1B	2.60	1.50	1.46
2	A	401	ANP	PB-O1B	2.55	1.50	1.46
2	B	401	ANP	PB-O1B	2.51	1.50	1.46
2	A	401	ANP	PB-O2B	-2.13	1.51	1.56
2	B	401	ANP	PB-O2B	-2.11	1.51	1.56
2	D	401	ANP	PB-O2B	-2.10	1.51	1.56
2	C	401	ANP	PB-O2B	-2.09	1.51	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ANP	O2B-PB-O1B	5.79	122.29	109.87
2	D	401	ANP	O2B-PB-O1B	5.50	121.67	109.87
2	A	401	ANP	O2B-PB-O1B	5.31	121.26	109.87
2	B	401	ANP	O2B-PB-O1B	5.26	121.15	109.87
2	A	401	ANP	O1G-PG-N3B	-4.49	105.15	111.77
2	B	401	ANP	O1G-PG-N3B	-3.54	106.56	111.77
2	D	401	ANP	O1G-PG-N3B	-3.45	106.70	111.77
2	C	401	ANP	O1G-PG-N3B	-2.97	107.40	111.77
2	C	401	ANP	O2G-PG-O3G	2.54	114.43	107.59
2	C	401	ANP	O3A-PB-N3B	-2.39	99.97	106.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ANP	O2G-PG-O3G	2.38	113.98	107.59
2	D	401	ANP	O2G-PG-O3G	2.31	113.80	107.59
2	B	401	ANP	O2G-PG-O3G	2.30	113.77	107.59
2	C	401	ANP	O3A-PA-O1A	2.08	116.95	110.70

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ANP	PB-N3B-PG-O1G
2	B	401	ANP	PB-N3B-PG-O1G
2	B	401	ANP	PG-N3B-PB-O3A
2	C	401	ANP	PB-N3B-PG-O1G
2	C	401	ANP	PG-N3B-PB-O3A
2	C	401	ANP	C5'-O5'-PA-O2A
2	D	401	ANP	PB-N3B-PG-O1G
2	D	401	ANP	PG-N3B-PB-O3A
2	D	401	ANP	C5'-O5'-PA-O2A
2	D	401	ANP	O4'-C4'-C5'-O5'
2	B	401	ANP	O4'-C4'-C5'-O5'
2	D	401	ANP	C3'-C4'-C5'-O5'
2	B	401	ANP	C3'-C4'-C5'-O5'
2	C	401	ANP	C5'-O5'-PA-O1A
2	D	401	ANP	C5'-O5'-PA-O1A
2	D	401	ANP	C5'-O5'-PA-O3A
2	C	401	ANP	O4'-C4'-C5'-O5'
2	B	401	ANP	PA-O3A-PB-O1B
2	C	401	ANP	PA-O3A-PB-O1B

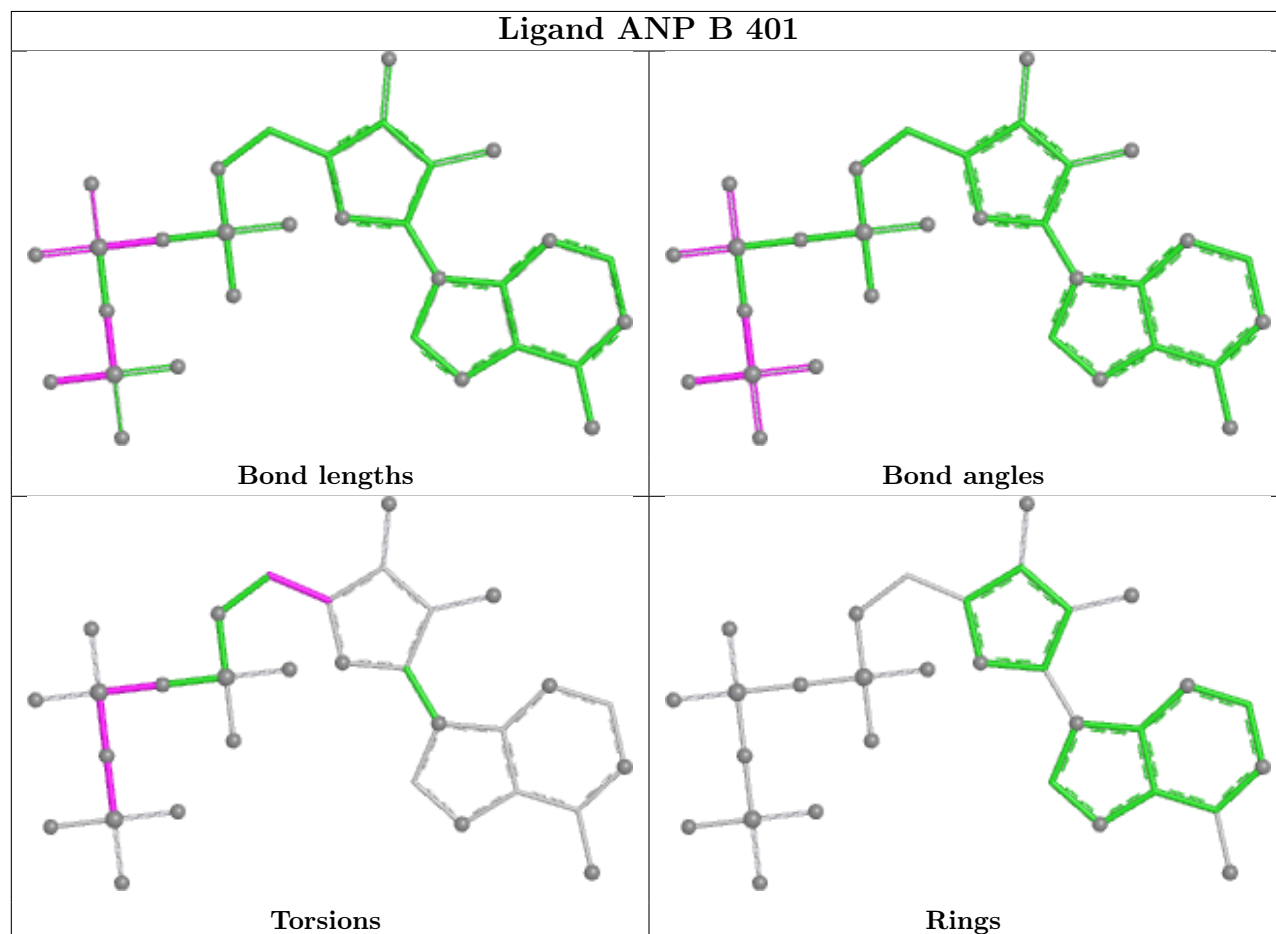
There are no ring outliers.

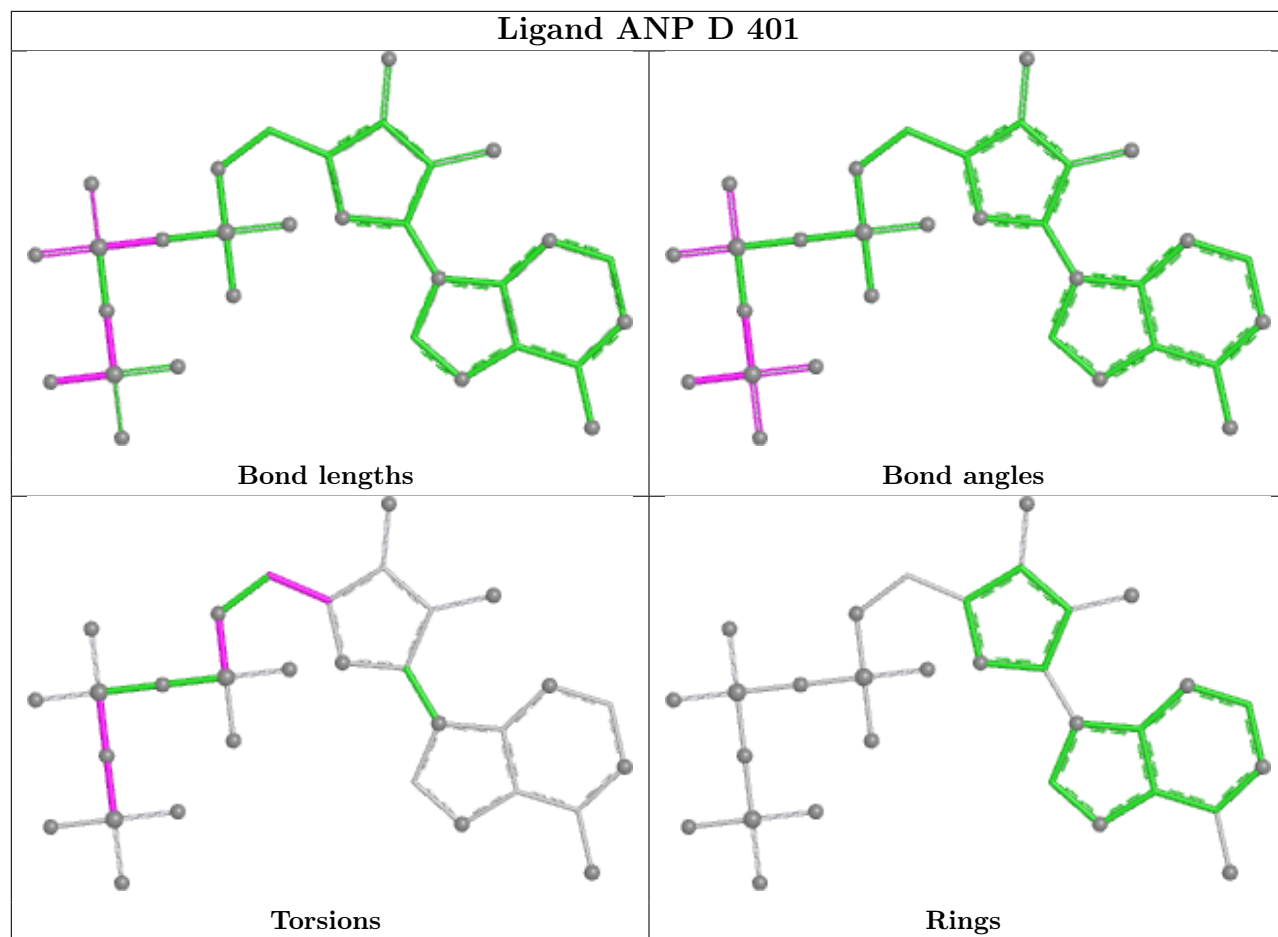
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ANP	1	0

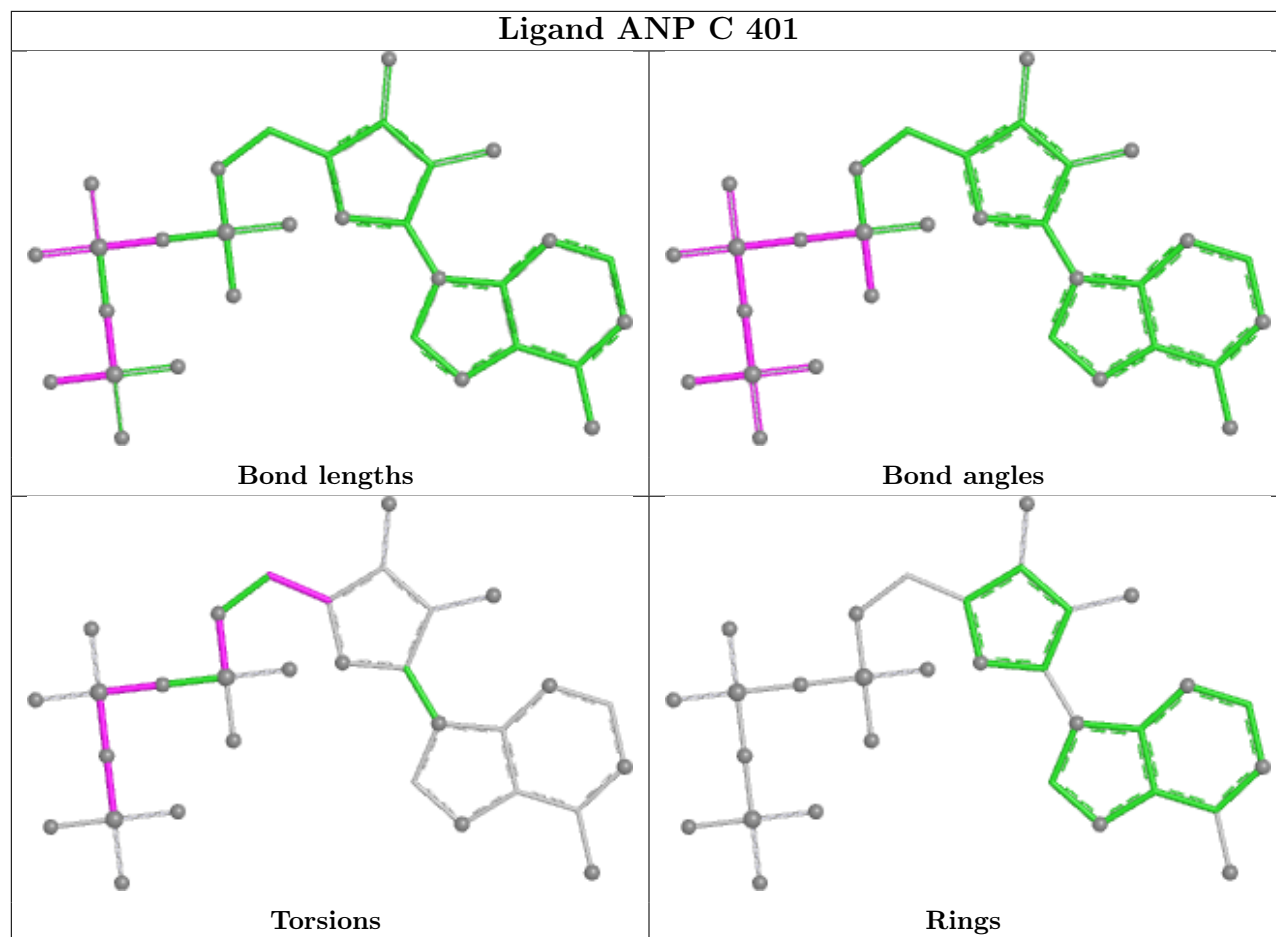
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

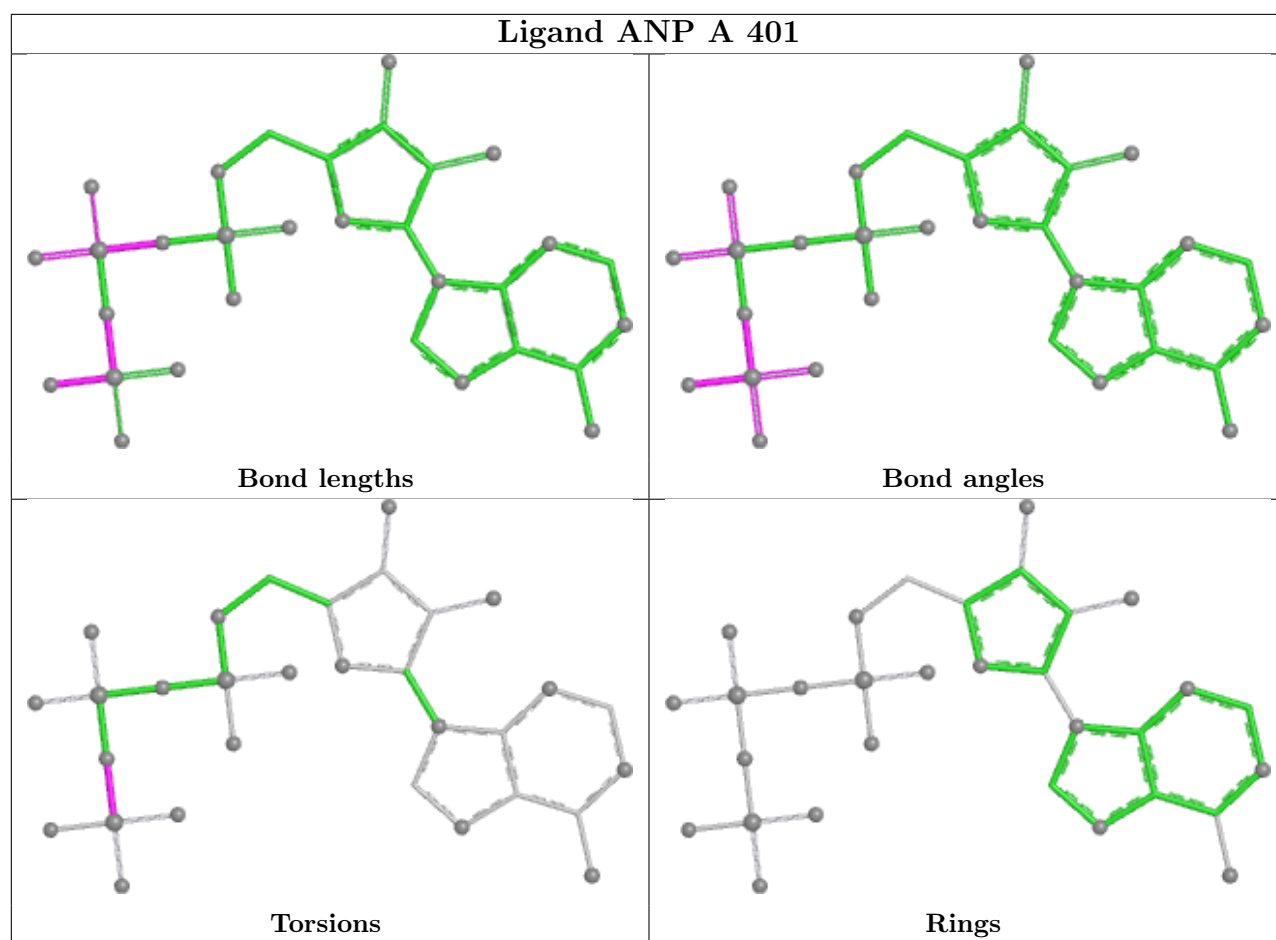
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	344/355 (96%)	-0.06	24 (6%) 22 25	13, 28, 73, 108	0
1	B	327/355 (92%)	0.49	34 (10%) 11 13	23, 44, 82, 112	0
1	C	338/355 (95%)	0.09	24 (7%) 22 25	17, 34, 74, 103	0
1	D	333/355 (93%)	0.61	44 (13%) 7 8	19, 49, 84, 133	0
All	All	1342/1420 (94%)	0.28	126 (9%) 14 15	13, 39, 81, 133	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	GLY	8.2
1	B	66	GLY	7.9
1	B	318	TYR	7.7
1	B	321	TRP	7.7
1	D	321	TRP	6.6
1	C	68	VAL	5.9
1	D	324	GLY	5.8
1	A	324	GLY	5.6
1	D	42	ALA	5.1
1	C	190	HIS	4.9
1	A	331	PHE	4.9
1	A	70	PRO	4.9
1	D	72	ALA	4.8
1	B	185	THR	4.7
1	A	67	PRO	4.5
1	A	122	THR	4.4
1	C	122	THR	4.4
1	C	184	LYS	4.3
1	C	4	GLY	4.3
1	D	266	GLY	4.3
1	D	185	THR	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	319	TYR	4.2
1	B	42	ALA	4.1
1	B	319	TYR	4.1
1	D	320	ARG	4.1
1	B	262	VAL	4.1
1	A	71	LYS	4.1
1	B	265	TYR	4.0
1	C	187	GLU	4.0
1	B	335	GLY	4.0
1	C	322	LYS	3.9
1	A	321	TRP	3.8
1	C	355	ARG	3.8
1	B	270	PRO	3.8
1	B	4	GLY	3.8
1	D	318	TYR	3.7
1	B	269	LYS	3.7
1	C	162	ILE	3.7
1	D	322	LYS	3.6
1	A	72	ALA	3.5
1	B	73	HIS	3.5
1	B	338	VAL	3.5
1	D	126	ALA	3.5
1	B	336	GLY	3.5
1	C	121	ASP	3.4
1	A	351	ARG	3.3
1	A	68	VAL	3.3
1	A	3	LYS	3.3
1	B	122	THR	3.3
1	B	350	GLU	3.2
1	C	318	TYR	3.2
1	D	122	THR	3.2
1	B	257	HIS	3.2
1	A	4	GLY	3.2
1	B	322	LYS	3.1
1	D	6	VAL	3.1
1	B	317	ILE	3.1
1	B	72	ALA	3.1
1	B	44	HIS	3.0
1	C	72	ALA	3.0
1	C	183	ALA	3.0
1	D	44	HIS	3.0
1	C	331	PHE	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	42	ALA	2.9
1	B	126	ALA	2.9
1	D	323	LYS	2.9
1	A	123	GLY	2.9
1	B	187	GLU	2.9
1	B	43	GLY	2.9
1	D	73	HIS	2.9
1	D	159	LEU	2.8
1	C	321	TRP	2.8
1	C	325	GLN	2.7
1	C	324	GLY	2.7
1	D	265	TYR	2.6
1	D	184	LYS	2.6
1	A	69	ALA	2.6
1	D	315	GLN	2.5
1	D	268	GLY	2.5
1	D	352	GLY	2.5
1	B	337	PHE	2.5
1	B	340	GLY	2.5
1	C	73	HIS	2.5
1	D	182	ARG	2.5
1	C	67	PRO	2.4
1	C	42	ALA	2.4
1	A	5	GLU	2.4
1	D	188	ILE	2.4
1	D	316	GLN	2.4
1	D	191	VAL	2.4
1	A	66	GLY	2.4
1	D	160	GLY	2.4
1	D	187	GLU	2.4
1	B	320	ARG	2.4
1	D	41	ALA	2.4
1	B	186	GLU	2.4
1	C	44	HIS	2.4
1	D	190	HIS	2.4
1	D	43	GLY	2.3
1	A	44	HIS	2.3
1	B	347	HIS	2.3
1	A	337	PHE	2.3
1	D	55	SER	2.3
1	B	188	ILE	2.3
1	B	271	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	320	ARG	2.3
1	D	120	LEU	2.3
1	B	300	HIS	2.2
1	D	317	ILE	2.2
1	D	189	PRO	2.2
1	C	333	ARG	2.2
1	A	121	ASP	2.2
1	D	161	ASP	2.2
1	A	352	GLY	2.2
1	D	339	ARG	2.2
1	D	77	ARG	2.2
1	D	121	ASP	2.2
1	D	163	GLY	2.1
1	D	181	GLU	2.1
1	A	332	ALA	2.1
1	D	225	GLU	2.1
1	A	333	ARG	2.1
1	D	162	ILE	2.1
1	C	5	GLU	2.1
1	B	339	ARG	2.0
1	A	185	THR	2.0

## 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, 95<sup>th</sup> 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.

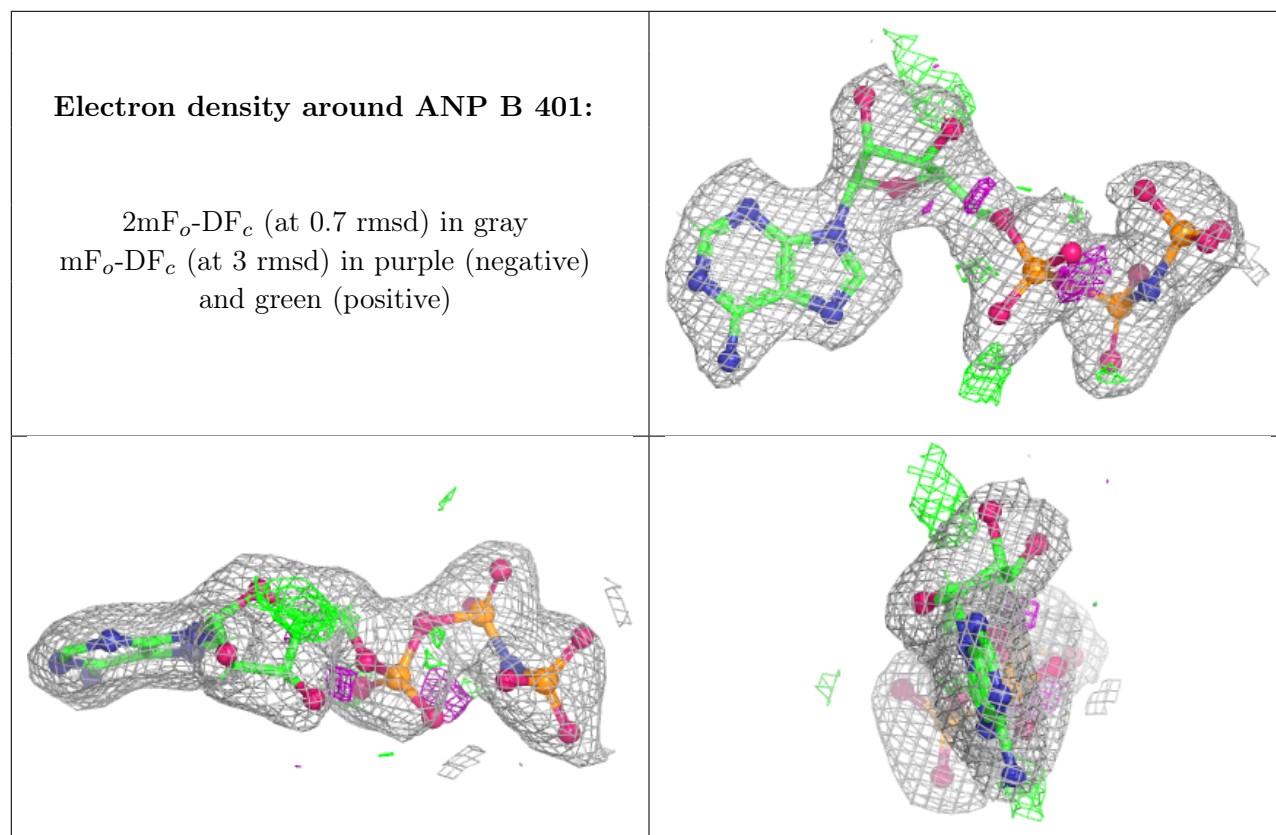
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	B	401	31/31	0.93	0.10	25,37,59,65	0
2	ANP	D	401	31/31	0.93	0.09	26,47,56,60	0

*Continued on next page...*

*Continued from previous page...*

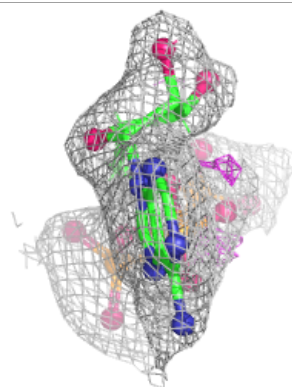
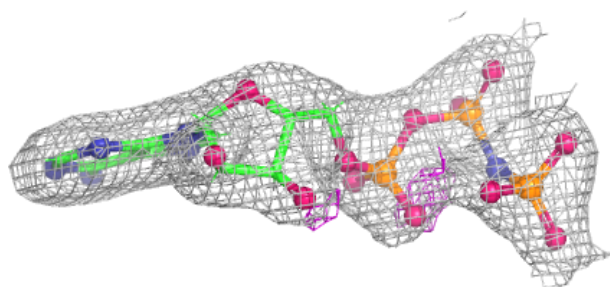
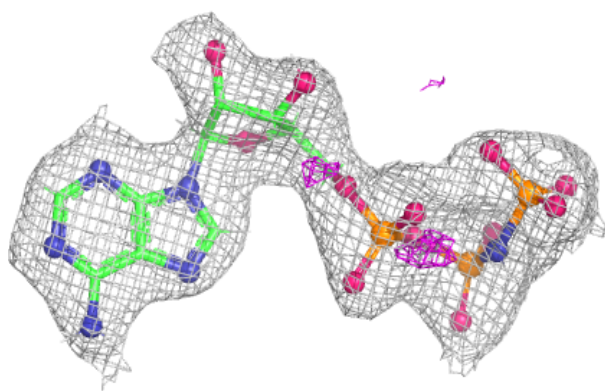
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	C	401	31/31	0.94	0.09	22,35,49,59	0
2	ANP	A	401	31/31	0.98	0.05	13,24,39,49	0

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.

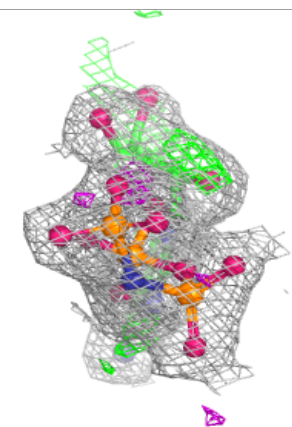
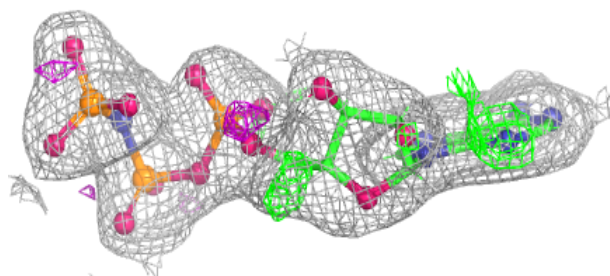
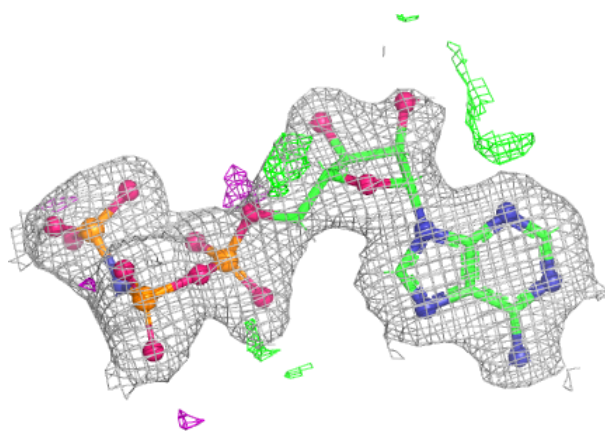


**Electron density around ANP D 401:**

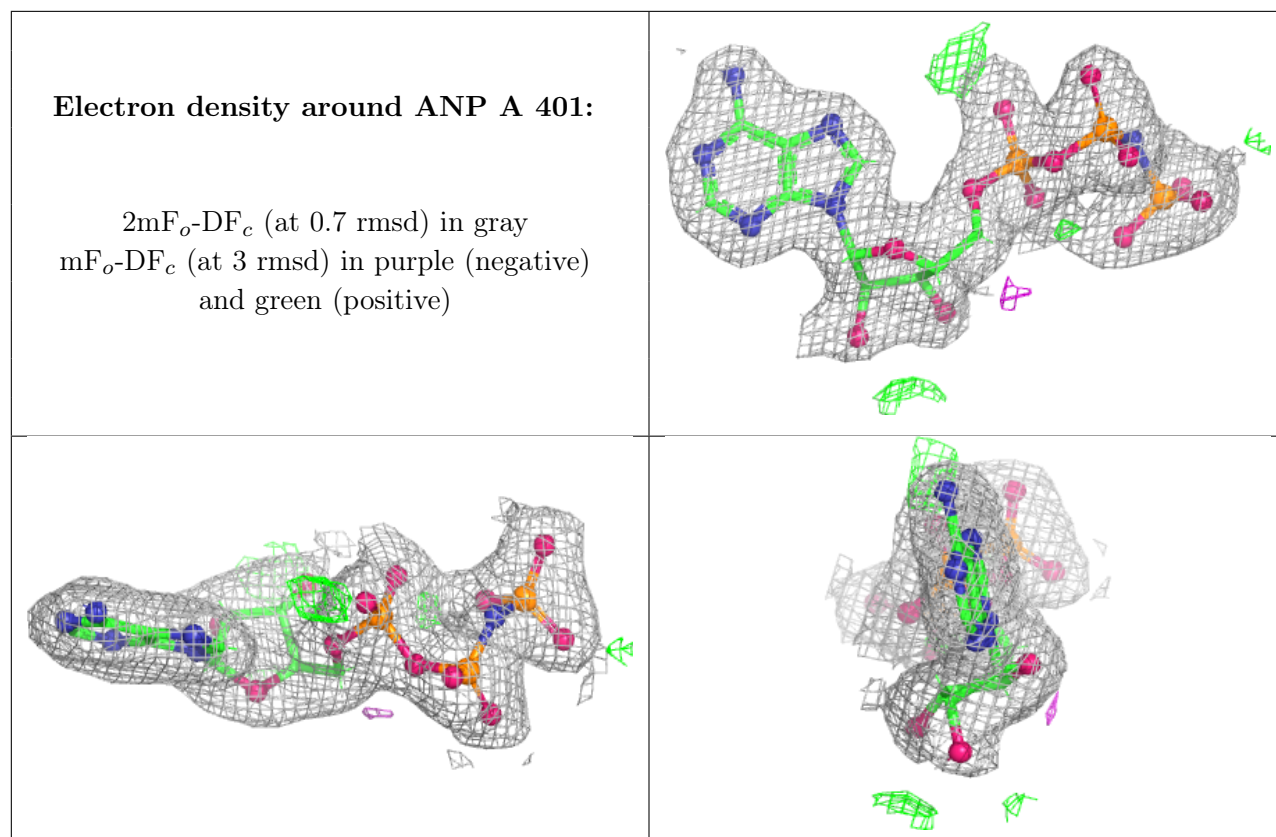
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP C 401:**

$2mF_o-DF_c$  (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.