



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:21 am BST

PDB ID : 3TSU  
Title : Crystal structure of E. coli HypF with AMP-PNP and carbamoyl phosphate  
Authors : Petkun, S.; Shi, R.; Li, Y.; Cygler, M.  
Deposited on : 2011-09-13  
Resolution : 1.92 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 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

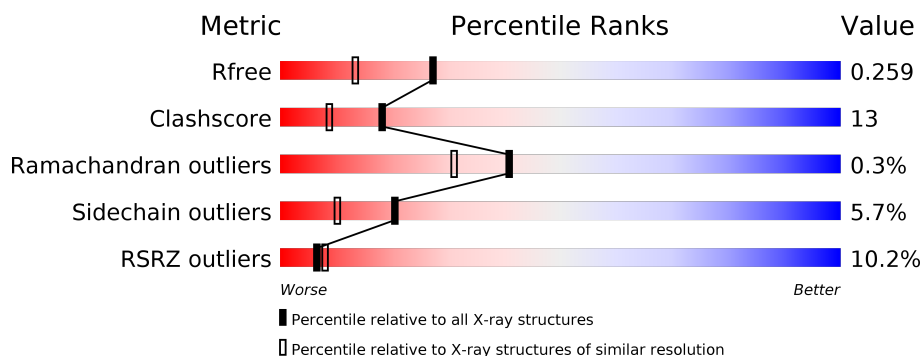
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.92 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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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	657	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5220 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 Transcriptional regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	646	Total	C	N	O	S	0	2	0
			4939	3119	889	893	38			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	GLY	-	EXPRESSION TAG	UNP Q7ABC4
A	91	SER	-	EXPRESSION TAG	UNP Q7ABC4
A	571	ALA	GLN	CONFLICT	UNP Q7ABC4
A	572	ALA	GLN	CONFLICT	UNP Q7ABC4
A	573	ALA	GLN	CONFLICT	UNP Q7ABC4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

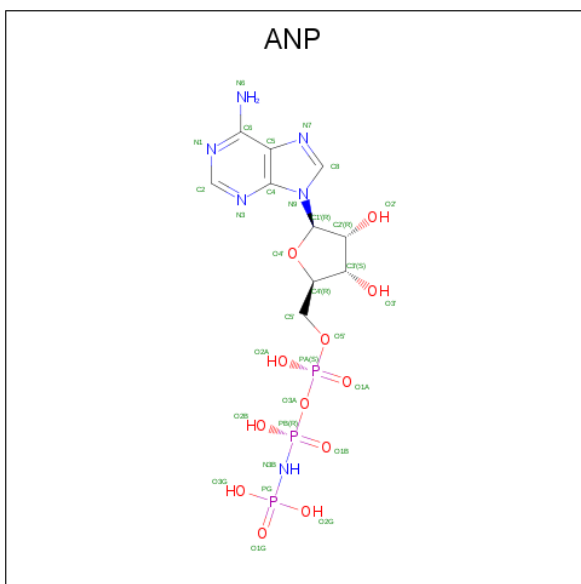
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 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
5	A	1	Total 31	C 10	N 6	O 12	P 3	0	0

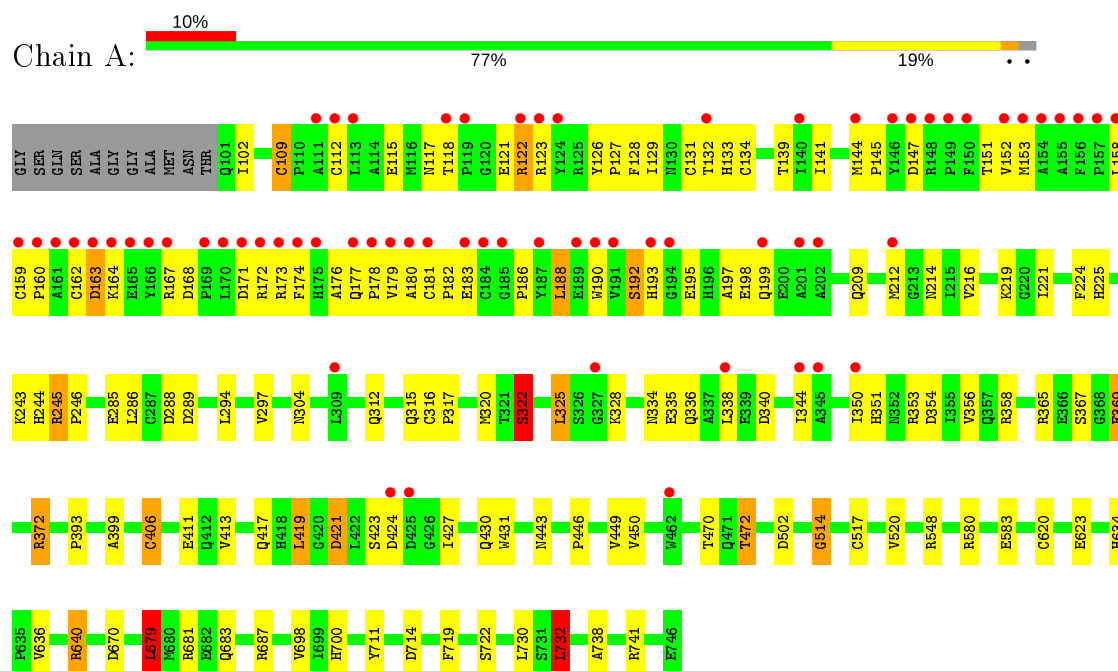
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	219	Total 219	O 219	0	0

### 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: Transcriptional regulatory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.33Å 75.05Å 201.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.66 – 1.92 50.03 – 1.92	Depositor EDS
% Data completeness (in resolution range)	84.8 (100.66-1.92) 80.7 (50.03-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.199 , 0.248 0.213 , 0.259	Depositor DCC
$R_{free}$ test set	2228 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, ZN, 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	1.04	10/5064 (0.2%)	0.94	11/6913 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	CYS	CB-SG	-9.89	1.65	1.82
1	A	109	CYS	CB-SG	6.66	1.93	1.82
1	A	472	THR	CB-CG2	-6.64	1.30	1.52
1	A	520	VAL	CB-CG2	-5.80	1.40	1.52
1	A	322	SER	CB-OG	-5.76	1.34	1.42
1	A	369	GLU	CG-CD	5.69	1.60	1.51
1	A	719	PHE	CD2-CE2	5.56	1.50	1.39
1	A	711	TYR	CE2-CZ	5.54	1.45	1.38
1	A	411	GLU	CG-CD	5.20	1.59	1.51
1	A	620	CYS	CB-SG	5.07	1.90	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	A	580	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	A	681	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	580	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	741	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	109	CYS	CA-CB-SG	6.57	125.82	114.00
1	A	732	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	640	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	548	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	679	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	A	732	LEU	CB-CG-CD2	5.18	119.80	111.00



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	4939	0	4851	131	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	27	0	12	1	0
5	A	31	0	12	8	0
6	A	219	0	0	27	0
All	All	5220	0	4875	132	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 13.

All (132) 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:122:ARG:NH2	1:A:162:CYS:SG	1.97	1.37
1:A:322:SER:HB2	5:A:748:ANP:O2B	1.51	1.11
1:A:117:ASN:HB3	6:A:64:HOH:O	1.52	1.09
1:A:517:CYS:HB2	6:A:758:HOH:O	0.90	1.06
1:A:109:CYS:SG	6:A:786:HOH:O	2.12	1.04
1:A:244:HIS:C	6:A:769:HOH:O	1.98	1.01
1:A:164:LYS:O	1:A:168:ASP:HB2	1.60	1.00
1:A:322:SER:CB	5:A:748:ANP:O2B	2.15	0.95
1:A:109:CYS:CB	6:A:786:HOH:O	2.15	0.94
5:A:748:ANP:O2G	5:A:748:ANP:PA	2.27	0.93
1:A:153:MET:HA	1:A:153:MET:HE2	1.47	0.93
1:A:127:PRO:HG2	1:A:188:LEU:HD11	1.48	0.93
1:A:153:MET:HG3	1:A:178:PRO:HA	1.49	0.92
1:A:244:HIS:O	1:A:246:PRO:HD3	1.70	0.92
1:A:180:ALA:HB3	6:A:764:HOH:O	1.72	0.88
1:A:134:CYS:HB3	6:A:786:HOH:O	1.73	0.87
1:A:188:LEU:N	1:A:188:LEU:HD12	1.94	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:H	1:A:188:LEU:CD1	1.93	0.81
1:A:449:VAL:CG1	1:A:470:THR:HG22	2.11	0.81
1:A:152:VAL:HG13	1:A:153:MET:HE3	1.63	0.80
1:A:683:GLN:OE1	1:A:687:ARG:NH2	2.15	0.79
1:A:640:ARG:HD2	6:A:45:HOH:O	1.83	0.78
1:A:152:VAL:CG2	1:A:354:ASP:HB2	2.14	0.77
1:A:583:GLU:HG3	6:A:77:HOH:O	1.86	0.75
1:A:640:ARG:NH1	6:A:45:HOH:O	1.97	0.75
1:A:188:LEU:N	1:A:188:LEU:CD1	2.49	0.74
1:A:369:GLU:OE2	1:A:700:HIS:HD2	1.70	0.73
1:A:152:VAL:HG23	1:A:354:ASP:HB2	1.71	0.72
1:A:224:PHE:HE1	1:A:350:ILE:HG22	1.56	0.71
1:A:173:ARG:HD3	1:A:179:VAL:HG21	1.73	0.70
1:A:225:HIS:CD2	1:A:320:MET:HG3	2.28	0.69
1:A:634:HIS:HD2	1:A:636:VAL:H	1.42	0.68
1:A:450:VAL:HG21	1:A:738:ALA:HB2	1.76	0.68
1:A:449:VAL:HG11	1:A:470:THR:HG22	1.77	0.66
1:A:182:PRO:HD2	6:A:73:HOH:O	1.97	0.65
1:A:351:HIS:HD2	1:A:353:ARG:H	1.45	0.64
1:A:178:PRO:HD2	6:A:890:HOH:O	1.97	0.64
1:A:219:LYS:NZ	1:A:334:ASN:HD21	1.96	0.64
1:A:623:GLU:OE1	4:A:747:ADP:N6	2.29	0.62
1:A:325:LEU:HD12	1:A:344:ILE:HD11	1.83	0.61
1:A:365:ARG:NH2	1:A:700:HIS:O	2.34	0.60
1:A:322:SER:OG	5:A:748:ANP:O2B	2.19	0.59
1:A:163:ASP:O	1:A:167:ARG:HB2	2.02	0.59
1:A:322:SER:CB	5:A:748:ANP:PB	2.91	0.59
1:A:152:VAL:HG21	1:A:354:ASP:HB2	1.84	0.58
1:A:173:ARG:HG3	6:A:38:HOH:O	2.03	0.58
1:A:128:PHE:HZ	1:A:351:HIS:CB	2.17	0.58
1:A:186:PRO:HD2	6:A:764:HOH:O	2.03	0.57
1:A:193:HIS:NE2	6:A:84:HOH:O	2.19	0.57
1:A:399:ALA:HB2	1:A:730:LEU:HD22	1.87	0.57
1:A:188:LEU:H	1:A:188:LEU:HD13	1.68	0.57
1:A:421:ASP:OD1	1:A:423:SER:N	2.35	0.56
1:A:199:GLN:HB3	6:A:70:HOH:O	2.05	0.56
1:A:424:ASP:O	1:A:427:ILE:HG22	2.06	0.55
1:A:153:MET:CA	1:A:153:MET:HE2	2.29	0.55
1:A:139:THR:O	1:A:356:VAL:HG12	2.07	0.55
1:A:224:PHE:CE1	1:A:350:ILE:HG22	2.42	0.54
1:A:450:VAL:HG21	1:A:738:ALA:CB	2.38	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:HB3	1:A:171:ASP:HB2	1.91	0.53
1:A:164:LYS:HG2	6:A:865:HOH:O	2.09	0.53
1:A:245:ARG:N	6:A:769:HOH:O	2.33	0.52
1:A:322:SER:HB2	5:A:748:ANP:PB	2.48	0.52
1:A:312:GLN:HA	1:A:315:GLN:NE2	2.24	0.52
1:A:244:HIS:O	6:A:769:HOH:O	2.18	0.52
1:A:109:CYS:HB3	6:A:786:HOH:O	1.99	0.52
1:A:325:LEU:CD1	1:A:344:ILE:HD11	2.40	0.52
1:A:122:ARG:HH11	1:A:122:ARG:HB3	1.75	0.51
1:A:190:TRP:HZ2	1:A:209:GLN:HE21	1.58	0.51
1:A:417:GLN:HG2	1:A:419:LEU:HD13	1.92	0.51
1:A:634:HIS:HE1	1:A:670:ASP:OD2	1.94	0.51
1:A:190:TRP:CH2	1:A:209:GLN:HG3	2.46	0.50
1:A:212:MET:HG3	1:A:214:ASN:ND2	2.27	0.50
1:A:190:TRP:CZ2	1:A:209:GLN:HG3	2.46	0.50
1:A:312:GLN:C	1:A:315:GLN:HE21	2.15	0.49
1:A:128:PHE:CZ	1:A:351:HIS:CG	3.01	0.49
1:A:640:ARG:HG3	1:A:679:LEU:HD12	1.95	0.48
1:A:285:GLU:HB2	6:A:26:HOH:O	2.13	0.48
1:A:312:GLN:O	1:A:315:GLN:NE2	2.42	0.48
1:A:212:MET:HG3	1:A:214:ASN:HD22	1.78	0.48
1:A:153:MET:HA	1:A:153:MET:CE	2.34	0.48
1:A:197:ALA:O	1:A:198:GLU:HG3	2.13	0.48
1:A:117:ASN:CB	6:A:64:HOH:O	2.32	0.47
1:A:640:ARG:CD	6:A:45:HOH:O	2.54	0.47
1:A:243:LYS:NZ	5:A:748:ANP:HNB1	2.13	0.47
1:A:168:ASP:O	1:A:174:PHE:HB2	2.15	0.47
1:A:316:CYS:HB2	1:A:317:PRO:HD2	1.97	0.47
1:A:147:ASP:HA	1:A:177:GLN:CD	2.35	0.46
1:A:153:MET:CE	1:A:353:ARG:HG3	2.46	0.46
1:A:517:CYS:CB	6:A:758:HOH:O	1.78	0.46
1:A:244:HIS:O	1:A:246:PRO:CD	2.53	0.46
1:A:449:VAL:HG12	1:A:470:THR:HG22	1.94	0.46
1:A:123:ARG:NH1	1:A:162:CYS:SG	2.89	0.46
1:A:358:ARG:HD2	1:A:430:GLN:NE2	2.31	0.46
1:A:336:GLN:HE21	1:A:340:ASP:HB2	1.81	0.45
1:A:128:PHE:HZ	1:A:351:HIS:CG	2.34	0.45
1:A:393:PRO:HB2	1:A:446:PRO:HA	1.99	0.45
1:A:583:GLU:CG	6:A:77:HOH:O	2.56	0.45
1:A:419:LEU:HD23	1:A:431:TRP:CD1	2.52	0.44
1:A:188:LEU:H	1:A:188:LEU:HD12	1.60	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HD23	6:A:758:HOH:O	2.17	0.44
1:A:172:ARG:O	1:A:172:ARG:HG2	2.18	0.43
1:A:351:HIS:HD2	1:A:353:ARG:N	2.16	0.43
1:A:413:VAL:HG11	1:A:732:LEU:CD2	2.49	0.43
1:A:141:ILE:O	1:A:356:VAL:HG11	2.18	0.43
1:A:634:HIS:HD2	1:A:636:VAL:N	2.12	0.43
1:A:714:ASP:N	1:A:714:ASP:OD1	2.50	0.43
1:A:192:SER:HB3	1:A:195:GLU:HB2	2.00	0.42
1:A:219:LYS:HE2	1:A:351:HIS:NE2	2.34	0.42
1:A:177:GLN:N	1:A:178:PRO:CD	2.82	0.42
1:A:351:HIS:CD2	1:A:353:ARG:HB3	2.54	0.42
1:A:102:ILE:HA	1:A:102:ILE:HD12	1.85	0.42
1:A:118:THR:O	1:A:121:GLU:HB2	2.20	0.42
1:A:243:LYS:HZ1	5:A:748:ANP:HNB1	1.66	0.42
1:A:171:ASP:C	1:A:173:ARG:H	2.23	0.42
1:A:181:CYS:HB2	1:A:182:PRO:HD2	2.01	0.42
1:A:419:LEU:O	1:A:427:ILE:HD11	2.19	0.42
1:A:158:LEU:N	6:A:800:HOH:O	2.53	0.42
1:A:144:MET:SD	1:A:145:PRO:HA	2.60	0.42
1:A:502:ASP:HA	1:A:698:VAL:HG23	2.02	0.41
1:A:181:CYS:HB2	1:A:182:PRO:CD	2.50	0.41
1:A:225:HIS:CG	1:A:320:MET:HG3	2.56	0.41
1:A:115:GLU:HG2	1:A:121:GLU:OE1	2.20	0.41
1:A:413:VAL:HG11	1:A:732:LEU:HD23	2.02	0.41
1:A:159:CYS:HB2	1:A:160:PRO:HD2	2.03	0.41
1:A:112:CYS:SG	1:A:129:ILE:HG12	2.61	0.41
1:A:334:ASN:O	1:A:338:LEU:HG	2.21	0.41
1:A:126:TYR:HA	1:A:127:PRO:HD3	1.58	0.41
1:A:153:MET:HE1	1:A:353:ARG:HG3	2.01	0.41
1:A:502:ASP:OD2	1:A:514:GLY:HA2	2.21	0.40
1:A:312:GLN:HA	1:A:315:GLN:HE22	1.86	0.40
1:A:176:ALA:O	1:A:179:VAL:HG12	2.22	0.40
1:A:286:LEU:CD1	1:A:297:VAL:HG11	2.51	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	646/657 (98%)	615 (95%)	29 (4%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ARG
1	A	514	GLY

### 5.3.2 Protein sidechains [i](#)

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	509/513 (99%)	480 (94%)	29 (6%)	20	10

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	131	CYS
1	A	132	THR
1	A	133	HIS
1	A	151	THR
1	A	163	ASP
1	A	183	GLU
1	A	188	LEU
1	A	192	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	216	VAL
1	A	221	ILE
1	A	288	ASP
1	A	289	ASP
1	A	294	LEU
1	A	304	ASN
1	A	322	SER
1	A	325	LEU
1	A	328	LYS
1	A	335	GLU
1	A	367	SER
1	A	372	ARG
1	A	406	CYS
1	A	419	LEU
1	A	421	ASP
1	A	443	ASN
1	A	472	THR
1	A	679	LEU
1	A	722	SER
1	A	732	LEU

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	209	GLN
1	A	214	ASN
1	A	295	ASN
1	A	315	GLN
1	A	324	ASN
1	A	334	ASN
1	A	336	GLN
1	A	351	HIS
1	A	430	GLN
1	A	451	HIS
1	A	587	ASN
1	A	634	HIS
1	A	700	HIS

### 5.3.3 RNA ⓘ

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](#)

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$
5	ANP	A	748	-	29,33,33	2.12	10 (34%)	31,52,52	2.92	16 (51%)
4	ADP	A	747	2	24,29,29	1.63	4 (16%)	29,45,45	1.42	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
5	ANP	A	748	-	-	9/14/38/38	0/3/3/3
4	ADP	A	747	2	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	747	ADP	O4'-C1'	4.63	1.47	1.41
5	A	748	ANP	PG-O3G	-4.32	1.45	1.56
5	A	748	ANP	PB-O1B	3.88	1.52	1.46
5	A	748	ANP	PA-O5'	3.43	1.73	1.59
5	A	748	ANP	PG-O2G	-3.39	1.47	1.56
4	A	747	ADP	C5-C4	3.15	1.49	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	748	ANP	PA-O2A	-3.11	1.40	1.55
5	A	748	ANP	C5'-C4'	3.07	1.61	1.51
4	A	747	ADP	C2-N3	2.95	1.36	1.32
5	A	748	ANP	PB-O3A	2.92	1.62	1.59
5	A	748	ANP	PB-O2B	-2.90	1.48	1.56
5	A	748	ANP	C5-N7	-2.54	1.30	1.39
5	A	748	ANP	O4'-C1'	2.54	1.44	1.41
4	A	747	ADP	PA-O1A	2.11	1.58	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	748	ANP	O2A-PA-O5'	-7.99	70.62	107.75
5	A	748	ANP	O5'-PA-O1A	6.35	133.87	109.07
5	A	748	ANP	O4'-C4'-C5'	5.12	126.23	109.37
5	A	748	ANP	O5'-C5'-C4'	4.94	125.98	108.99
5	A	748	ANP	O4'-C1'-C2'	-4.39	100.51	106.93
5	A	748	ANP	C4-C5-N7	-3.99	105.24	109.40
5	A	748	ANP	O3'-C3'-C2'	-3.18	101.52	111.82
4	A	747	ADP	C4-C5-N7	-2.84	106.44	109.40
5	A	748	ANP	N3-C2-N1	-2.78	124.34	128.68
4	A	747	ADP	O3B-PB-O2B	2.75	118.15	107.64
4	A	747	ADP	O3A-PB-O1B	-2.63	96.57	111.19
4	A	747	ADP	N3-C2-N1	-2.62	124.58	128.68
5	A	748	ANP	O2G-PG-O1G	-2.55	107.04	113.45
5	A	748	ANP	C2'-C3'-C4'	2.41	107.33	102.64
5	A	748	ANP	O3'-C3'-C4'	-2.39	104.13	111.05
5	A	748	ANP	O2B-PB-O1B	2.37	114.90	109.92
5	A	748	ANP	PA-O5'-C5'	2.26	134.95	121.68
5	A	748	ANP	C1'-N9-C4	2.22	130.54	126.64
5	A	748	ANP	PA-O3A-PB	-2.22	124.80	132.62
4	A	747	ADP	O2'-C2'-C3'	-2.16	104.82	111.82
5	A	748	ANP	O4'-C4'-C3'	-2.01	101.14	105.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	748	ANP	PG-N3B-PB-O1B
5	A	748	ANP	C5'-O5'-PA-O1A
5	A	748	ANP	C4'-C5'-O5'-PA
5	A	748	ANP	O4'-C4'-C5'-O5'

*Continued on next page...*



*Continued from previous page...*

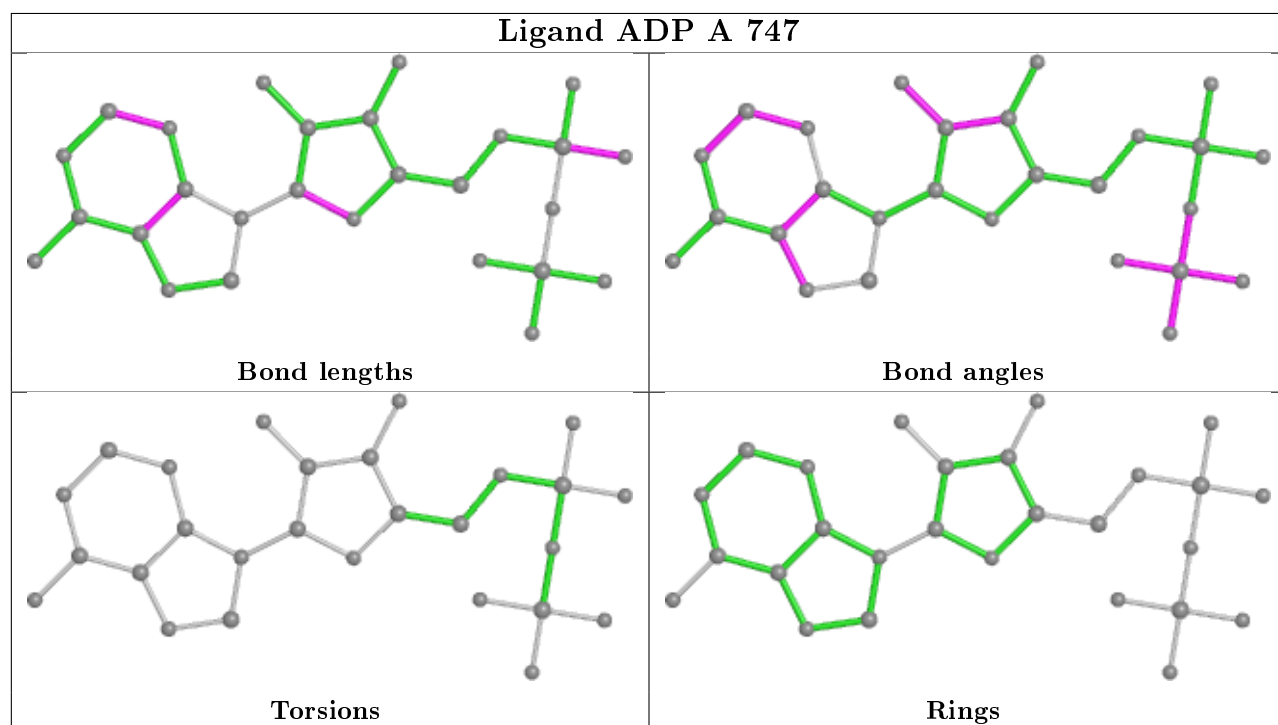
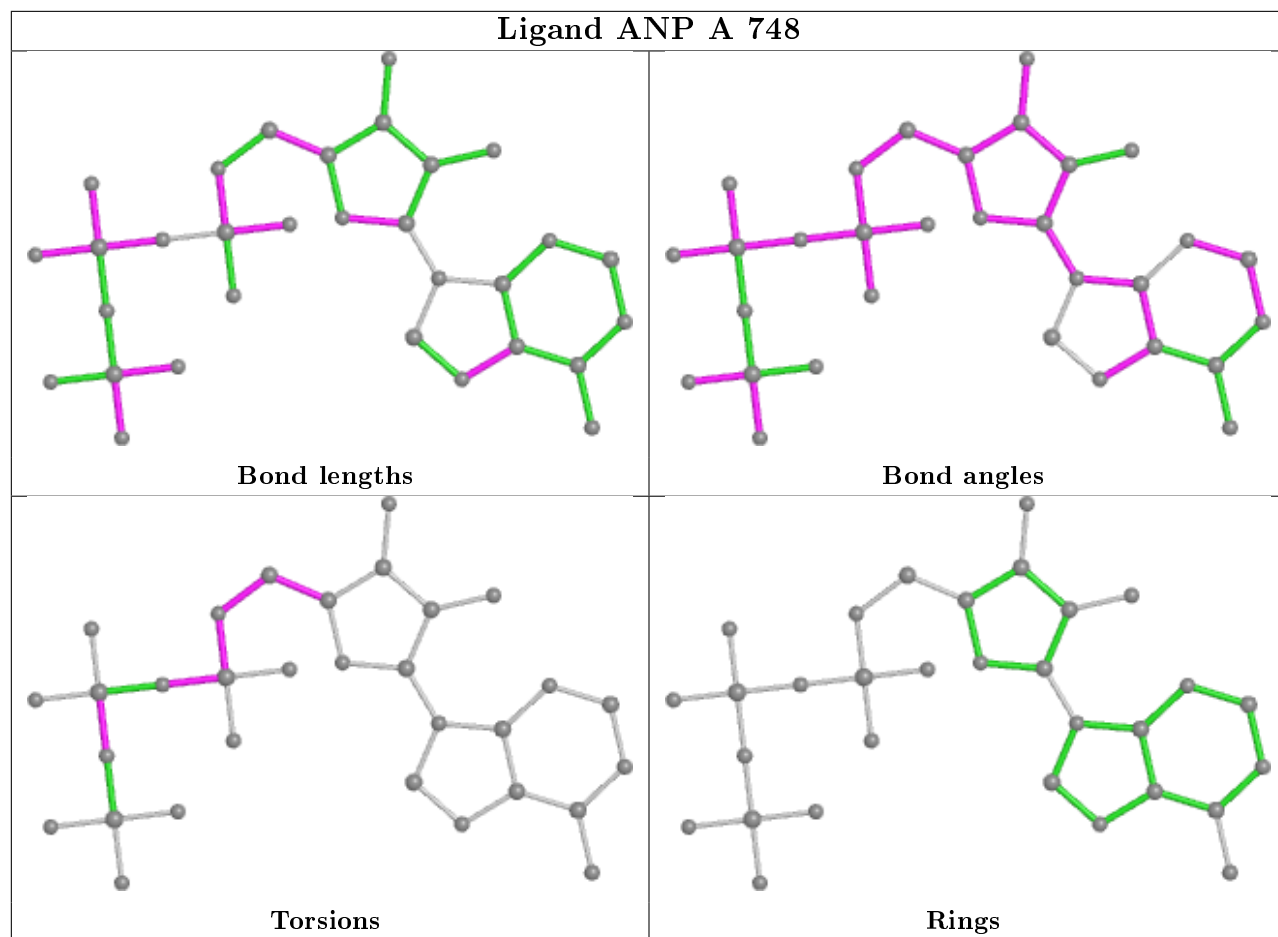
Mol	Chain	Res	Type	Atoms
5	A	748	ANP	C3'-C4'-C5'-O5'
5	A	748	ANP	PB-O3A-PA-O5'
5	A	748	ANP	C5'-O5'-PA-O3A
5	A	748	ANP	C5'-O5'-PA-O2A
5	A	748	ANP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	748	ANP	8	0
4	A	747	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 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

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	646/657 (98%)	0.63	66 (10%) 6 8	18, 29, 82, 112	4 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	TYR	13.5
1	A	170	LEU	9.0
1	A	174	PHE	8.4
1	A	175	HIS	7.4
1	A	146	TYR	7.0
1	A	149	PRO	6.4
1	A	160	PRO	6.1
1	A	150	PHE	6.0
1	A	180	ALA	5.8
1	A	159	CYS	5.7
1	A	179	VAL	5.4
1	A	157	PRO	5.2
1	A	167	ARG	5.0
1	A	327	GLY	4.9
1	A	172	ARG	4.8
1	A	154	ALA	4.8
1	A	163	ASP	4.7
1	A	156	PHE	4.7
1	A	144	MET	4.5
1	A	194	GLY	4.4
1	A	173	ARG	4.4
1	A	155	ALA	4.3
1	A	140	ILE	4.3
1	A	181	CYS	4.3
1	A	153	MET	4.2
1	A	424	ASP	4.2
1	A	164	LYS	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	112	CYS	4.0
1	A	169	PRO	4.0
1	A	178	PRO	4.0
1	A	185	GLY	3.8
1	A	184	CYS	3.6
1	A	202	ALA	3.6
1	A	158	LEU	3.5
1	A	193	HIS	3.3
1	A	113	LEU	3.3
1	A	124	TYR	3.2
1	A	147	ASP	3.2
1	A	152	VAL	3.2
1	A	344	ILE	3.1
1	A	425	ASP	3.0
1	A	191	VAL	3.0
1	A	187	TYR	2.9
1	A	177	GLN	2.8
1	A	148	ARG	2.7
1	A	350	ILE	2.7
1	A	183	GLU	2.7
1	A	201	ALA	2.7
1	A	189	GLU	2.7
1	A	111	ALA	2.5
1	A	190	TRP	2.4
1	A	161	ALA	2.4
1	A	123	ARG	2.4
1	A	309	LEU	2.4
1	A	165	GLU	2.4
1	A	171	ASP	2.3
1	A	338	LEU	2.3
1	A	119	PRO	2.3
1	A	122	ARG	2.2
1	A	118	THR	2.2
1	A	132	THR	2.2
1	A	212	MET	2.1
1	A	345	ALA	2.1
1	A	162	CYS	2.1
1	A	199	GLN	2.1
1	A	462	TRP	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

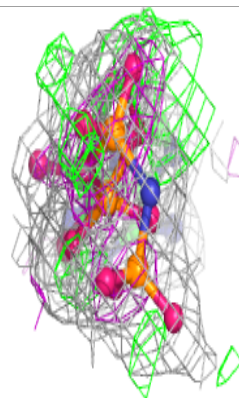
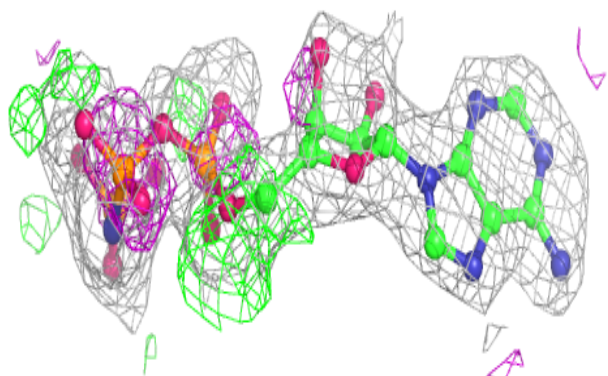
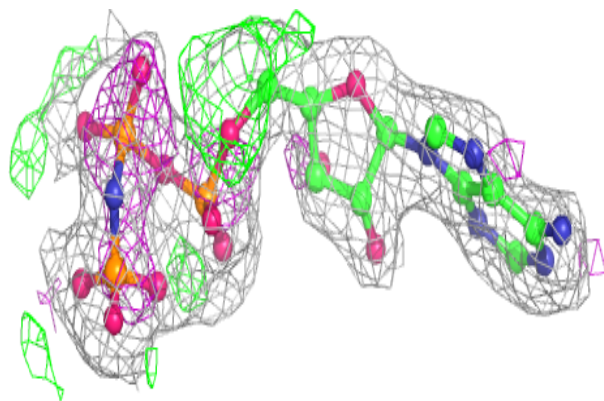
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	ANP	A	748	31/31	0.83	0.15	23,30,36,39	0
2	ZN	A	2	1/1	0.92	0.05	78,78,78,78	0
4	ADP	A	747	27/27	0.94	0.12	23,32,37,37	0
2	ZN	A	1	1/1	0.97	0.04	58,58,58,58	0
3	MG	A	4	1/1	0.98	0.06	19,19,19,19	0
2	ZN	A	3	1/1	0.99	0.05	35,35,35,35	0

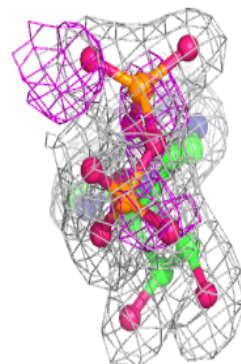
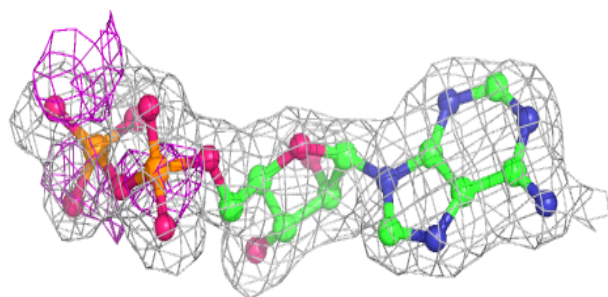
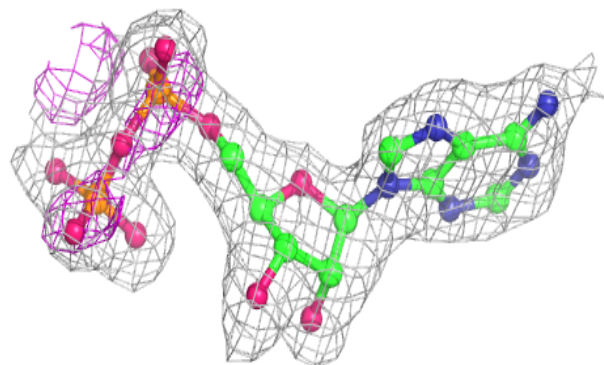
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ANP A 748:**

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

**Electron density around ADP A 747:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.