



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 11:31 AM UTC

PDB ID : 3CF2 / pdb_00003cf2
Title : Structure of P97/vcp in complex with ADP/AMP-PNP
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.
Deposited on : 2008-03-01
Resolution : 3.50 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 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 : **FAILED**
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

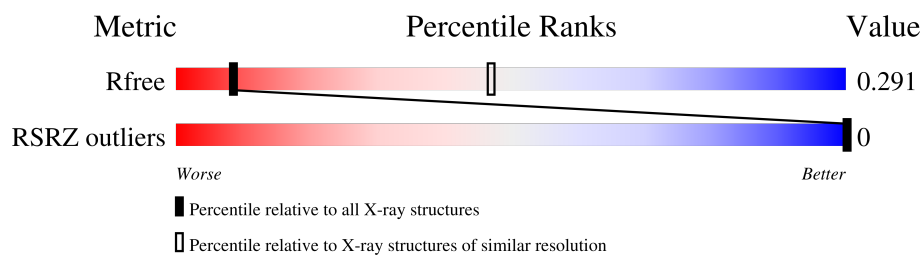
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20917 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	0	0
			5172	3263	903	977	29			
1	B	659	Total	C	N	O	S	0	0	0
			5172	3263	903	977	29			
1	C	659	Total	C	N	O	S	0	0	0
			5172	3263	903	977	29			
1	D	659	Total	C	N	O	S	0	0	0
			5169	3260	903	977	29			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



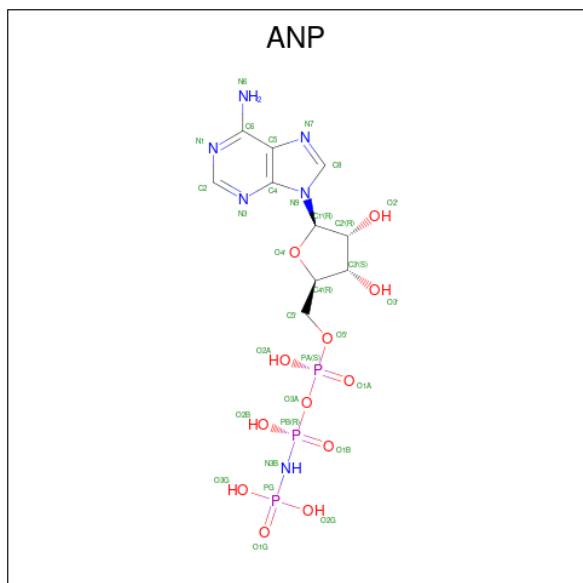
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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



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

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3 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	144.90Å 144.90Å 164.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.00 – 3.50 23.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.00-3.50) 99.5 (23.00-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.23Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.285 0.289 , 0.291	Depositor DCC
R_{free} test set	6358 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 89.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.369 for -h,-k,l 0.377 for h,-h-k,-l 0.369 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20917	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

8 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
3	ANP	A	901	-	33,33,33	2.06	12 (36%)	45,52,52	2.06	10 (22%)
2	ADP	B	807	-	28,29,29	1.89	4 (14%)	43,45,45	2.05	8 (18%)
2	ADP	C	807	-	28,29,29	1.89	4 (14%)	43,45,45	2.06	8 (18%)
2	ADP	D	807	-	28,29,29	1.89	4 (14%)	43,45,45	2.06	8 (18%)
3	ANP	B	901	-	33,33,33	2.06	12 (36%)	45,52,52	2.06	10 (22%)
3	ANP	D	901	-	33,33,33	2.06	12 (36%)	45,52,52	2.07	10 (22%)
2	ADP	A	807	-	28,29,29	1.89	4 (14%)	43,45,45	2.06	8 (18%)
3	ANP	C	901	-	33,33,33	2.05	12 (36%)	45,52,52	2.06	10 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	901	-	-	7/18/38/38	0/3/3/3
2	ADP	B	807	-	-	6/16/32/32	0/3/3/3
2	ADP	C	807	-	-	6/16/32/32	0/3/3/3
2	ADP	D	807	-	-	6/16/32/32	0/3/3/3
3	ANP	B	901	-	-	7/18/38/38	0/3/3/3
3	ANP	D	901	-	-	7/18/38/38	0/3/3/3
2	ADP	A	807	-	-	6/16/32/32	0/3/3/3
3	ANP	C	901	-	-	7/18/38/38	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	ADP	PA-O3A	-5.34	1.53	1.59
2	C	807	ADP	PA-O3A	-5.33	1.53	1.59
2	D	807	ADP	PA-O3A	-5.33	1.53	1.59
2	B	807	ADP	PA-O3A	-5.33	1.53	1.59
2	B	807	ADP	C5-N7	-5.13	1.29	1.39
2	A	807	ADP	C5-N7	-5.13	1.29	1.39
2	D	807	ADP	C5-N7	-5.12	1.29	1.39
2	C	807	ADP	C5-N7	-5.11	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	ANP	PB-N3B	-4.48	1.51	1.63
3	C	901	ANP	PB-N3B	-4.47	1.51	1.63
3	A	901	ANP	PB-N3B	-4.46	1.51	1.63
3	D	901	ANP	PB-N3B	-4.45	1.51	1.63
3	B	901	ANP	PG-N3B	-4.28	1.52	1.63
3	C	901	ANP	PG-N3B	-4.28	1.52	1.63
3	A	901	ANP	PG-N3B	-4.27	1.52	1.63
3	D	901	ANP	PG-N3B	-4.26	1.52	1.63
3	B	901	ANP	C5-N7	-4.08	1.31	1.39
3	A	901	ANP	C5-N7	-4.07	1.31	1.39
3	D	901	ANP	C5-N7	-4.06	1.31	1.39
3	C	901	ANP	C5-N7	-4.05	1.31	1.39
2	A	807	ADP	C4-N9	-3.10	1.31	1.37
2	D	807	ADP	C4-N9	-3.10	1.31	1.37
2	B	807	ADP	C4-N9	-3.08	1.31	1.37
2	C	807	ADP	C4-N9	-3.05	1.31	1.37
3	B	901	ANP	C1'-N9	2.99	1.54	1.46
3	C	901	ANP	C1'-N9	2.98	1.54	1.46
3	A	901	ANP	C1'-N9	2.98	1.54	1.46
3	D	901	ANP	C1'-N9	2.98	1.54	1.46
3	B	901	ANP	C5-C4	2.75	1.44	1.39
3	A	901	ANP	C5-C4	2.74	1.44	1.39
3	D	901	ANP	C5-C4	2.74	1.44	1.39
3	D	901	ANP	PG-O1G	2.73	1.50	1.46
3	C	901	ANP	C5-C4	2.73	1.44	1.39
3	B	901	ANP	PG-O1G	2.71	1.50	1.46
3	A	901	ANP	PG-O1G	2.69	1.50	1.46
3	C	901	ANP	PG-O1G	2.68	1.50	1.46
3	D	901	ANP	C4-N3	2.64	1.39	1.34
3	C	901	ANP	C4-N3	2.60	1.39	1.34
3	B	901	ANP	C4-N3	2.58	1.39	1.34
3	A	901	ANP	C4-N3	2.58	1.39	1.34
3	D	901	ANP	C5'-C4'	2.50	1.59	1.51
3	A	901	ANP	C5'-C4'	2.49	1.59	1.51
3	B	901	ANP	C5'-C4'	2.49	1.59	1.51
3	C	901	ANP	C5'-C4'	2.49	1.59	1.51
3	D	901	ANP	PG-O3G	-2.44	1.50	1.56
3	A	901	ANP	PG-O3G	-2.42	1.50	1.56
3	C	901	ANP	PG-O3G	-2.42	1.50	1.56
3	B	901	ANP	PG-O3G	-2.41	1.50	1.56
3	C	901	ANP	PB-O1B	2.38	1.49	1.46
3	D	901	ANP	PB-O1B	2.34	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ANP	PB-O1B	2.34	1.49	1.46
3	B	901	ANP	PB-O1B	2.33	1.49	1.46
2	A	807	ADP	PA-O2A	-2.07	1.45	1.55
2	C	807	ADP	PA-O2A	-2.07	1.45	1.55
2	B	807	ADP	PA-O2A	-2.07	1.45	1.55
2	D	807	ADP	PA-O2A	-2.07	1.45	1.55
3	B	901	ANP	PG-O2G	2.06	1.62	1.56
3	C	901	ANP	O4'-C1'	2.06	1.46	1.42
3	C	901	ANP	PG-O2G	2.05	1.62	1.56
3	A	901	ANP	PG-O2G	2.05	1.62	1.56
3	D	901	ANP	O4'-C1'	2.05	1.46	1.42
3	A	901	ANP	O4'-C1'	2.04	1.46	1.42
3	D	901	ANP	PG-O2G	2.03	1.62	1.56
3	B	901	ANP	O4'-C1'	2.01	1.46	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	807	ADP	N3-C2-N1	-6.95	118.06	128.58
2	A	807	ADP	N3-C2-N1	-6.94	118.07	128.58
2	D	807	ADP	N3-C2-N1	-6.93	118.08	128.58
2	B	807	ADP	N3-C2-N1	-6.92	118.11	128.58
3	B	901	ANP	N3-C2-N1	-6.90	118.14	128.58
3	A	901	ANP	N3-C2-N1	-6.89	118.16	128.58
3	D	901	ANP	N3-C2-N1	-6.88	118.17	128.58
3	C	901	ANP	N3-C2-N1	-6.87	118.18	128.58
2	A	807	ADP	C5-C4-N3	-5.33	119.38	126.72
2	C	807	ADP	C5-C4-N3	-5.31	119.41	126.72
2	D	807	ADP	C5-C4-N3	-5.31	119.41	126.72
3	D	901	ANP	C5-C4-N3	-5.30	119.42	126.72
2	B	807	ADP	C5-C4-N3	-5.29	119.44	126.72
3	C	901	ANP	C5-C4-N3	-5.27	119.45	126.72
3	B	901	ANP	C5-C4-N3	-5.27	119.46	126.72
3	A	901	ANP	C5-C4-N3	-5.26	119.47	126.72
3	B	901	ANP	C2-N3-C4	4.50	122.82	111.83
3	D	901	ANP	C2-N3-C4	4.50	122.81	111.83
3	A	901	ANP	C2-N3-C4	4.50	122.81	111.83
3	C	901	ANP	C2-N3-C4	4.49	122.80	111.83
2	A	807	ADP	C2-N3-C4	4.37	122.50	111.83
2	C	807	ADP	C2-N3-C4	4.37	122.49	111.83
2	D	807	ADP	C2-N3-C4	4.35	122.46	111.83
2	B	807	ADP	C2-N3-C4	4.34	122.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	ADP	N3-C4-N9	4.15	134.22	127.17
3	C	901	ANP	N3-C4-N9	4.15	134.22	127.17
2	C	807	ADP	N3-C4-N9	4.15	134.22	127.17
3	D	901	ANP	N3-C4-N9	4.14	134.21	127.17
3	A	901	ANP	N3-C4-N9	4.14	134.21	127.17
2	B	807	ADP	N3-C4-N9	4.14	134.20	127.17
2	D	807	ADP	N3-C4-N9	4.14	134.20	127.17
3	B	901	ANP	N3-C4-N9	4.13	134.19	127.17
3	D	901	ANP	C5-N7-C8	3.42	108.83	103.45
3	B	901	ANP	C5-N7-C8	3.40	108.79	103.45
3	A	901	ANP	C5-N7-C8	3.39	108.77	103.45
3	C	901	ANP	C5-N7-C8	3.38	108.76	103.45
2	D	807	ADP	C5-N7-C8	3.34	108.69	103.45
2	C	807	ADP	C5-N7-C8	3.33	108.68	103.45
2	A	807	ADP	C5-N7-C8	3.33	108.68	103.45
2	B	807	ADP	C5-N7-C8	3.31	108.65	103.45
2	D	807	ADP	N9-C8-N7	-2.86	109.88	113.94
2	A	807	ADP	N9-C8-N7	-2.85	109.89	113.94
2	C	807	ADP	N9-C8-N7	-2.84	109.91	113.94
2	B	807	ADP	N9-C8-N7	-2.82	109.94	113.94
2	A	807	ADP	C4-C5-N7	-2.76	107.42	110.58
2	C	807	ADP	C4-C5-N7	-2.75	107.43	110.58
2	D	807	ADP	C4-C5-N7	-2.75	107.43	110.58
2	B	807	ADP	C4-C5-N7	-2.74	107.45	110.58
3	D	901	ANP	C4-C5-N7	-2.70	107.50	110.58
3	C	901	ANP	C4-C5-N7	-2.63	107.57	110.58
3	B	901	ANP	C4-C5-N7	-2.63	107.57	110.58
3	A	901	ANP	C4-C5-N7	-2.63	107.58	110.58
2	B	807	ADP	C2'-C3'-C4'	2.62	107.66	102.61
2	D	807	ADP	C2'-C3'-C4'	2.60	107.63	102.61
2	C	807	ADP	C2'-C3'-C4'	2.59	107.62	102.61
2	A	807	ADP	C2'-C3'-C4'	2.59	107.62	102.61
3	B	901	ANP	N9-C8-N7	-2.58	110.28	113.94
3	A	901	ANP	N9-C8-N7	-2.56	110.31	113.94
3	D	901	ANP	N9-C8-N7	-2.56	110.31	113.94
3	C	901	ANP	N9-C8-N7	-2.55	110.32	113.94
3	D	901	ANP	C2'-C3'-C4'	2.50	107.43	102.61
3	A	901	ANP	C2'-C3'-C4'	2.49	107.42	102.61
3	B	901	ANP	C2'-C3'-C4'	2.48	107.41	102.61
3	C	901	ANP	C2'-C3'-C4'	2.48	107.41	102.61
3	B	901	ANP	C2-N1-C6	2.20	122.34	118.73
3	D	901	ANP	C2-N1-C6	2.19	122.33	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	ANP	C2-N1-C6	2.18	122.31	118.73
3	A	901	ANP	C2-N1-C6	2.18	122.31	118.73
3	D	901	ANP	O1G-PG-N3B	-2.11	108.66	111.77
3	A	901	ANP	O1G-PG-N3B	-2.09	108.69	111.77
3	C	901	ANP	O1G-PG-N3B	-2.07	108.72	111.77
3	B	901	ANP	O1G-PG-N3B	-2.05	108.75	111.77

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	807	ADP	C5'-O5'-PA-O1A
2	A	807	ADP	C5'-O5'-PA-O2A
2	A	807	ADP	C5'-O5'-PA-O3A
2	A	807	ADP	O4'-C4'-C5'-O5'
2	B	807	ADP	C5'-O5'-PA-O1A
2	B	807	ADP	C5'-O5'-PA-O2A
2	B	807	ADP	C5'-O5'-PA-O3A
2	B	807	ADP	O4'-C4'-C5'-O5'
2	C	807	ADP	C5'-O5'-PA-O1A
2	C	807	ADP	C5'-O5'-PA-O2A
2	C	807	ADP	C5'-O5'-PA-O3A
2	C	807	ADP	O4'-C4'-C5'-O5'
2	D	807	ADP	C5'-O5'-PA-O1A
2	D	807	ADP	C5'-O5'-PA-O2A
2	D	807	ADP	C5'-O5'-PA-O3A
2	D	807	ADP	O4'-C4'-C5'-O5'
3	A	901	ANP	PG-N3B-PB-O1B
3	A	901	ANP	PG-N3B-PB-O3A
3	A	901	ANP	C5'-O5'-PA-O1A
3	A	901	ANP	C5'-O5'-PA-O2A
3	A	901	ANP	C5'-O5'-PA-O3A
3	B	901	ANP	PG-N3B-PB-O1B
3	B	901	ANP	PG-N3B-PB-O3A
3	B	901	ANP	C5'-O5'-PA-O1A
3	B	901	ANP	C5'-O5'-PA-O2A
3	B	901	ANP	C5'-O5'-PA-O3A
3	C	901	ANP	PG-N3B-PB-O1B
3	C	901	ANP	PG-N3B-PB-O3A
3	C	901	ANP	C5'-O5'-PA-O1A
3	C	901	ANP	C5'-O5'-PA-O2A
3	C	901	ANP	C5'-O5'-PA-O3A

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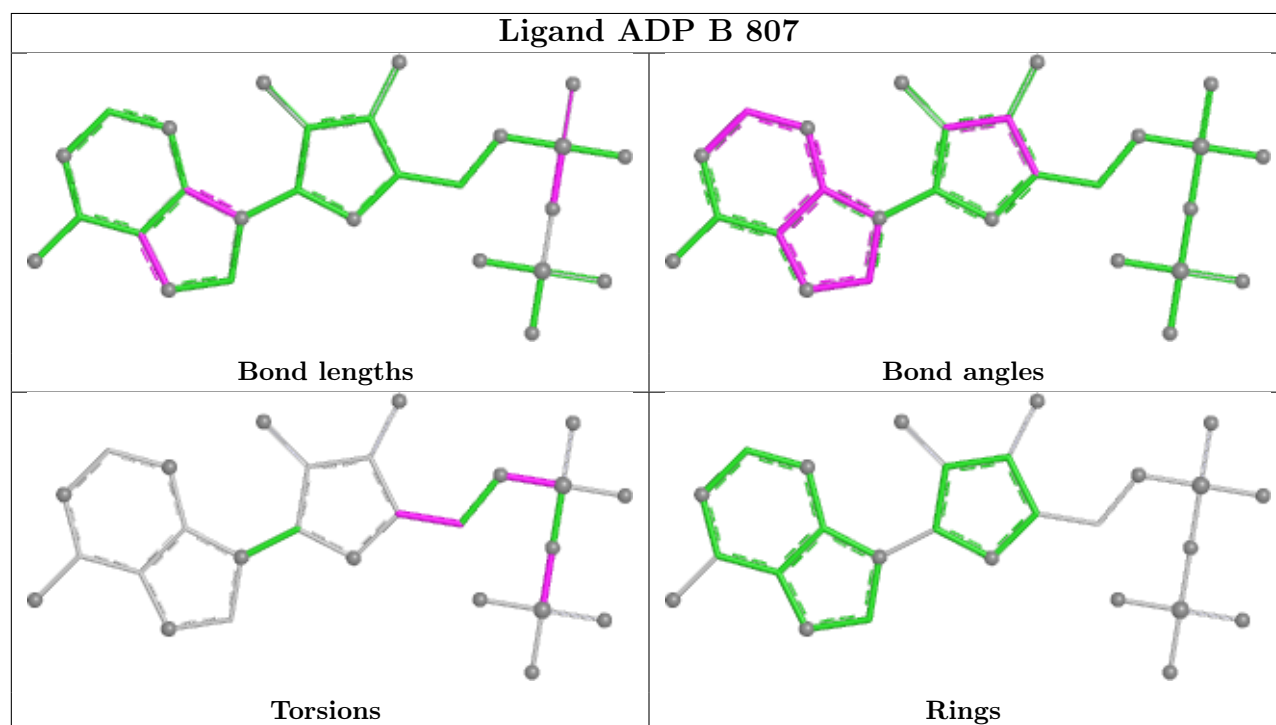
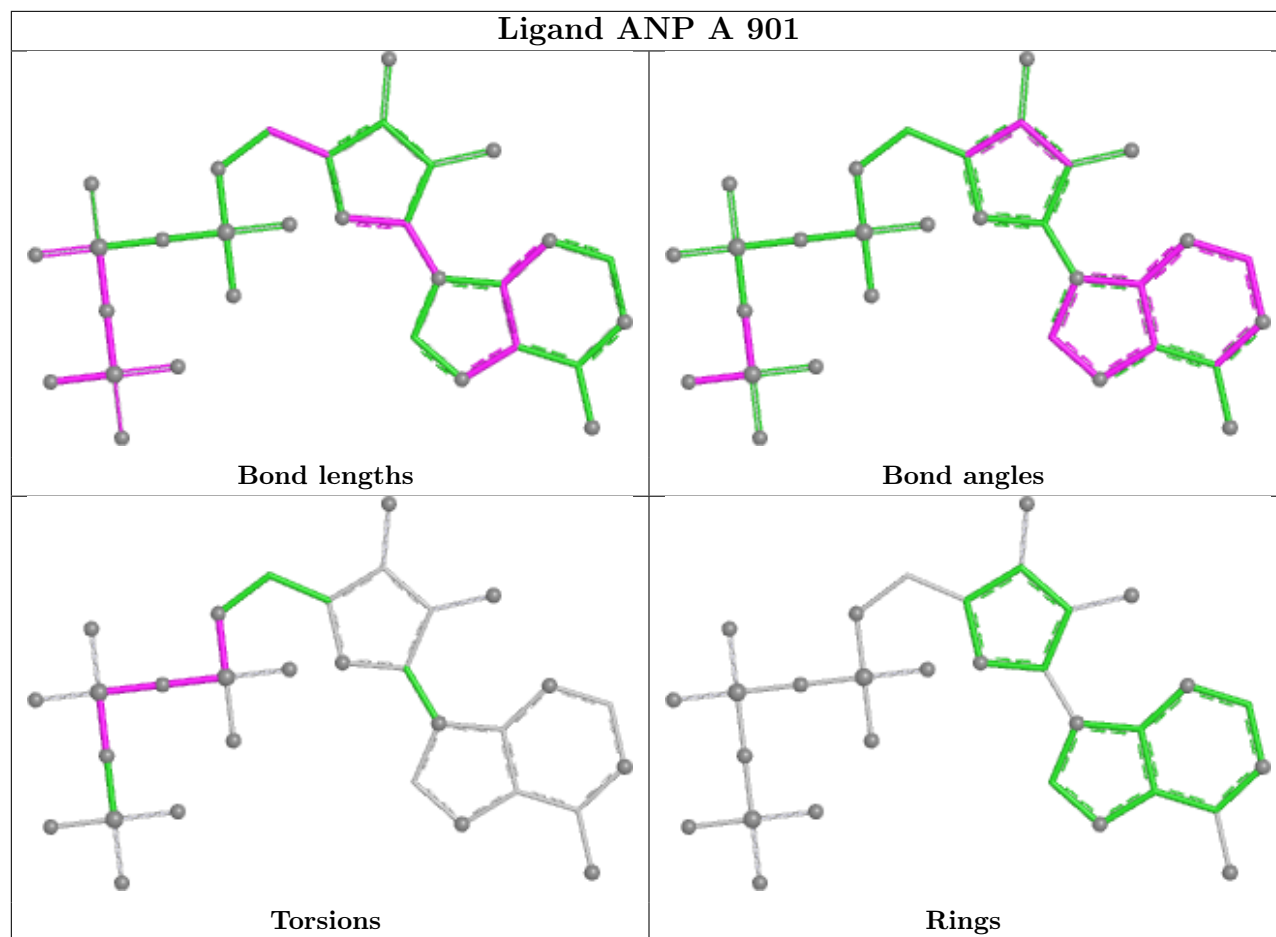
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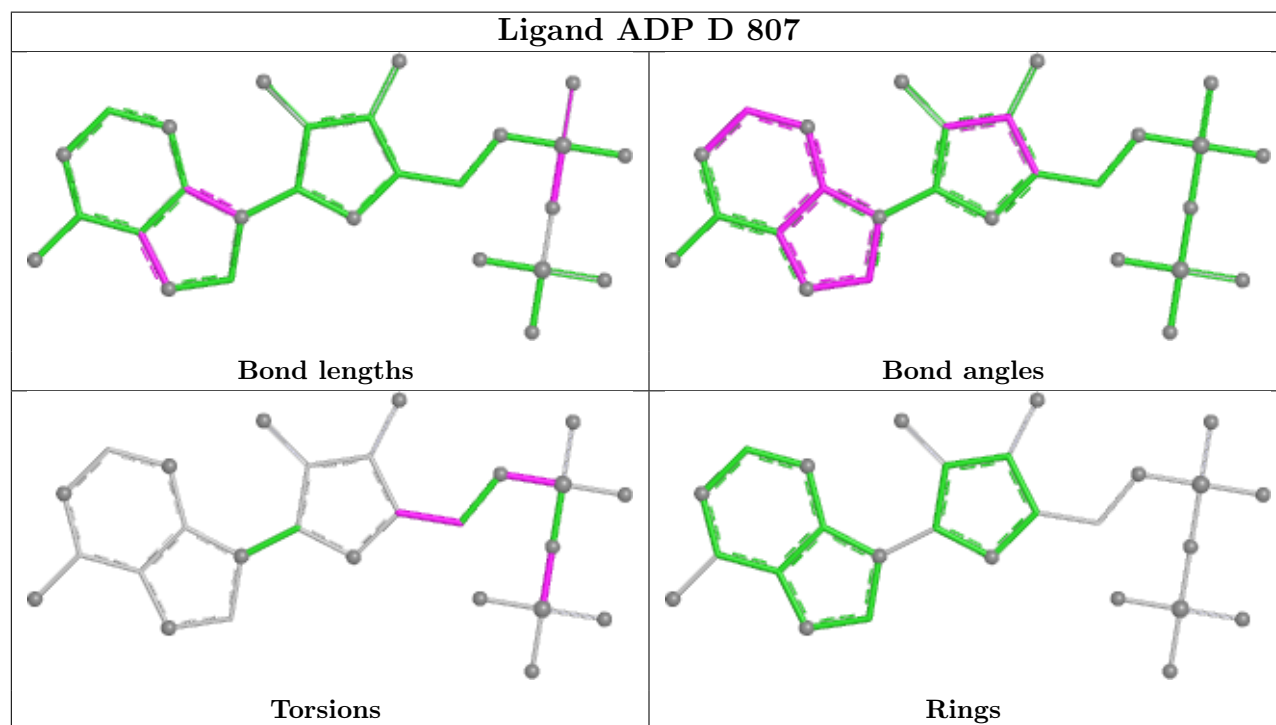
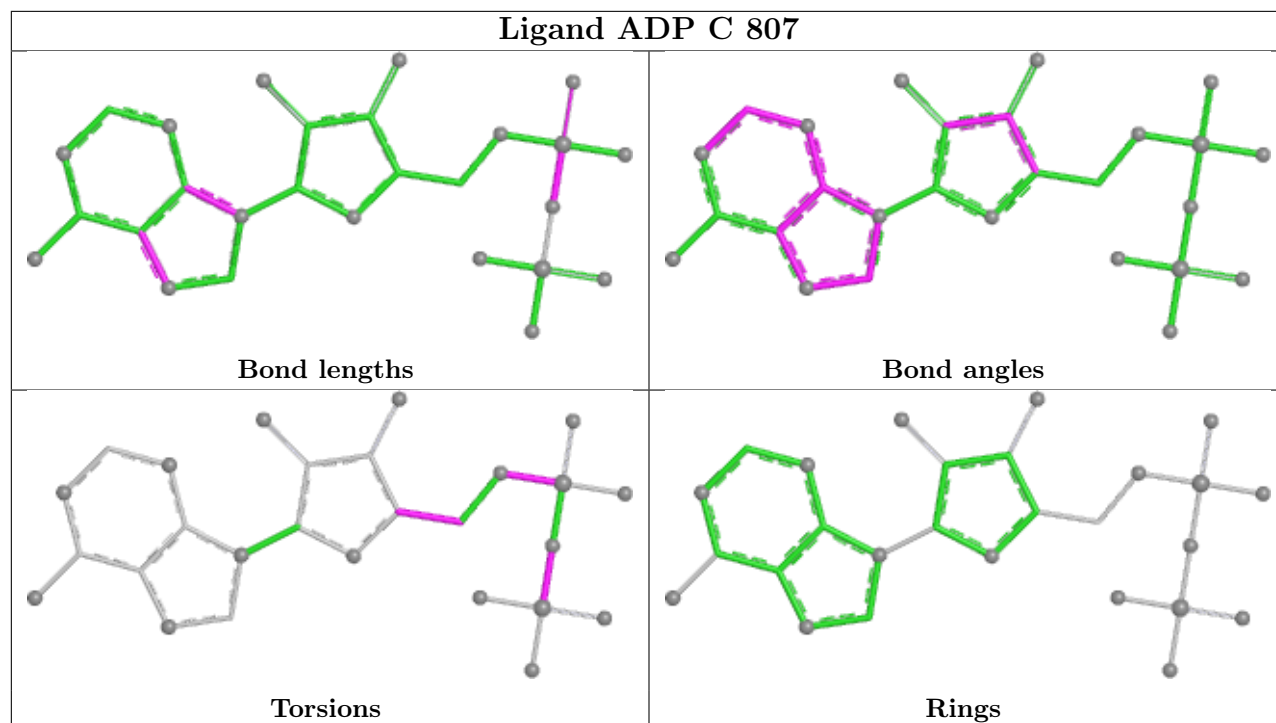
Mol	Chain	Res	Type	Atoms
3	D	901	ANP	PG-N3B-PB-O1B
3	D	901	ANP	PG-N3B-PB-O3A
3	D	901	ANP	C5'-O5'-PA-O1A
3	D	901	ANP	C5'-O5'-PA-O2A
3	D	901	ANP	C5'-O5'-PA-O3A
2	A	807	ADP	C3'-C4'-C5'-O5'
2	B	807	ADP	C3'-C4'-C5'-O5'
2	C	807	ADP	C3'-C4'-C5'-O5'
2	D	807	ADP	C3'-C4'-C5'-O5'
3	A	901	ANP	PB-O3A-PA-O1A
3	B	901	ANP	PB-O3A-PA-O1A
3	C	901	ANP	PB-O3A-PA-O1A
3	D	901	ANP	PB-O3A-PA-O1A
2	A	807	ADP	PA-O3A-PB-O3B
2	B	807	ADP	PA-O3A-PB-O3B
2	C	807	ADP	PA-O3A-PB-O3B
2	D	807	ADP	PA-O3A-PB-O3B
3	A	901	ANP	PA-O3A-PB-O1B
3	B	901	ANP	PA-O3A-PB-O1B
3	C	901	ANP	PA-O3A-PB-O1B
3	D	901	ANP	PA-O3A-PB-O1B

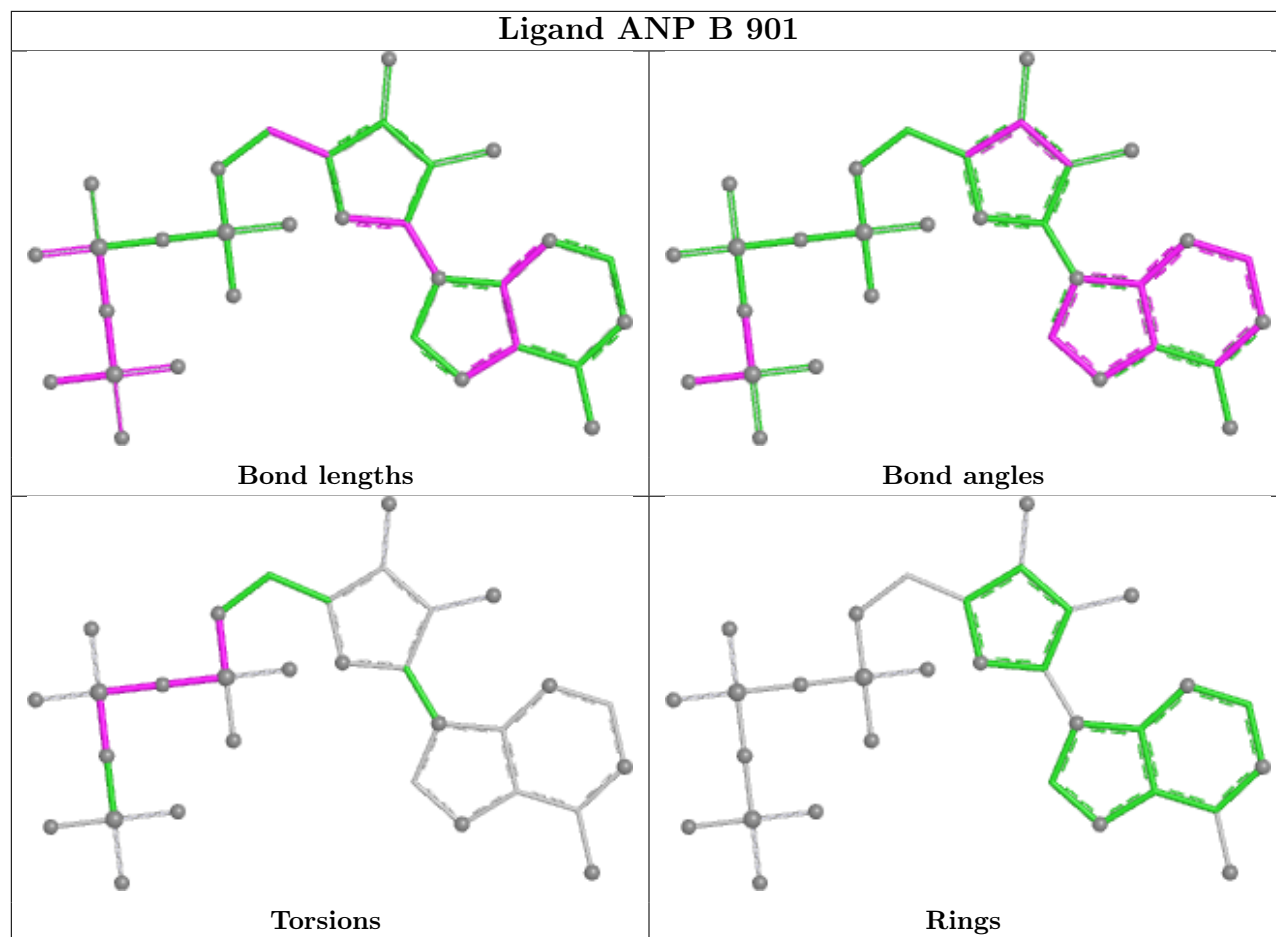
There are no ring outliers.

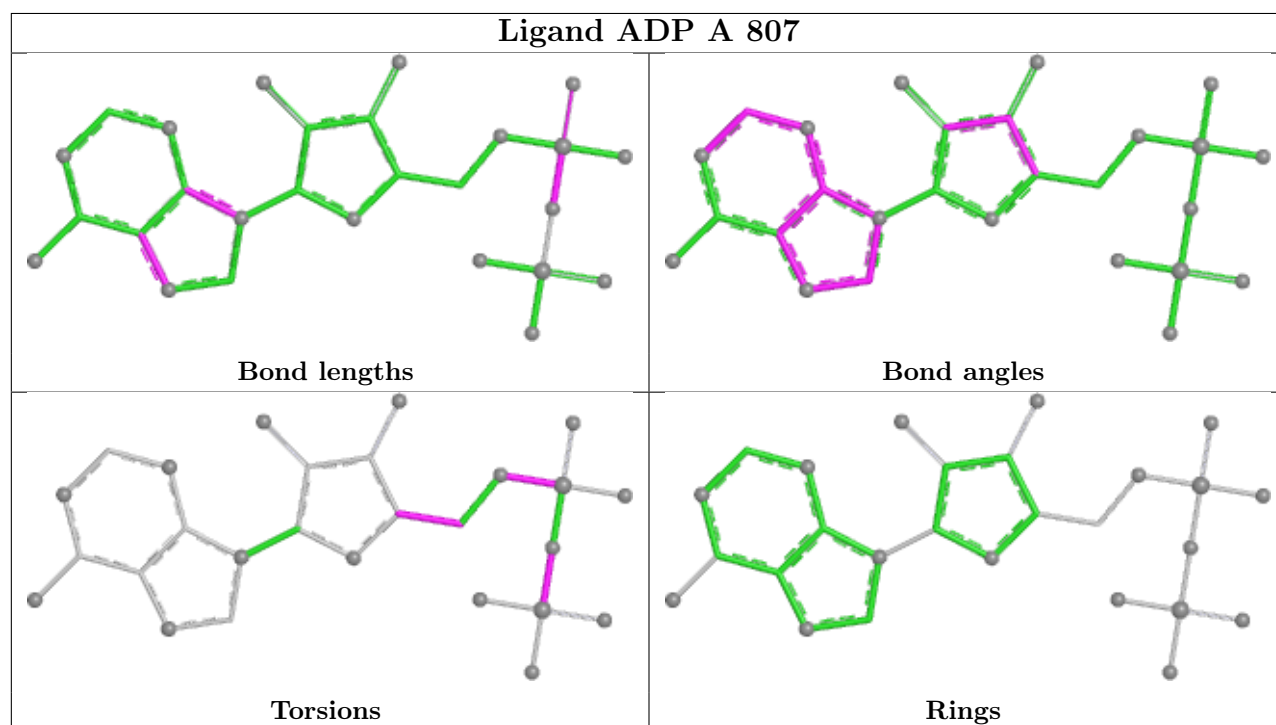
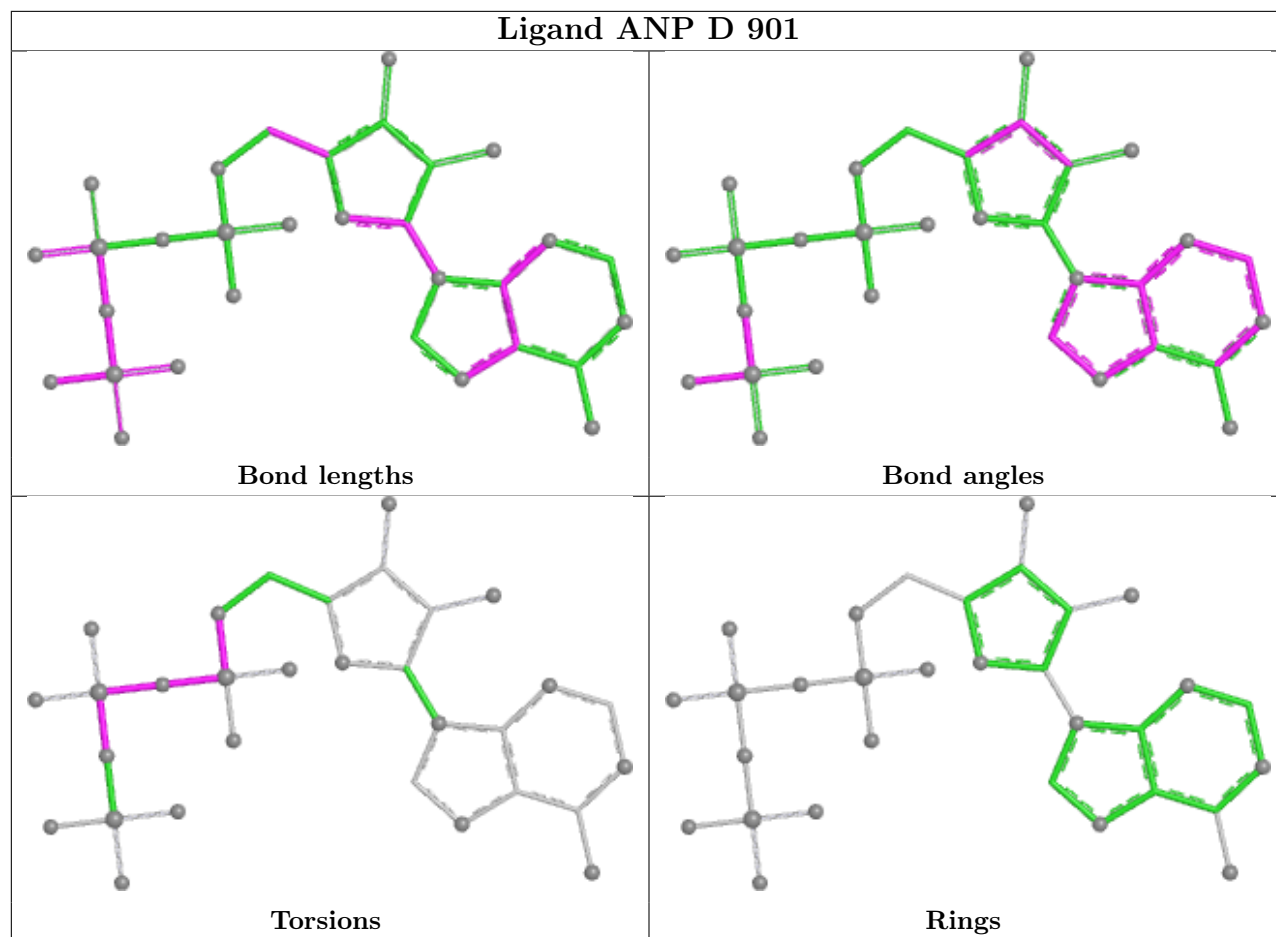
No monomer is involved in short contacts.

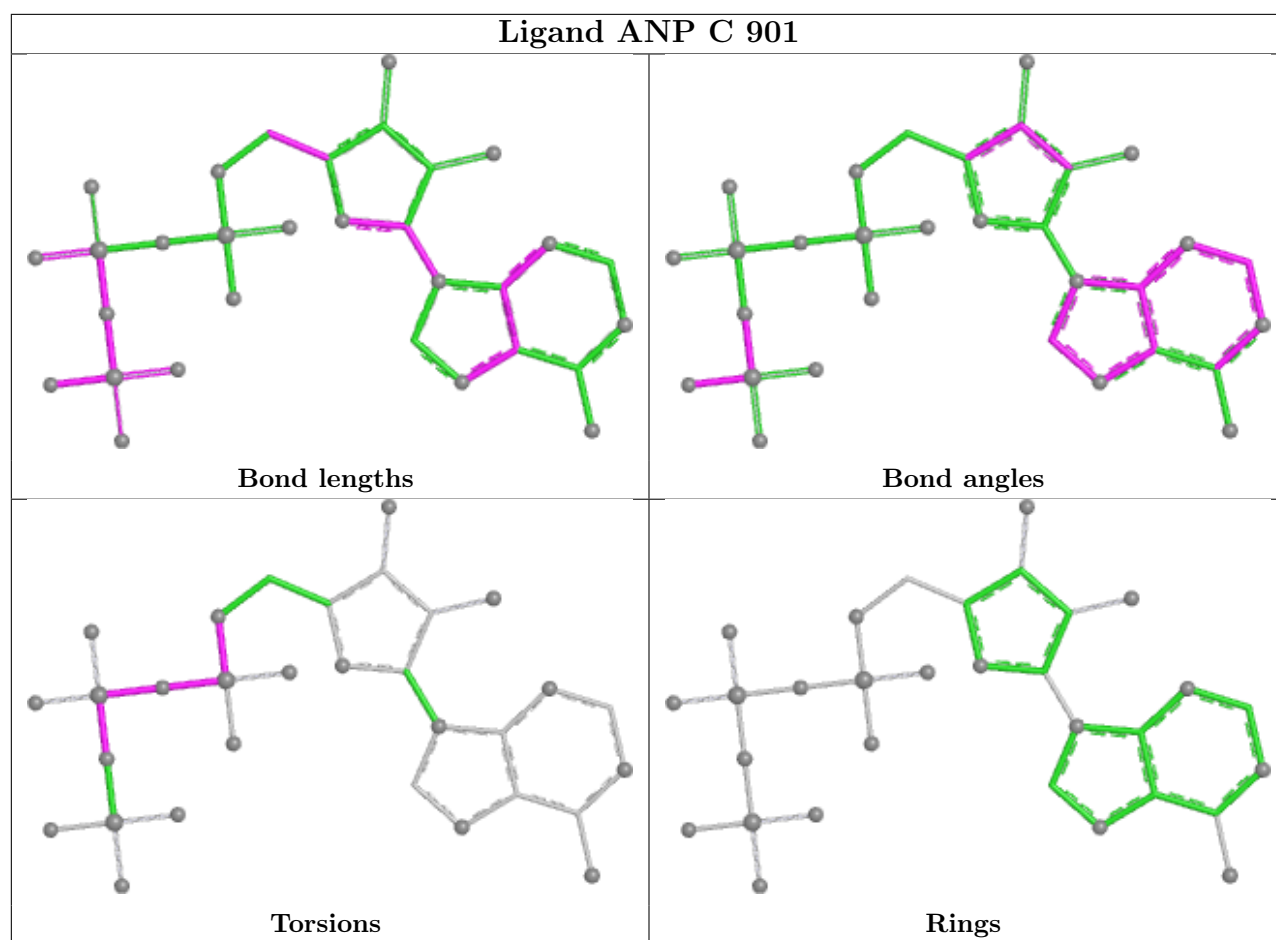
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2
1	C	2
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	438:ASP	C	439:ALA	N	1.17
1	B	438:ASP	C	439:ALA	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	438:ASP	C	439:ALA	N	1.17
1	D	438:ASP	C	439:ALA	N	1.17
1	A	425:LYS	C	426:LYS	N	1.06
1	B	425:LYS	C	426:LYS	N	1.06
1	C	425:LYS	C	426:LYS	N	1.06
1	D	425:LYS	C	426:LYS	N	1.06

5 Fit of model and data [i](#)

5.1 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	659/806 (81%)	-1.23	0 100 100	17, 128, 281, 412	0
1	B	659/806 (81%)	-1.22	0 100 100	17, 128, 281, 412	0
1	C	659/806 (81%)	-1.21	0 100 100	17, 128, 281, 412	0
1	D	659/806 (81%)	-1.24	0 100 100	17, 128, 281, 412	0
All	All	2636/3224 (81%)	-1.22	0 100 100	17, 128, 281, 412	0

There are no RSRZ outliers to report.

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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.

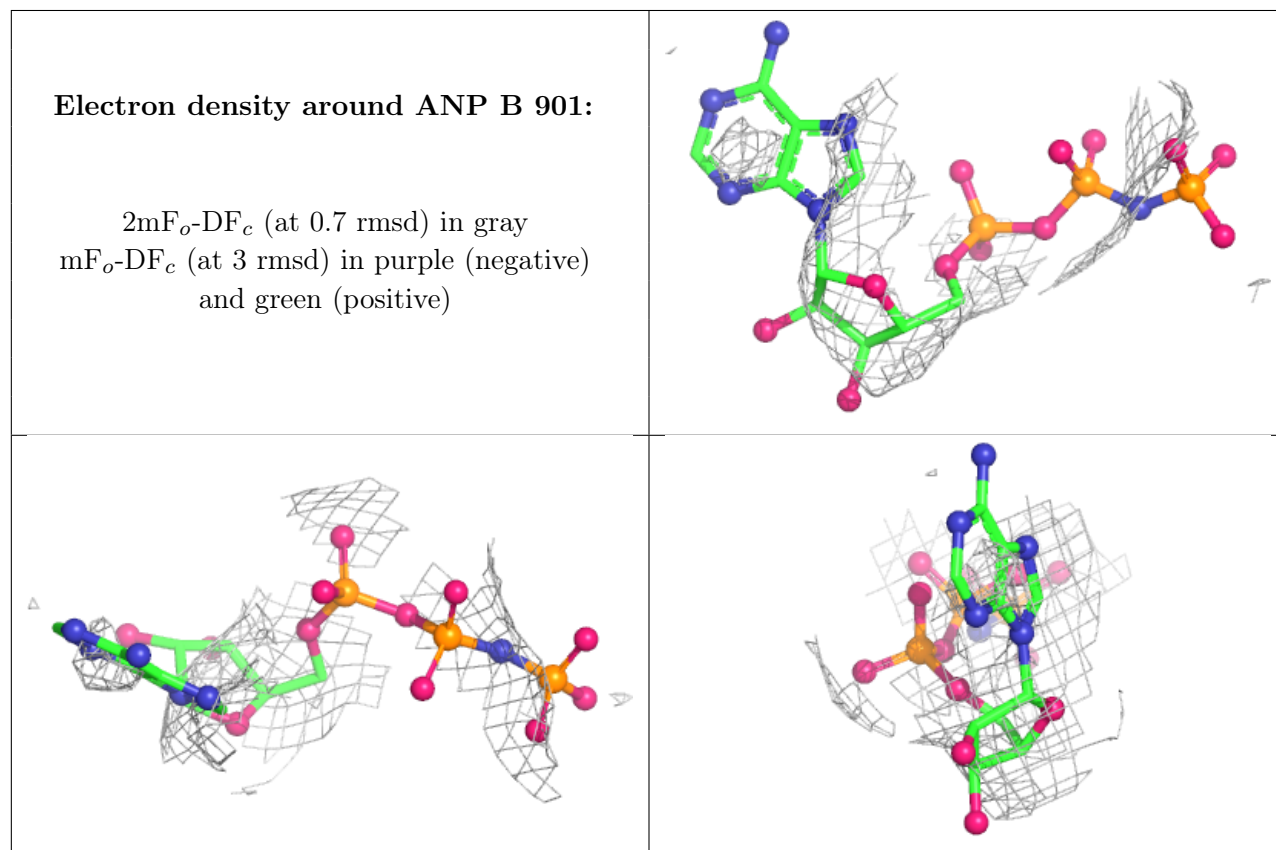
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	B	901	31/31	0.98	0.03	150,150,150,150	0
3	ANP	C	901	31/31	0.98	0.04	150,150,150,150	0
2	ADP	C	807	27/27	0.99	0.04	163,163,163,163	0
2	ADP	D	807	27/27	0.99	0.04	163,163,163,163	0

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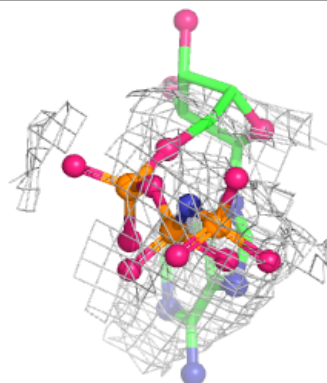
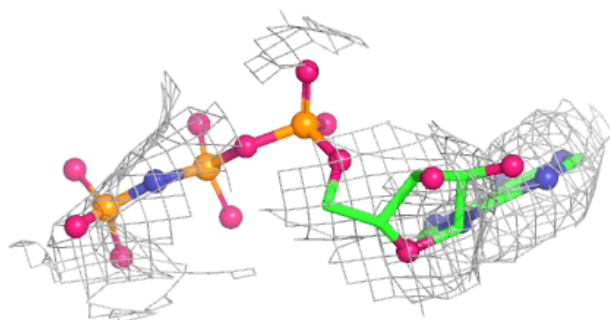
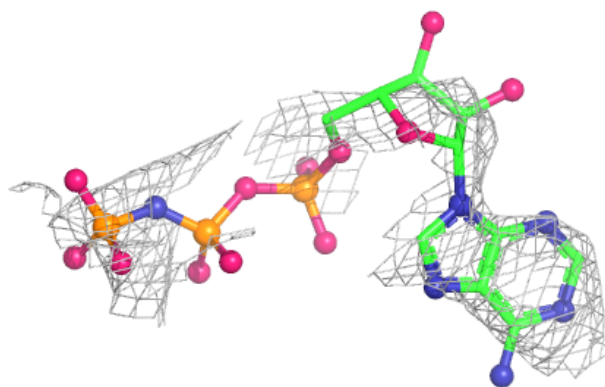
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	A	901	31/31	0.99	0.03	150,150,150,150	0
2	ADP	A	807	27/27	0.99	0.04	163,163,163,163	0
2	ADP	B	807	27/27	0.99	0.04	163,163,163,163	0
3	ANP	D	901	31/31	0.99	0.03	150,150,150,150	0

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.



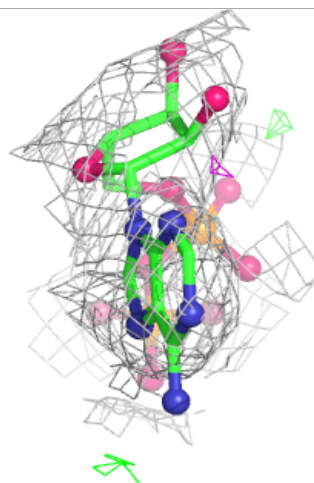
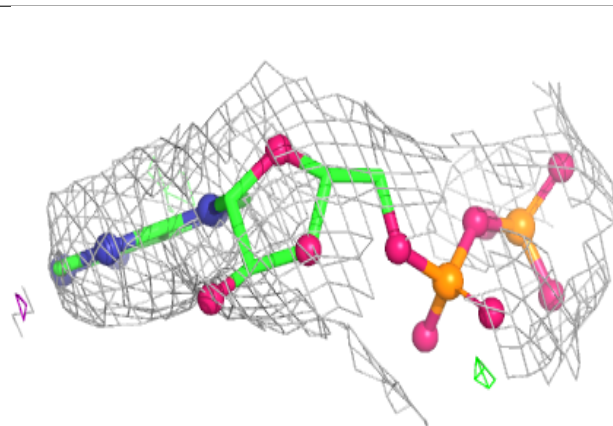
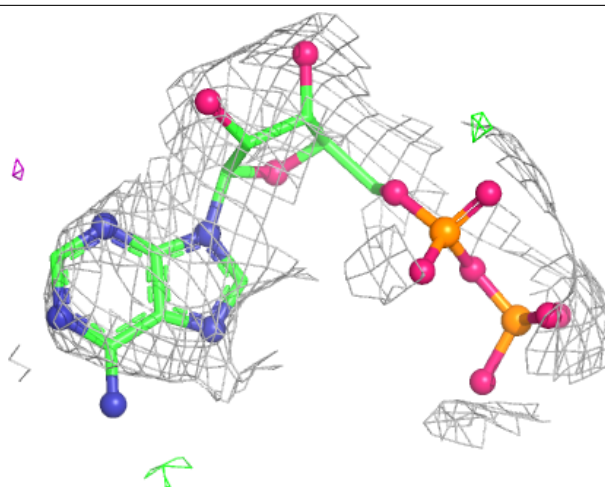
Electron density around ANP C 901:

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



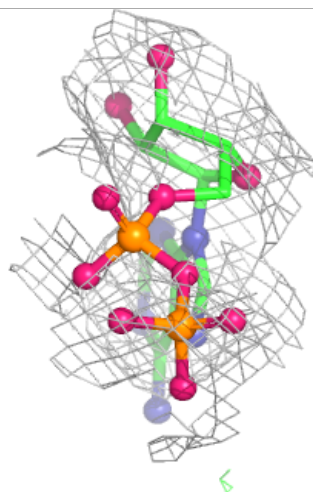
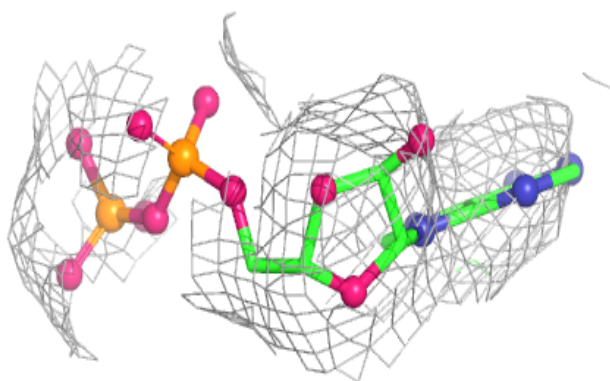
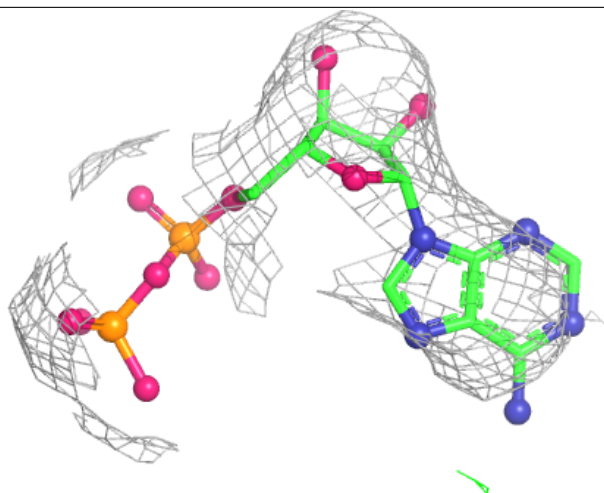
Electron density around ADP C 807:

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



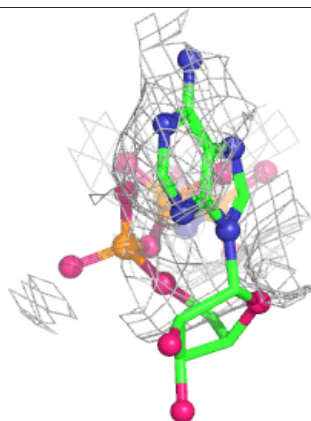
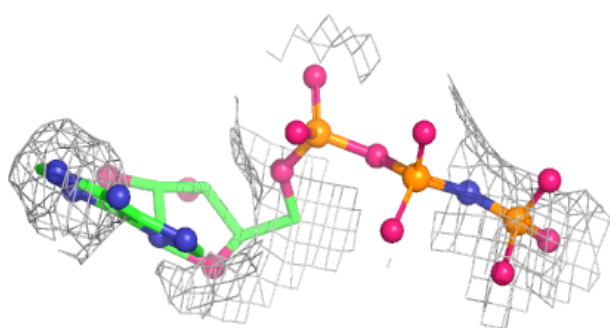
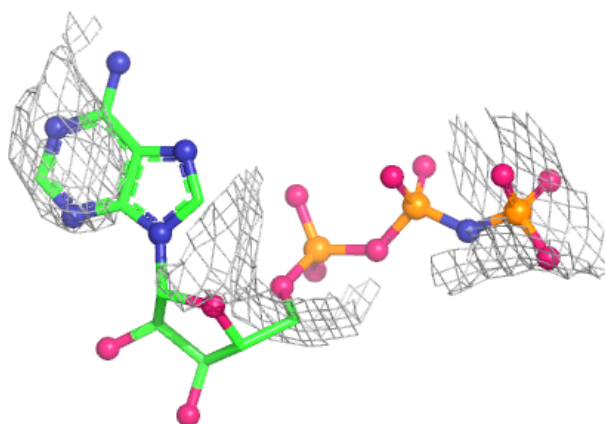
Electron density around ADP D 807:

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



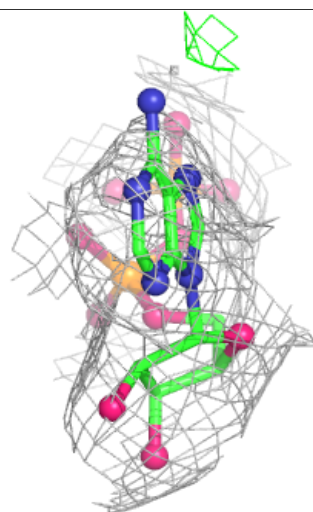
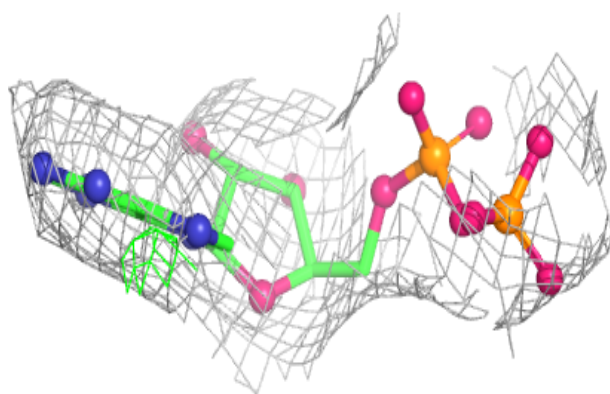
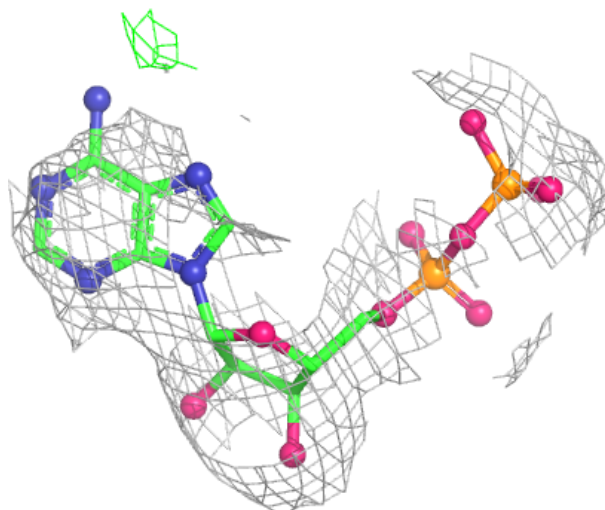
Electron density around ANP A 901:

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



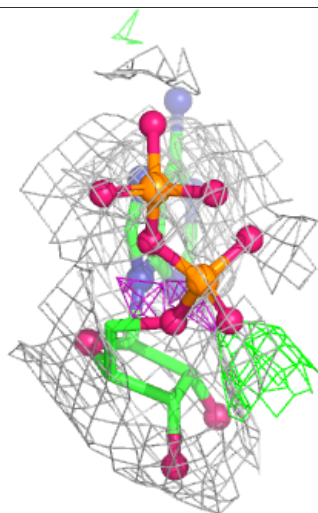
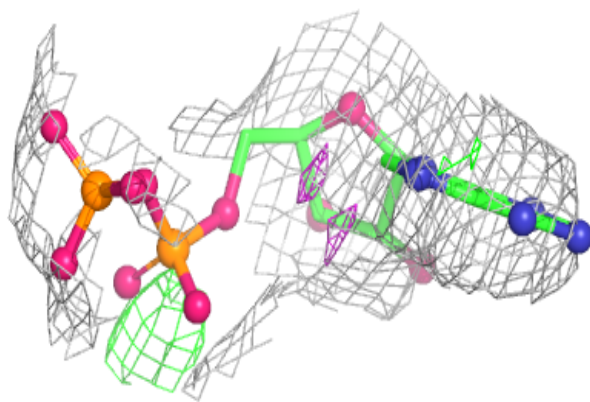
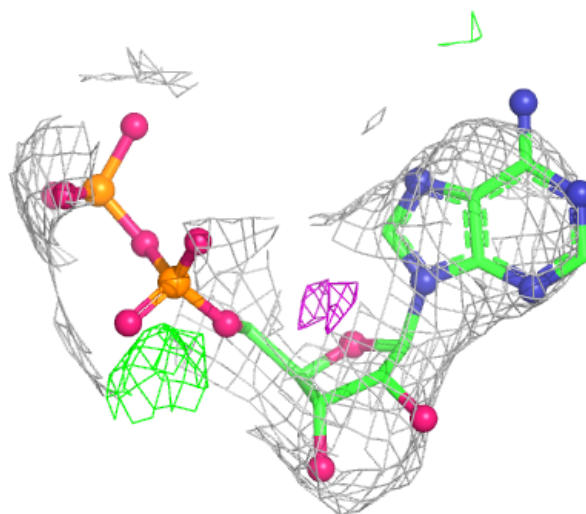
Electron density around ADP A 807:

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



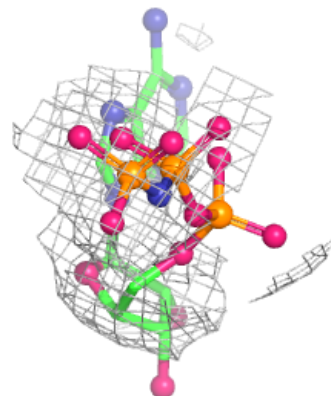
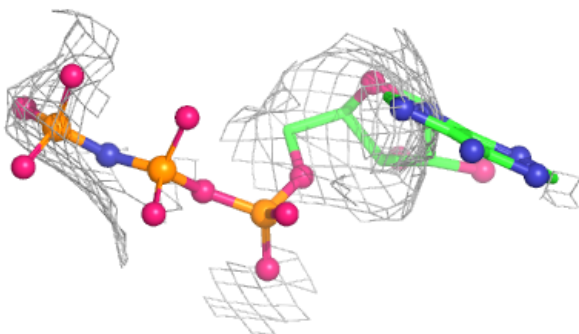
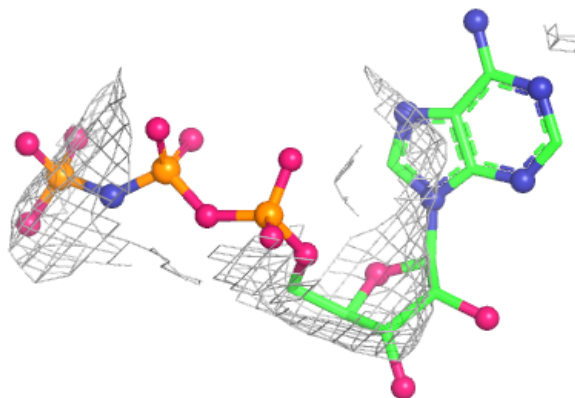
Electron density around ADP B 807:

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



Electron density around ANP D 901:

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



5.5 Other polymers ⓘ

There are no such residues in this entry.