Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 04:31 am GMT

PDB ID	:	2C39
Title	:	RNase PH core of the archaeal exosome in complex with ADP
Authors	:	Lorentzen, E.; Conti, E.
Deposited on	:	2005-10-05
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

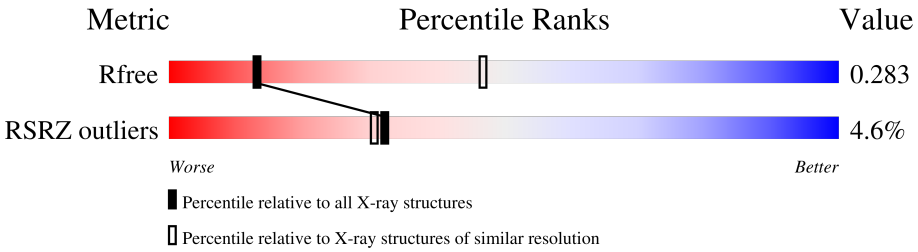
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 45814 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 PROBABLE EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1944	1239	320	380	5			
1	C	260	Total	C	N	O	S	0	0	0
			1947	1243	321	378	5			
1	E	260	Total	C	N	O	S	0	0	0
			1968	1253	325	385	5			
1	G	260	Total	C	N	O	S	0	0	0
			1961	1250	323	383	5			
1	I	260	Total	C	N	O	S	0	0	0
			1954	1247	323	379	5			
1	K	260	Total	C	N	O	S	0	0	0
			1958	1249	323	381	5			
1	M	260	Total	C	N	O	S	0	0	0
			1960	1249	324	382	5			
1	O	260	Total	C	N	O	S	0	0	0
			1951	1246	323	377	5			
1	Q	260	Total	C	N	O	S	0	0	0
			1953	1245	322	381	5			
1	S	259	Total	C	N	O	S	0	0	0
			1955	1245	323	382	5			
1	U	255	Total	C	N	O	S	0	0	0
			1908	1219	317	367	5			
1	W	259	Total	C	N	O	S	0	0	0
			1950	1245	322	378	5			

- Molecule 2 is a protein called PROBABLE EXOSOME COMPLEX EXONUCLEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1812	1145	317	340	10			
2	D	248	Total	C	N	O	S	0	0	0
			1900	1198	330	360	12			

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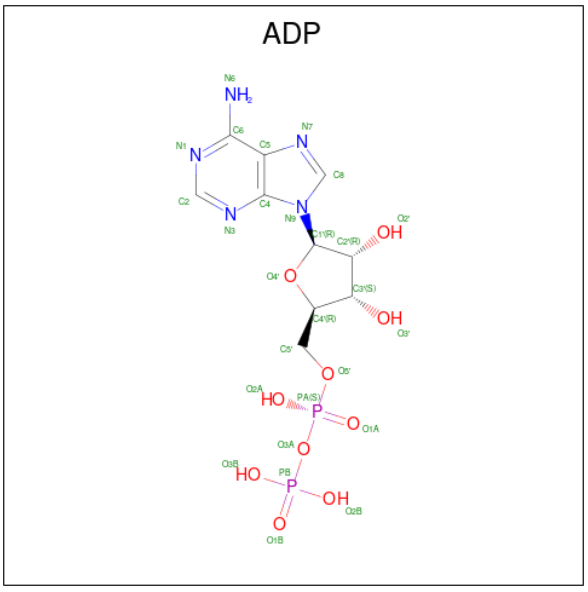
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	241	Total	C	N	O	S	0	0	0
			1838	1161	317	350	10			
2	H	230	Total	C	N	O	S	0	0	0
			1732	1094	302	327	9			
2	J	241	Total	C	N	O	S	0	0	0
			1844	1165	321	348	10			
2	L	247	Total	C	N	O	S	0	0	0
			1890	1194	328	357	11			
2	N	239	Total	C	N	O	S	0	0	0
			1809	1144	313	342	10			
2	P	248	Total	C	N	O	S	0	0	0
			1904	1202	332	358	12			
2	R	248	Total	C	N	O	S	0	0	0
			1880	1188	332	348	12			
2	T	248	Total	C	N	O	S	0	0	0
			1884	1193	328	351	12			
2	V	239	Total	C	N	O	S	0	0	0
			1815	1148	318	339	10			
2	X	239	Total	C	N	O	S	0	0	0
			1821	1148	315	348	10			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O P 27 10 5 10 2	0	0
3	F	1	Total C O P 17 5 10 2	0	0
3	H	1	Total C N O P 27 10 5 10 2	0	0
3	J	1	Total O P 9 7 2	0	0
3	L	1	Total C N O P 27 10 5 10 2	0	0
3	N	1	Total C N O P 27 10 5 10 2	0	0
3	P	1	Total C N O P 27 10 5 10 2	0	0
3	R	1	Total C N O P 27 10 5 10 2	0	0
3	T	1	Total C N O P 27 10 5 10 2	0	0
3	V	1	Total C O P 17 5 10 2	0	0
3	X	1	Total C O P 17 5 10 2	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	206.20Å 214.00Å 432.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.25 – 3.30 93.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (93.25-3.30) 93.5 (93.06-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.274 , 0.295 0.265 , 0.283	Depositor DCC
R_{free} test set	4015 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	86.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 21.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.048 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	45814	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

12 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	ADP	T	404	-	24,29,29	0.96	2 (8%)	29,45,45	1.26	3 (10%)
3	ADP	D	404	2	24,29,29	1.16	3 (12%)	29,45,45	1.48	3 (10%)
3	ADP	J	404	-	6,8,29	0.90	0	13,13,45	1.14	1 (7%)
3	ADP	F	404	-	15,17,29	1.66	2 (13%)	21,26,45	1.15	1 (4%)
3	ADP	P	404	-	24,29,29	1.08	2 (8%)	29,45,45	1.59	4 (13%)
3	ADP	L	404	-	24,29,29	1.12	3 (12%)	29,45,45	1.59	5 (17%)
3	ADP	R	404	2	24,29,29	1.22	4 (16%)	29,45,45	1.30	5 (17%)
3	ADP	V	404	-	15,17,29	0.88	1 (6%)	21,26,45	1.25	2 (9%)
3	ADP	B	404	-	24,29,29	1.12	3 (12%)	29,45,45	1.20	2 (6%)
3	ADP	N	404	-	24,29,29	1.17	2 (8%)	29,45,45	1.22	2 (6%)
3	ADP	X	404	-	15,17,29	1.95	2 (13%)	21,26,45	1.47	3 (14%)
3	ADP	H	404	-	24,29,29	1.06	2 (8%)	29,45,45	1.34	4 (13%)

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	ADP	T	404	-	-	3/12/32/32	0/3/3/3
3	ADP	D	404	2	-	1/12/32/32	0/3/3/3
3	ADP	J	404	-	-	0/6/6/32	-
3	ADP	F	404	-	-	2/12/25/32	0/1/1/3
3	ADP	P	404	-	-	5/12/32/32	0/3/3/3
3	ADP	L	404	-	-	3/12/32/32	0/3/3/3
3	ADP	R	404	2	-	3/12/32/32	0/3/3/3
3	ADP	V	404	-	-	0/12/25/32	0/1/1/3
3	ADP	B	404	-	-	6/12/32/32	0/3/3/3
3	ADP	N	404	-	-	5/12/32/32	0/3/3/3
3	ADP	X	404	-	-	6/12/25/32	0/1/1/3
3	ADP	H	404	-	-	4/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	404	ADP	O4'-C1'	6.17	1.57	1.43
3	F	404	ADP	O4'-C1'	5.34	1.55	1.43
3	X	404	ADP	C1'-C2'	3.31	1.57	1.51
3	B	404	ADP	C5-C4	2.87	1.48	1.40
3	R	404	ADP	C5-C4	2.83	1.48	1.40
3	N	404	ADP	C5-C4	2.76	1.48	1.40
3	L	404	ADP	C5-C4	2.74	1.48	1.40
3	H	404	ADP	C5-C4	2.64	1.47	1.40
3	F	404	ADP	C1'-C2'	2.51	1.56	1.51
3	D	404	ADP	C5-C4	2.51	1.47	1.40
3	N	404	ADP	O4'-C1'	2.47	1.44	1.41
3	R	404	ADP	O4'-C1'	2.42	1.44	1.41
3	D	404	ADP	C2-N3	2.41	1.36	1.32
3	R	404	ADP	C2-N3	2.39	1.35	1.32
3	P	404	ADP	C5-C4	2.39	1.47	1.40
3	P	404	ADP	C2-N3	2.38	1.35	1.32
3	D	404	ADP	O4'-C1'	2.29	1.44	1.41
3	B	404	ADP	O4'-C1'	2.28	1.44	1.41
3	L	404	ADP	C2-N3	2.24	1.35	1.32
3	B	404	ADP	C2-N3	2.22	1.35	1.32
3	H	404	ADP	O4'-C1'	2.22	1.44	1.41
3	T	404	ADP	C5-C4	2.18	1.46	1.40
3	V	404	ADP	O4'-C1'	2.13	1.48	1.43
3	T	404	ADP	C2-N3	2.12	1.35	1.32
3	L	404	ADP	C6-C5	2.07	1.51	1.43
3	R	404	ADP	C2'-C1'	-2.00	1.50	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	404	ADP	N3-C2-N1	-4.06	122.33	128.68
3	X	404	ADP	C1'-C2'-C3'	3.89	107.55	101.63
3	P	404	ADP	PA-O3A-PB	-3.87	119.53	132.83
3	D	404	ADP	N3-C2-N1	-3.76	122.80	128.68
3	L	404	ADP	C4-C5-N7	-3.67	105.58	109.40
3	L	404	ADP	PA-O3A-PB	-3.65	120.29	132.83
3	V	404	ADP	C1'-C2'-C3'	3.61	107.13	101.63
3	N	404	ADP	N3-C2-N1	-3.60	123.05	128.68
3	H	404	ADP	N3-C2-N1	-3.52	123.17	128.68
3	B	404	ADP	N3-C2-N1	-3.43	123.31	128.68
3	T	404	ADP	N3-C2-N1	-3.24	123.62	128.68
3	F	404	ADP	C1'-C2'-C3'	3.18	106.47	101.63
3	L	404	ADP	N3-C2-N1	-3.06	123.90	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	404	ADP	PA-O3A-PB	-3.00	122.54	132.83
3	D	404	ADP	PA-O3A-PB	-3.00	122.54	132.83
3	R	404	ADP	N3-C2-N1	-2.96	124.04	128.68
3	X	404	ADP	PA-O3A-PB	-2.83	123.10	132.83
3	D	404	ADP	C4-C5-N7	-2.83	106.45	109.40
3	H	404	ADP	PA-O3A-PB	-2.79	123.24	132.83
3	P	404	ADP	C4-C5-N7	-2.76	106.53	109.40
3	X	404	ADP	O4'-C1'-C2'	-2.71	100.75	105.99
3	B	404	ADP	C4-C5-N7	-2.54	106.75	109.40
3	R	404	ADP	C4-C5-N7	-2.51	106.78	109.40
3	L	404	ADP	O3B-PB-O2B	2.50	117.19	107.64
3	V	404	ADP	PA-O3A-PB	-2.27	125.04	132.83
3	H	404	ADP	C3'-C2'-C1'	2.18	104.26	100.98
3	N	404	ADP	PA-O3A-PB	-2.16	125.41	132.83
3	H	404	ADP	C4-C5-N7	-2.15	107.16	109.40
3	R	404	ADP	O3B-PB-O2B	2.15	115.84	107.64
3	P	404	ADP	O3B-PB-O2B	2.10	115.65	107.64
3	T	404	ADP	N6-C6-N1	2.06	122.85	118.57
3	J	404	ADP	O3B-PB-O1B	2.04	118.67	110.68
3	L	404	ADP	C5-C6-N6	2.02	123.42	120.35
3	R	404	ADP	O2'-C2'-C1'	-2.02	103.41	110.85
3	R	404	ADP	PA-O3A-PB	-2.01	125.92	132.83

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	ADP	C5'-O5'-PA-O2A
3	B	404	ADP	C5'-O5'-PA-O3A
3	H	404	ADP	C5'-O5'-PA-O3A
3	L	404	ADP	PB-O3A-PA-O5'
3	L	404	ADP	C3'-C4'-C5'-O5'
3	N	404	ADP	C5'-O5'-PA-O1A
3	P	404	ADP	C5'-O5'-PA-O1A
3	P	404	ADP	C5'-O5'-PA-O3A
3	R	404	ADP	C5'-O5'-PA-O1A
3	T	404	ADP	C5'-O5'-PA-O1A
3	T	404	ADP	C5'-O5'-PA-O3A
3	X	404	ADP	C5'-O5'-PA-O1A
3	X	404	ADP	C5'-O5'-PA-O3A
3	B	404	ADP	O4'-C4'-C5'-O5'
3	L	404	ADP	O4'-C4'-C5'-O5'

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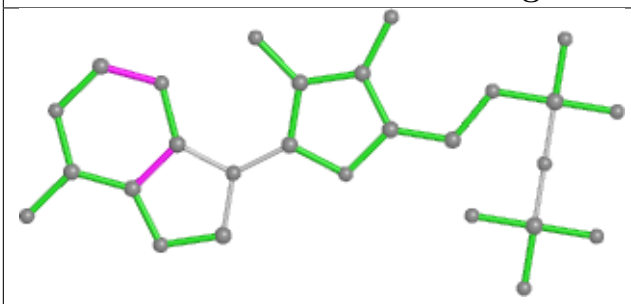
Mol	Chain	Res	Type	Atoms
3	X	404	ADP	O4'-C4'-C5'-O5'
3	X	404	ADP	C3'-C4'-C5'-O5'
3	B	404	ADP	C3'-C4'-C5'-O5'
3	N	404	ADP	O4'-C4'-C5'-O5'
3	F	404	ADP	C3'-C4'-C5'-O5'
3	N	404	ADP	C3'-C4'-C5'-O5'
3	B	404	ADP	PB-O3A-PA-O5'
3	D	404	ADP	PB-O3A-PA-O5'
3	P	404	ADP	PA-O3A-PB-O1B
3	N	404	ADP	C5'-O5'-PA-O3A
3	H	404	ADP	C5'-O5'-PA-O1A
3	N	404	ADP	C5'-O5'-PA-O2A
3	P	404	ADP	C5'-O5'-PA-O2A
3	T	404	ADP	C5'-O5'-PA-O2A
3	X	404	ADP	C5'-O5'-PA-O2A
3	F	404	ADP	O4'-C4'-C5'-O5'
3	H	404	ADP	O4'-C4'-C5'-O5'
3	R	404	ADP	O4'-C4'-C5'-O5'
3	R	404	ADP	PB-O3A-PA-O5'
3	B	404	ADP	PA-O3A-PB-O1B
3	P	404	ADP	PA-O3A-PB-O2B
3	H	404	ADP	C3'-C4'-C5'-O5'
3	X	404	ADP	PA-O3A-PB-O1B

There are no ring outliers.

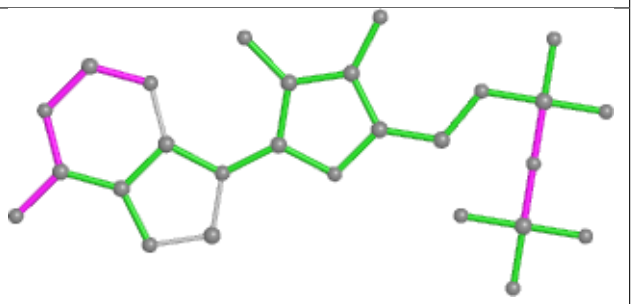
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

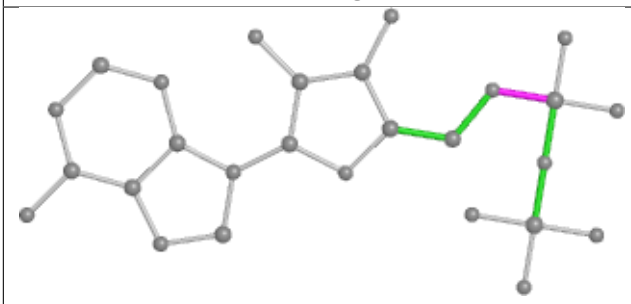
Ligand ADP T 404



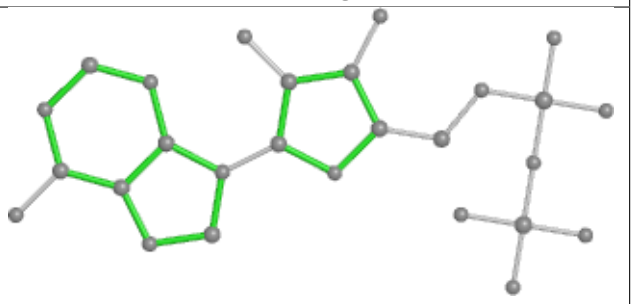
Bond lengths



Bond angles

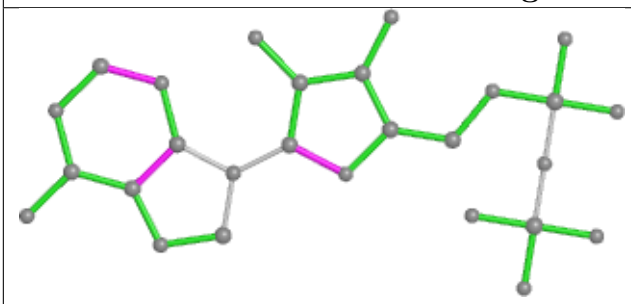


Torsions

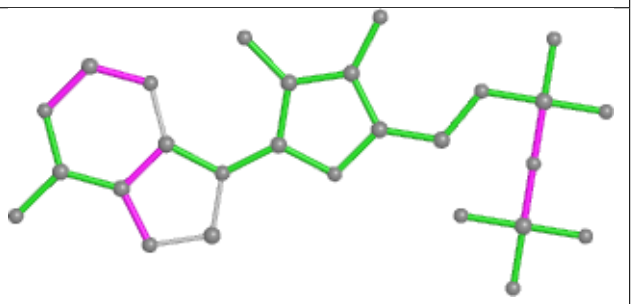


Rings

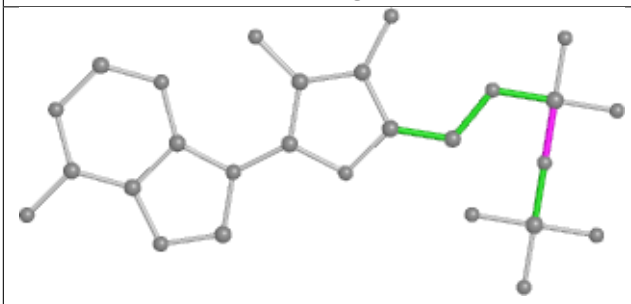
Ligand ADP D 404



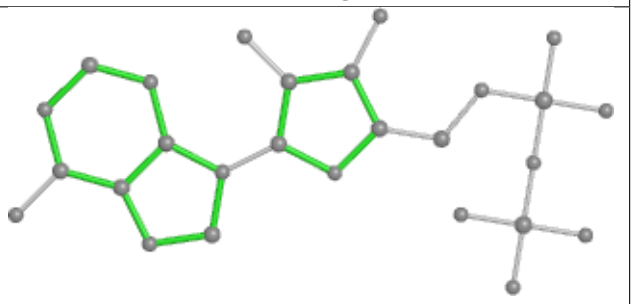
Bond lengths



Bond angles

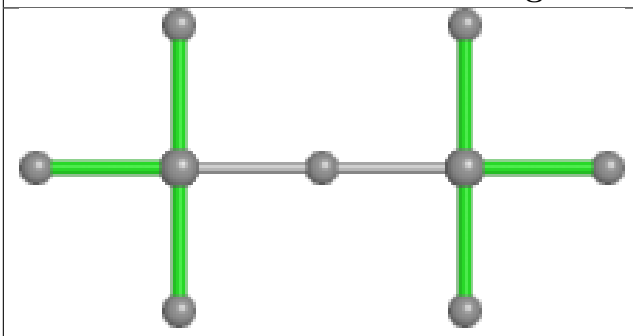


Torsions

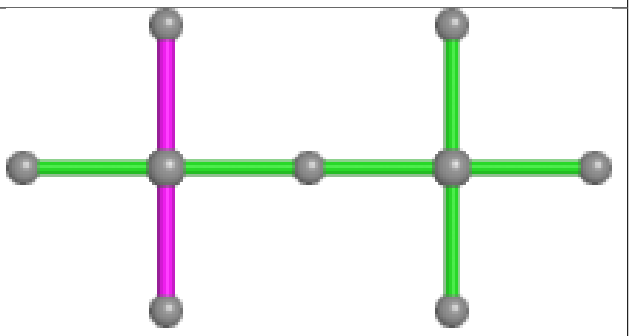


Rings

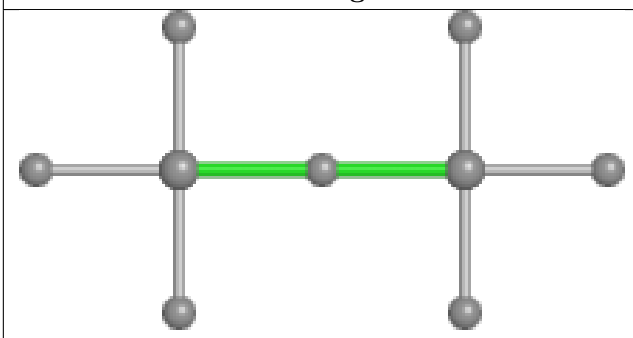
Ligand ADP J 404



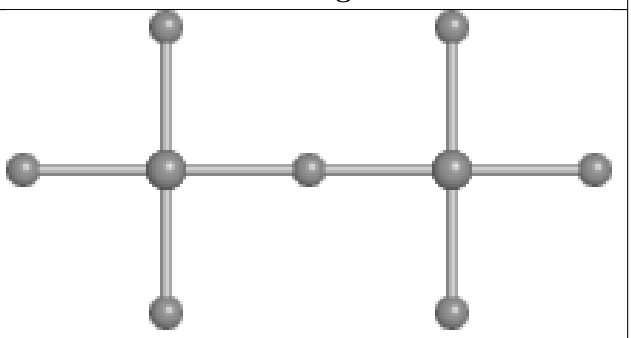
Bond lengths



Bond angles

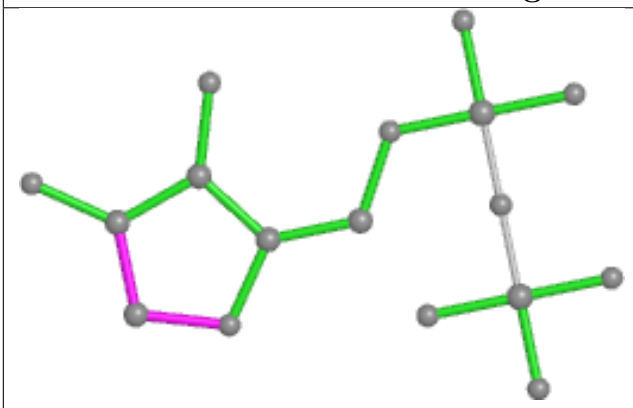


Torsions

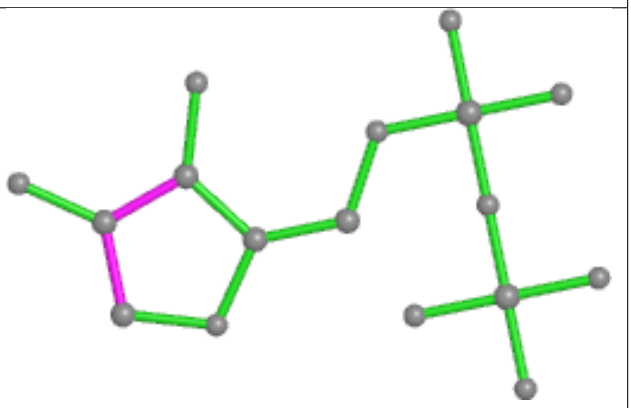


Rings

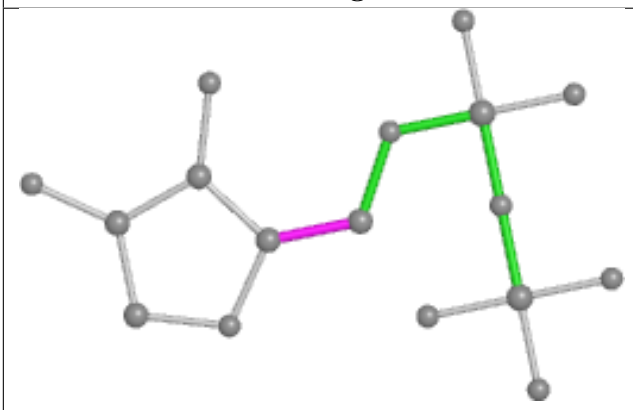
Ligand ADP F 404



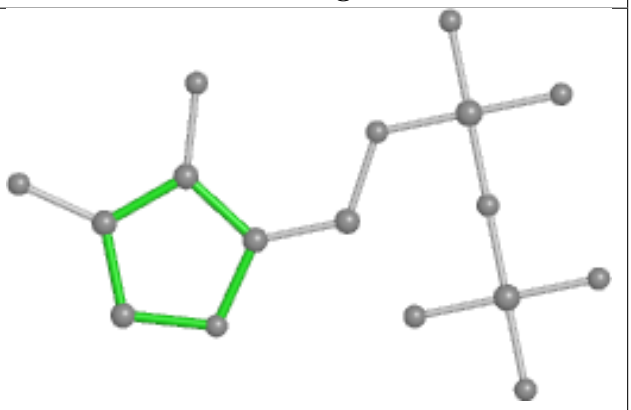
Bond lengths



Bond angles

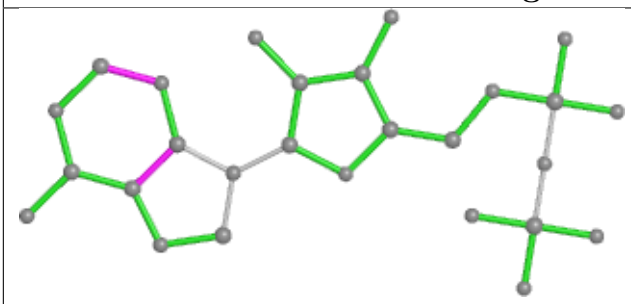


Torsions

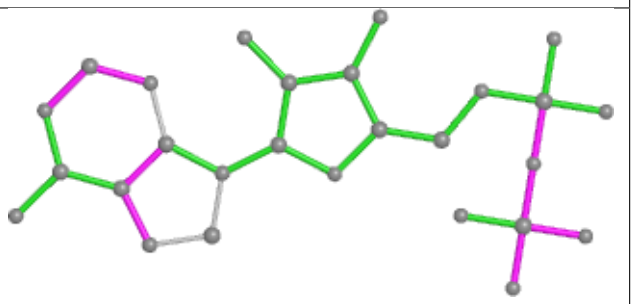


Rings

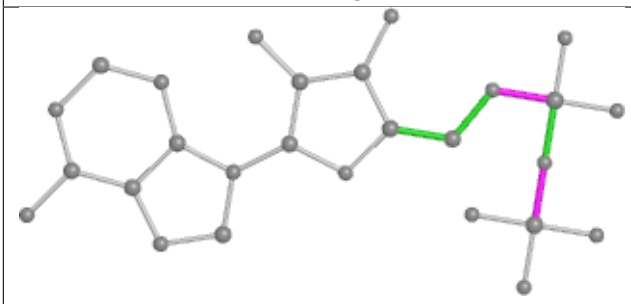
Ligand ADP P 404



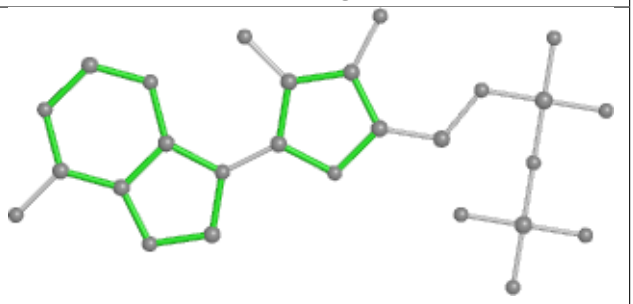
Bond lengths



Bond angles

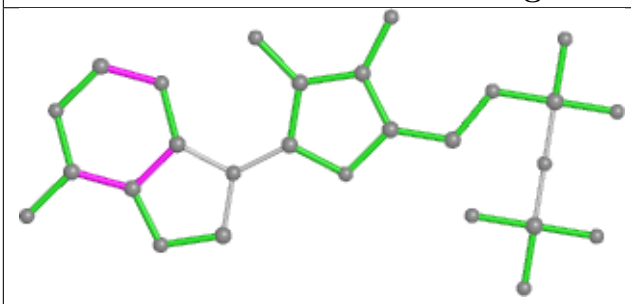


Torsions

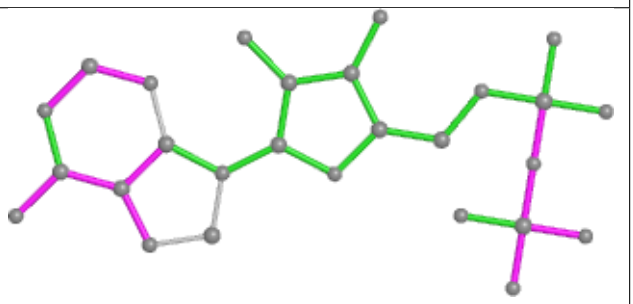


Rings

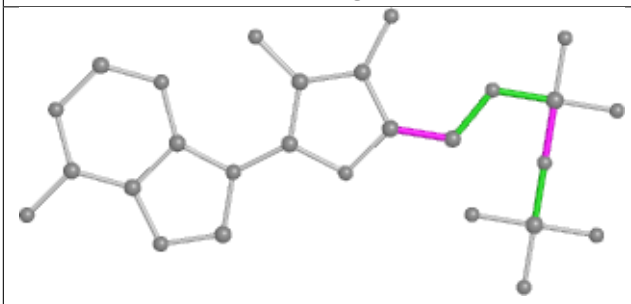
Ligand ADP L 404



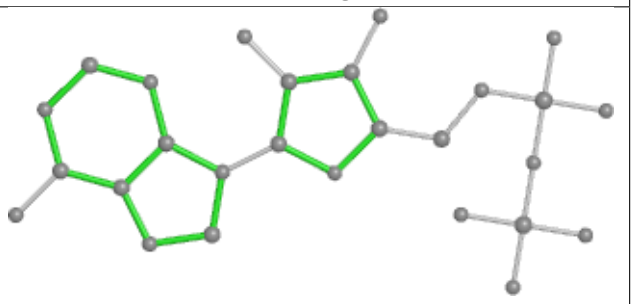
Bond lengths



Bond angles

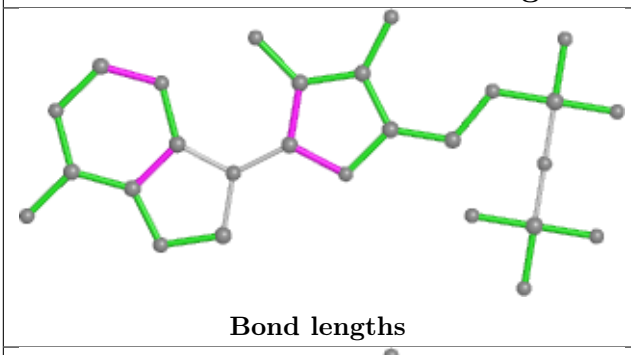


Torsions

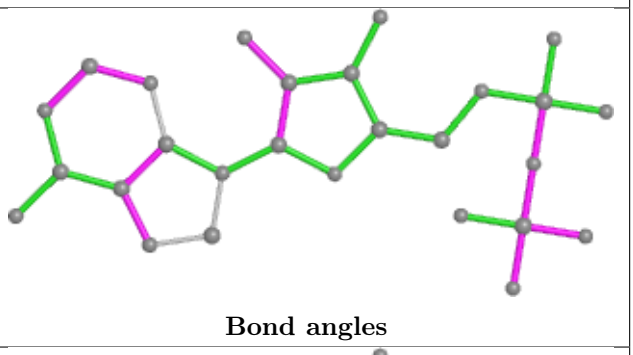


Rings

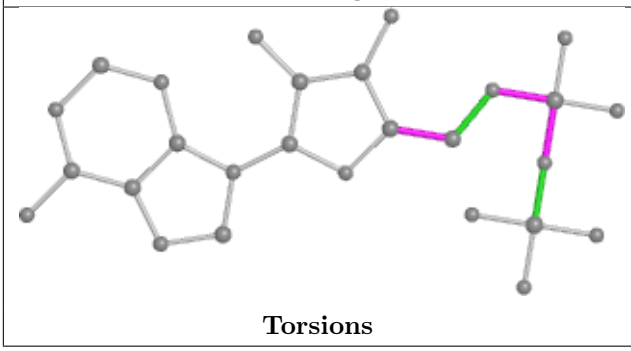
Ligand ADP R 404



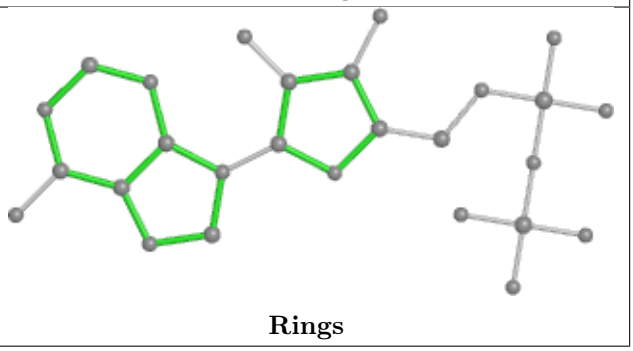
Bond lengths



Bond angles

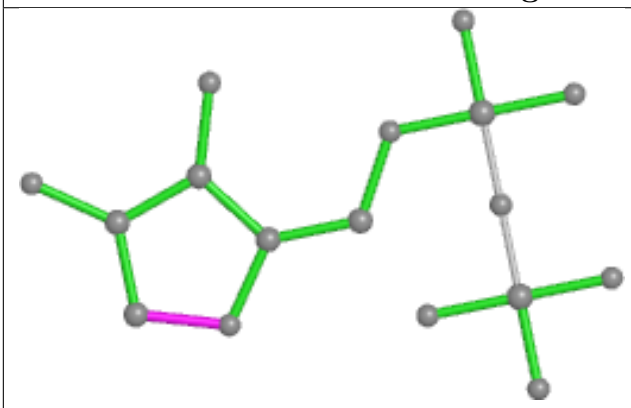


Torsions

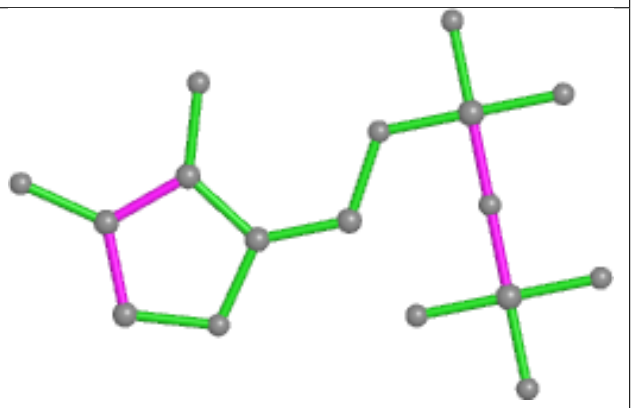


Rings

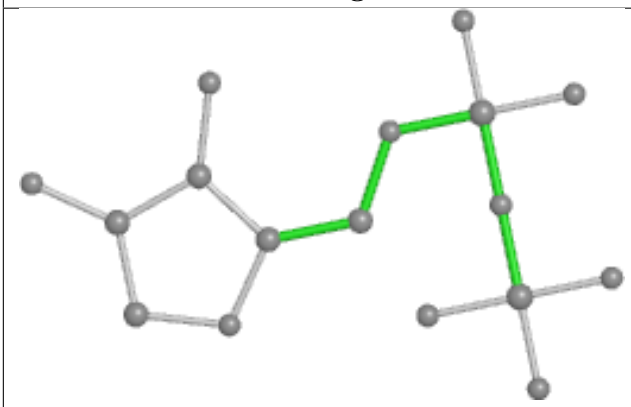
Ligand ADP V 404



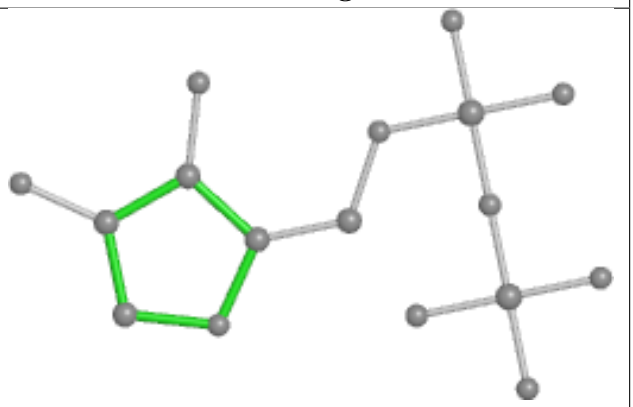
Bond lengths



Bond angles

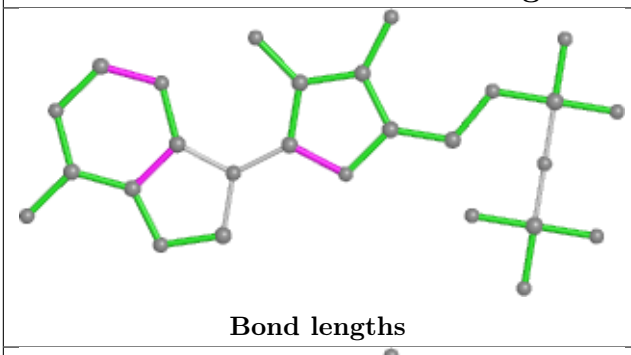


Torsions

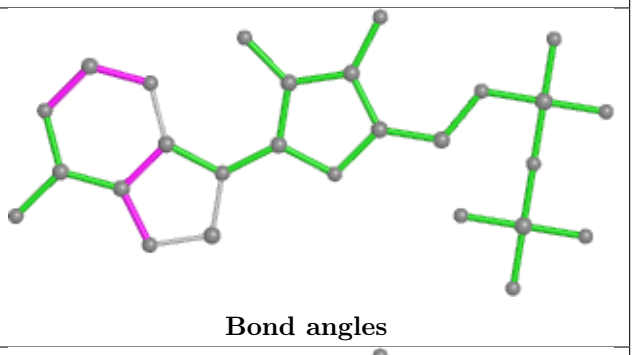


Rings

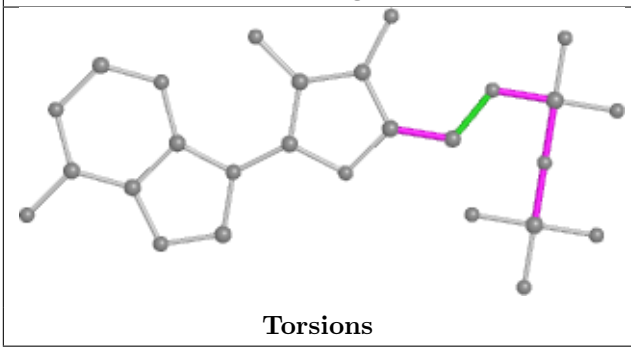
Ligand ADP B 404



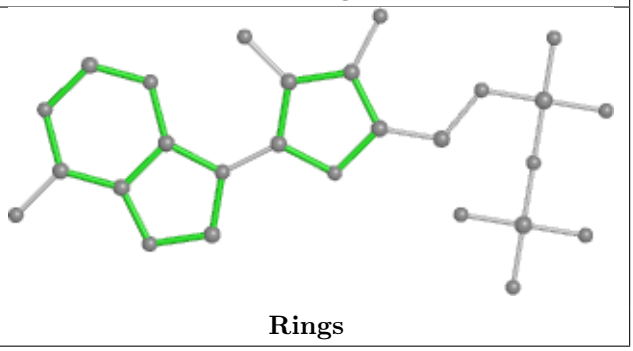
Bond lengths



Bond angles

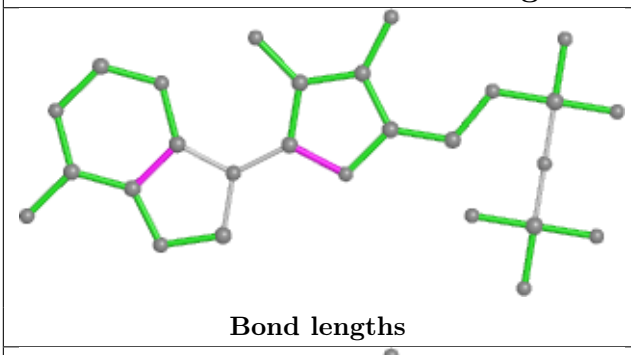


Torsions

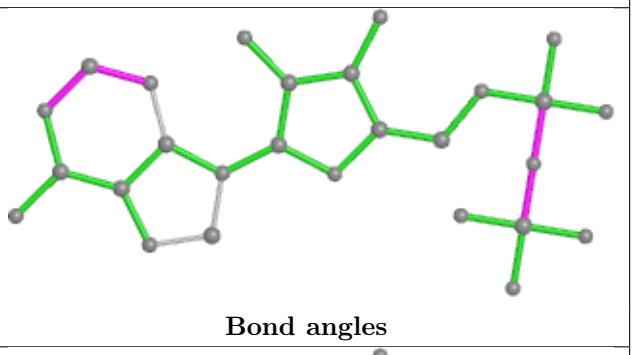


Rings

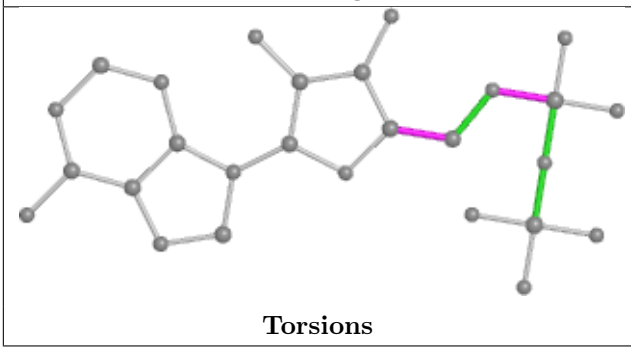
Ligand ADP N 404



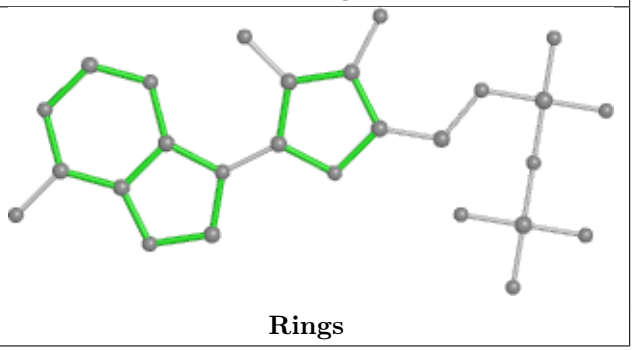
Bond lengths



Bond angles

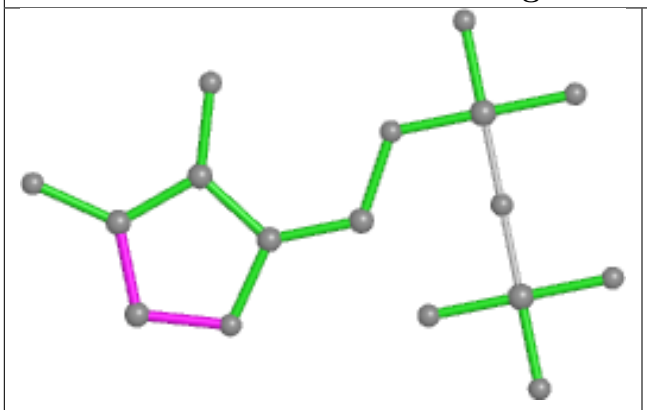


Torsions

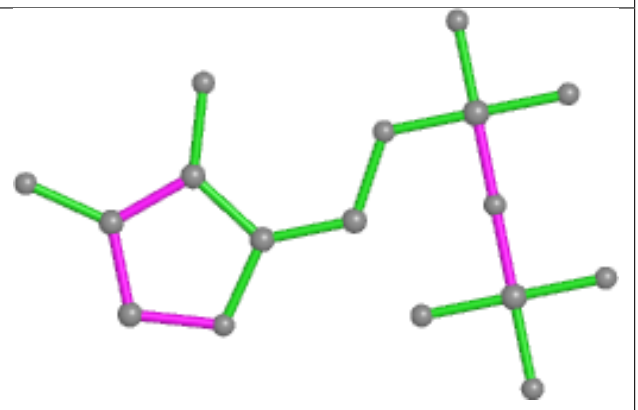


Rings

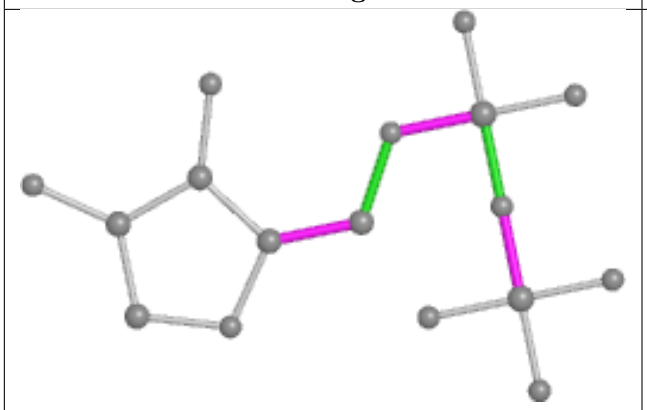
Ligand ADP X 404



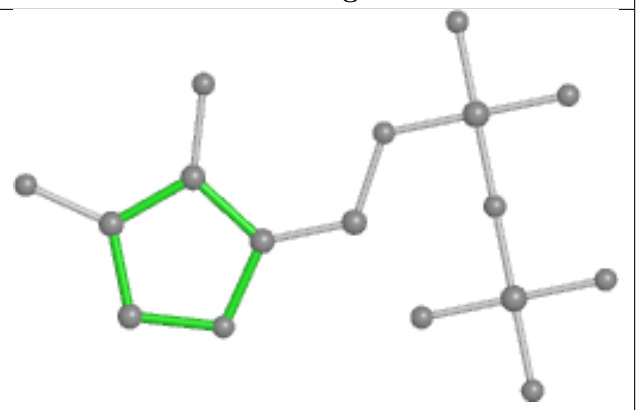
Bond lengths



Bond angles

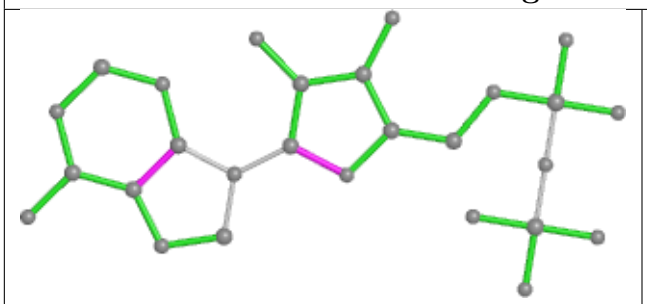


Torsions

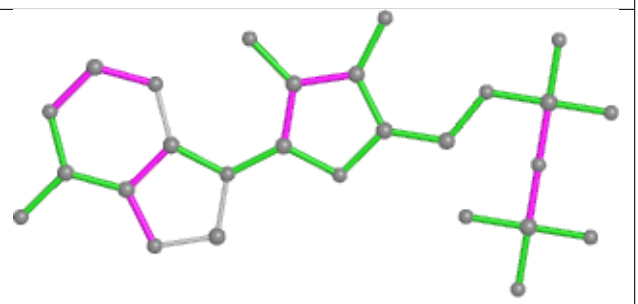


Rings

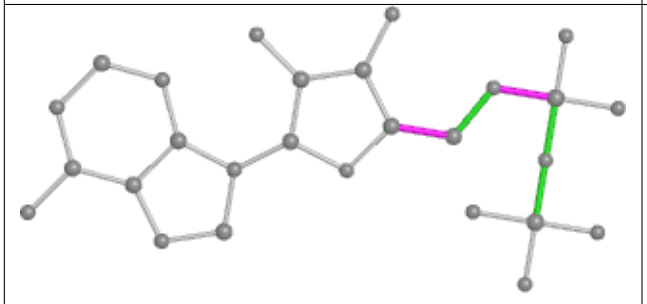
Ligand ADP H 404



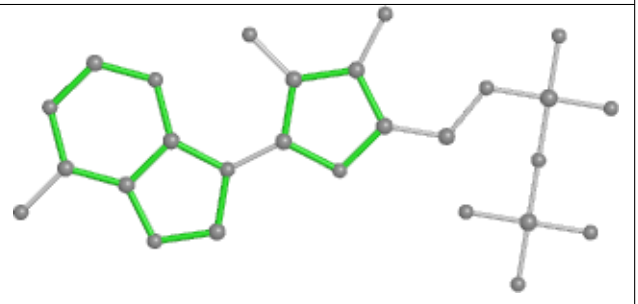
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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^{th} 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	260/275 (94%)	0.57	6 (2%) 60 59	46, 53, 67, 74	0
1	C	260/275 (94%)	0.68	6 (2%) 60 59	46, 53, 67, 75	0
1	E	260/275 (94%)	0.59	6 (2%) 60 59	46, 53, 67, 74	0
1	G	260/275 (94%)	0.64	14 (5%) 25 24	46, 53, 67, 74	0
1	I	260/275 (94%)	0.67	18 (6%) 16 16	46, 53, 67, 73	0
1	K	260/275 (94%)	0.75	6 (2%) 60 59	46, 53, 67, 75	0
1	M	260/275 (94%)	0.63	6 (2%) 60 59	46, 53, 67, 75	0
1	O	260/275 (94%)	0.69	3 (1%) 79 78	46, 53, 67, 75	0
1	Q	260/275 (94%)	0.64	6 (2%) 60 59	46, 53, 67, 74	0
1	S	259/275 (94%)	0.73	26 (10%) 7 7	46, 53, 67, 73	0
1	U	255/275 (92%)	0.72	18 (7%) 16 16	46, 53, 66, 73	0
1	W	259/275 (94%)	0.74	13 (5%) 28 27	46, 53, 67, 75	0
2	B	241/248 (97%)	0.75	16 (6%) 18 18	46, 52, 68, 80	0
2	D	248/248 (100%)	0.68	8 (3%) 47 46	45, 52, 68, 80	0
2	F	241/248 (97%)	0.65	11 (4%) 32 30	46, 52, 68, 80	0
2	H	230/248 (92%)	0.86	23 (10%) 7 7	46, 52, 69, 80	0
2	J	241/248 (97%)	0.78	19 (7%) 12 12	46, 52, 68, 80	0
2	L	247/248 (99%)	0.67	5 (2%) 65 64	45, 52, 68, 80	0
2	N	239/248 (96%)	0.65	4 (1%) 70 68	46, 52, 69, 79	0
2	P	248/248 (100%)	0.71	6 (2%) 59 56	45, 52, 68, 80	0
2	R	248/248 (100%)	0.65	4 (1%) 72 70	45, 52, 69, 80	0
2	T	248/248 (100%)	0.67	7 (2%) 53 51	45, 52, 69, 79	0
2	V	239/248 (96%)	0.92	29 (12%) 4 3	46, 52, 68, 79	0
2	X	239/248 (96%)	0.68	18 (7%) 14 13	46, 52, 69, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	6022/6276 (95%)	0.70	278 (4%)	32	30	45, 52, 68, 80	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	171	TYR	5.0
2	V	132	LEU	4.7
2	L	248	VAL	4.6
1	S	138	TRP	4.5
1	S	90	LEU	4.4
2	B	248	VAL	4.3
2	H	248	VAL	4.1
1	I	275	ILE	4.0
2	N	248	VAL	4.0
1	U	1	MET	3.9
2	V	55	ILE	3.9
2	B	15	ASP	3.9
1	S	88	VAL	3.8
1	I	124	LEU	3.8
2	V	107	ILE	3.7
2	H	55	ILE	3.7
1	U	173	VAL	3.7
2	R	248	VAL	3.5
2	F	248	VAL	3.5
1	U	170	VAL	3.5
1	I	248	LEU	3.5
1	C	12	PRO	3.4
2	X	12	LEU	3.4
2	V	204	GLN	3.4
2	V	116	LEU	3.4
2	H	60	GLY	3.4
2	T	248	VAL	3.4
2	V	133	GLN	3.4
2	X	132	LEU	3.4
2	J	18	LYS	3.3
2	D	161	ILE	3.3
1	U	44	LEU	3.3
2	D	248	VAL	3.2
2	V	53	LYS	3.2
2	V	64	MET	3.2
2	J	14	LEU	3.2
1	S	166	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	14	ILE	3.2
1	S	83	ASN	3.2
1	S	142	LEU	3.1
1	W	58	LEU	3.1
2	V	170	ASP	3.1
1	S	144	VAL	3.1
1	I	66	GLY	3.1
2	V	128	PHE	3.1
1	W	265	LEU	3.1
2	V	209	MET	3.1
1	U	235	ILE	3.0
2	X	172	VAL	3.0
1	M	37	TYR	3.0
2	X	161	ILE	3.0
2	P	248	VAL	3.0
2	V	25	PRO	3.0
2	J	148	LEU	3.0
1	A	275	ILE	3.0
1	W	130	VAL	2.9
1	W	275	ILE	2.9
2	H	107	ILE	2.9
2	L	161	ILE	2.9
2	V	201	THR	2.9
1	S	167	ASN	2.9
1	E	124	LEU	2.9
2	V	131	ILE	2.9
2	V	123	THR	2.9
1	A	37	TYR	2.9
2	V	153	ALA	2.9
2	J	15	ASP	2.8
1	U	202	VAL	2.8
2	B	12	LEU	2.8
1	W	196	PRO	2.8
1	W	213	PRO	2.8
2	H	111	LEU	2.8
1	U	225	ILE	2.7
1	I	154	LEU	2.7
1	S	37	TYR	2.7
1	S	225	ILE	2.7
1	S	69	LEU	2.7
2	H	160	LEU	2.7
2	H	80	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	X	221	ALA	2.7
2	D	160	LEU	2.7
1	O	63	VAL	2.7
1	W	61	THR	2.6
1	I	90	LEU	2.6
2	H	57	ALA	2.6
1	G	233	LEU	2.6
2	J	169	ALA	2.6
2	X	160	LEU	2.6
2	T	125	ILE	2.6
1	G	129	LEU	2.6
1	G	47	ALA	2.6
1	I	203	ALA	2.6
1	G	131	ILE	2.6
1	Q	54	ALA	2.6
2	H	232	GLU	2.6
2	J	163	GLY	2.6
2	B	55	ILE	2.6
2	H	127	VAL	2.6
1	G	29	GLN	2.5
2	V	35	LEU	2.5
2	J	193	MET	2.5
2	L	162	ALA	2.5
1	A	173	VAL	2.5
1	S	66	GLY	2.5
2	H	132	LEU	2.5
2	X	107	ILE	2.5
1	E	196	PRO	2.5
2	V	231	LEU	2.5
2	X	47	PHE	2.5
2	T	148	LEU	2.5
1	S	89	GLU	2.5
2	F	165	ALA	2.5
1	G	248	LEU	2.5
2	J	79	VAL	2.5
2	V	56	ALA	2.5
2	V	84	THR	2.5
2	H	116	LEU	2.5
1	I	14	ILE	2.5
1	S	53	SER	2.5
1	W	67	THR	2.5
1	S	171	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	28	LEU	2.5
2	J	231	LEU	2.4
2	V	166	VAL	2.4
2	V	169	ALA	2.4
1	I	209	LEU	2.4
1	K	63	VAL	2.4
2	R	128	PHE	2.4
2	V	54	ALA	2.4
1	M	6	SER	2.4
2	J	220	LEU	2.4
1	C	37	TYR	2.4
1	S	220	ILE	2.4
2	F	247	GLY	2.4
2	R	218	PHE	2.4
1	I	251	ILE	2.4
2	B	17	GLY	2.4
1	G	171	TYR	2.4
1	I	37	TYR	2.4
1	I	225	ILE	2.4
1	M	63	VAL	2.4
2	D	145	ALA	2.4
2	F	246	GLU	2.4
2	H	192	ALA	2.4
2	B	125	ILE	2.4
2	J	223	LYS	2.4
2	J	110	ALA	2.4
1	I	146	VAL	2.4
2	V	138	SER	2.4
1	K	37	TYR	2.3
1	G	273	LEU	2.3
1	S	202	VAL	2.3
1	G	136	SER	2.3
1	E	248	LEU	2.3
2	T	160	LEU	2.3
2	B	188	ASP	2.3
1	S	248	LEU	2.3
2	D	177	LEU	2.3
1	U	257	THR	2.3
2	J	162	ALA	2.3
2	J	61	PRO	2.3
2	J	248	VAL	2.3
2	L	191	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	140	VAL	2.3
2	X	124	ALA	2.3
1	S	56	VAL	2.3
1	A	136	SER	2.3
1	A	161	SER	2.3
2	V	208	SER	2.3
2	N	191	ILE	2.3
1	S	63	VAL	2.3
1	U	137	VAL	2.3
2	H	247	GLY	2.3
1	G	169	LYS	2.3
1	G	71	ILE	2.3
2	J	217	ALA	2.3
1	I	67	THR	2.3
2	T	201	THR	2.3
2	N	239	LYS	2.3
1	S	146	VAL	2.3
2	H	164	VAL	2.3
1	G	12	PRO	2.3
2	J	70	SER	2.3
1	K	157	CYS	2.3
1	Q	65	ALA	2.3
2	X	126	ASP	2.3
1	E	225	ILE	2.3
1	G	275	ILE	2.3
1	E	138	TRP	2.2
1	I	158	THR	2.2
2	P	217	ALA	2.2
1	U	269	LEU	2.2
2	F	202	LEU	2.2
2	H	101	ILE	2.2
2	X	141	VAL	2.2
2	X	166	VAL	2.2
1	Q	266	LEU	2.2
2	J	120	PHE	2.2
1	S	173	VAL	2.2
2	P	48	GLU	2.2
1	W	124	LEU	2.2
2	X	101	ILE	2.2
1	W	168	THR	2.2
1	W	191	LEU	2.2
2	B	132	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	71	ILE	2.2
2	H	23	ARG	2.2
2	B	57	ALA	2.2
2	F	117	VAL	2.2
2	P	125	ILE	2.2
2	P	164	VAL	2.2
1	M	149	TYR	2.2
1	O	65	ALA	2.2
2	T	162	ALA	2.2
2	B	236	LEU	2.2
2	R	79	VAL	2.2
2	L	147	SER	2.2
2	D	128	PHE	2.2
1	K	108	ILE	2.2
1	U	28	ARG	2.2
1	I	18	SER	2.2
1	W	223	ALA	2.2
2	B	116	LEU	2.2
2	V	103	LEU	2.2
1	U	12	PRO	2.2
2	F	148	LEU	2.1
2	H	175	LEU	2.1
2	B	187	ALA	2.1
2	D	141	VAL	2.1
2	X	232	GLU	2.1
1	A	134	GLY	2.1
1	Q	64	LEU	2.1
1	I	89	GLU	2.1
1	S	14	ILE	2.1
2	X	142	SER	2.1
1	W	165	LEU	2.1
1	C	223	ALA	2.1
2	H	56	ALA	2.1
2	X	54	ALA	2.1
1	C	14	ILE	2.1
1	S	198	VAL	2.1
2	H	79	VAL	2.1
2	N	76	VAL	2.1
1	E	1	MET	2.1
1	C	11	ILE	2.1
1	S	140	VAL	2.1
2	F	173	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	193	MET	2.1
2	H	202	LEU	2.1
2	X	128	PHE	2.1
2	H	54	ALA	2.1
2	V	57	ALA	2.1
2	H	228	ILE	2.1
2	B	176	ASP	2.1
2	T	60	GLY	2.1
2	P	178	ASN	2.1
2	V	129	THR	2.1
1	K	149	TYR	2.1
1	Q	213	PRO	2.1
1	M	275	ILE	2.1
1	Q	209	LEU	2.1
2	J	224	GLY	2.1
1	M	225	ILE	2.1
2	F	161	ILE	2.1
1	K	86	VAL	2.0
1	U	42	ILE	2.0
1	U	196	PRO	2.0
1	U	52	GLY	2.0
2	V	199	GLN	2.0
1	U	56	VAL	2.0
2	B	214	PHE	2.0
1	S	82	GLY	2.0
2	D	142	SER	2.0
2	B	107	ILE	2.0
2	F	35	LEU	2.0
2	X	202	LEU	2.0
1	U	157	CYS	2.0
1	O	142	LEU	2.0

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 monosaccharides in this entry.

5.4 Ligands (i)

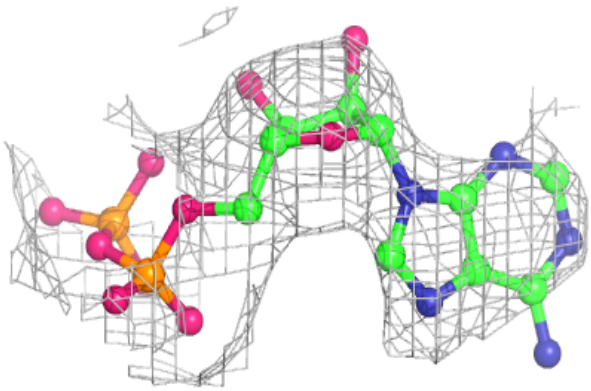
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

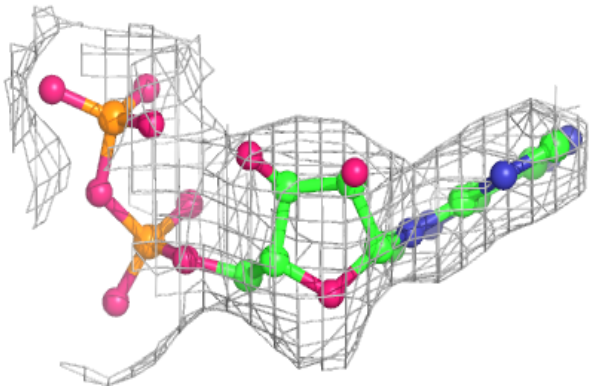
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	H	404	27/27	0.86	0.24	116,117,119,119	0
3	ADP	V	404	17/27	0.86	0.28	90,93,95,95	0
3	ADP	F	404	17/27	0.88	0.22	91,94,95,95	0
3	ADP	X	404	17/27	0.88	0.20	86,87,89,89	0
3	ADP	J	404	9/27	0.92	0.14	100,100,101,101	0
3	ADP	N	404	27/27	0.92	0.25	59,62,64,64	0
3	ADP	B	404	27/27	0.93	0.20	79,90,95,95	0
3	ADP	R	404	27/27	0.95	0.22	47,55,58,58	0
3	ADP	L	404	27/27	0.95	0.23	52,54,56,58	0
3	ADP	D	404	27/27	0.95	0.25	48,50,51,51	0
3	ADP	T	404	27/27	0.96	0.24	55,60,63,63	0
3	ADP	P	404	27/27	0.97	0.23	33,39,41,42	0

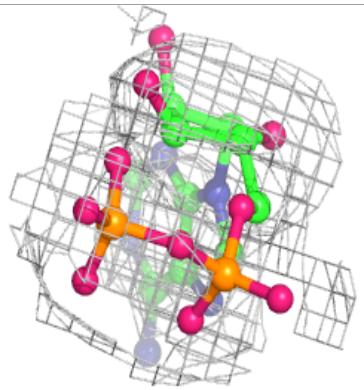
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP H 404:

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

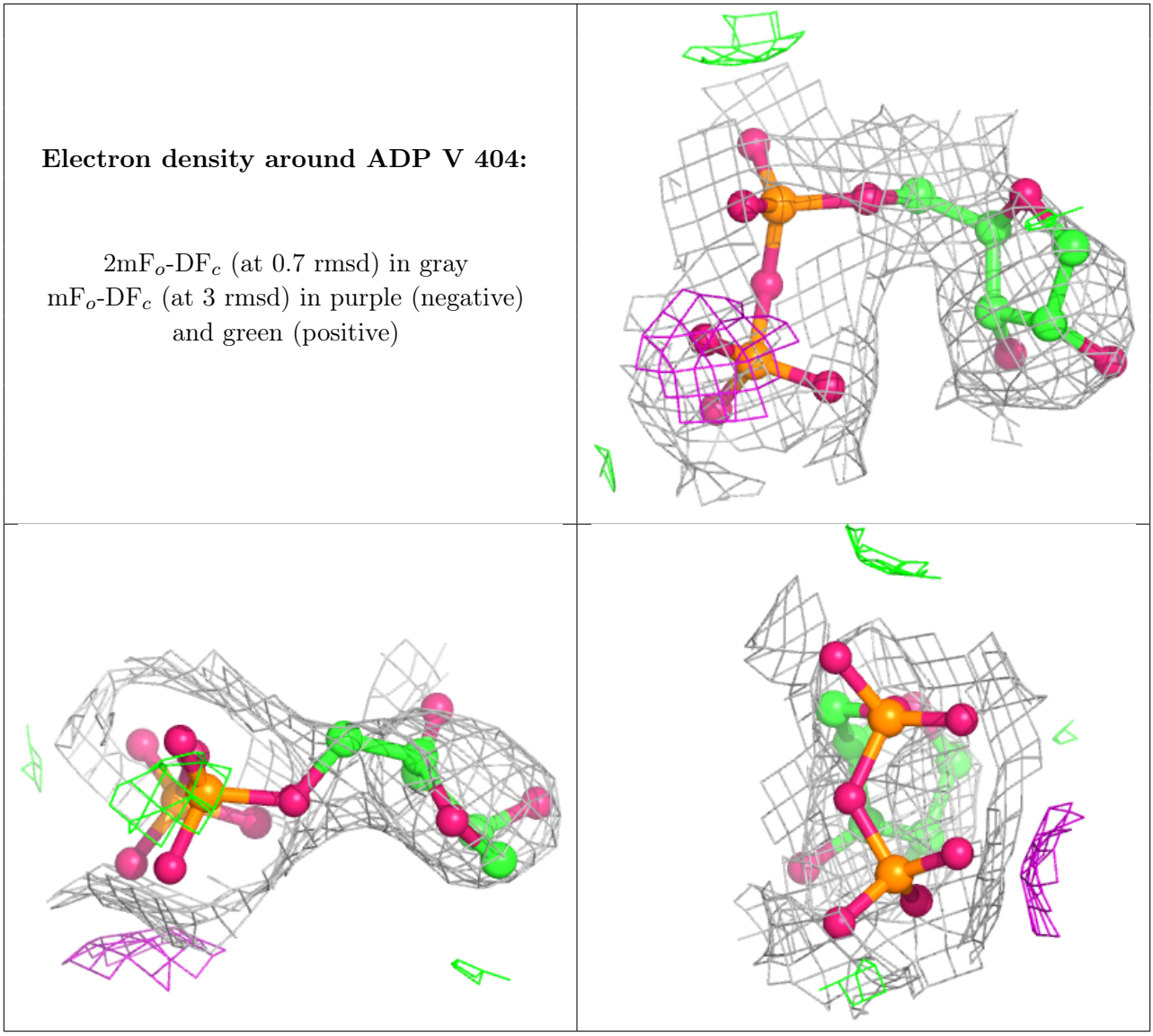






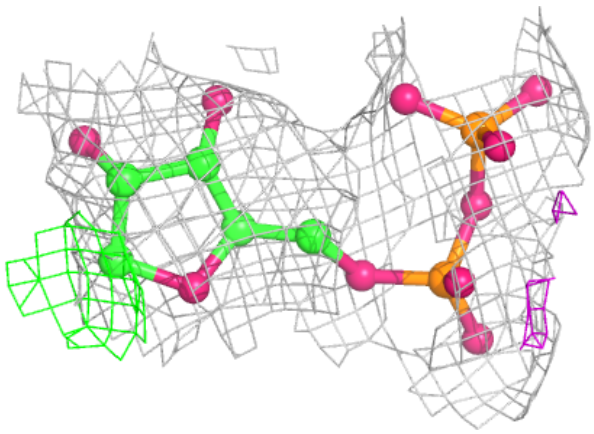
Electron density around ADP V 404:

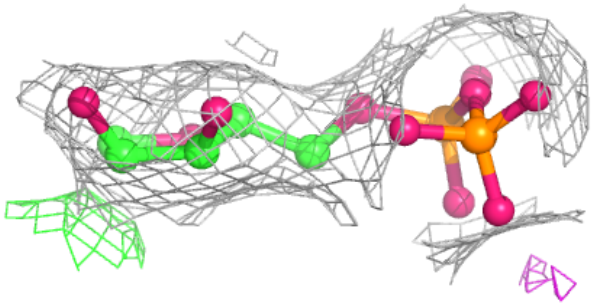
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

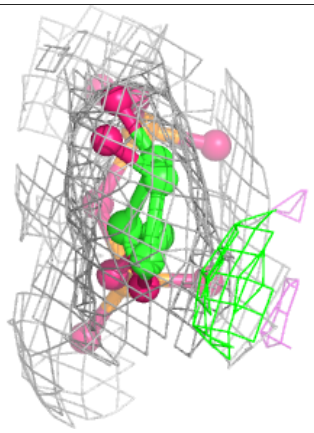


Electron density around ADP F 404:

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

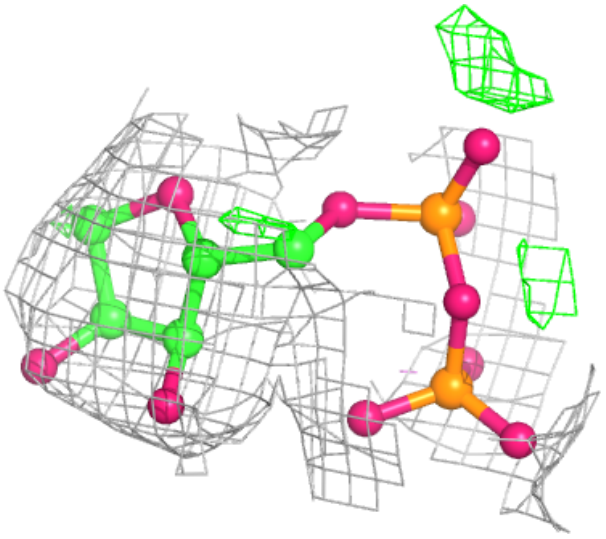


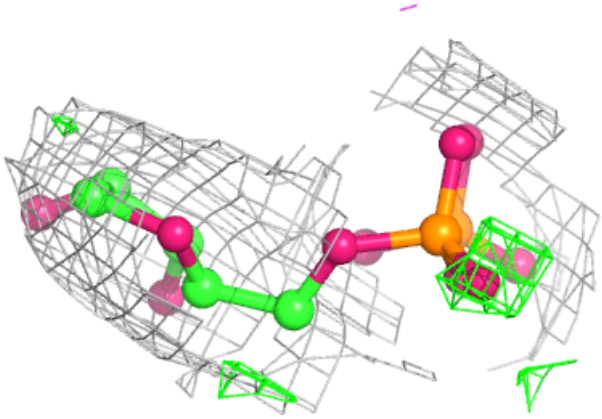


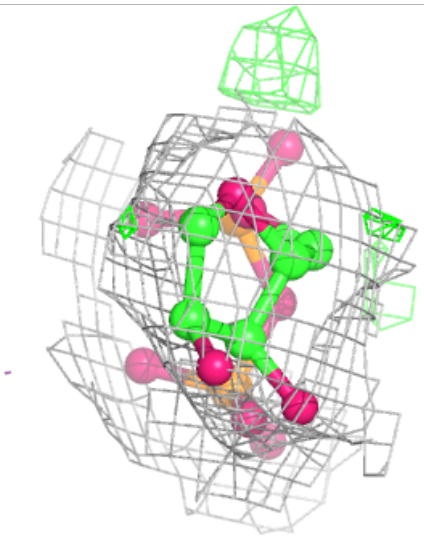


Electron density around ADP X 404:

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

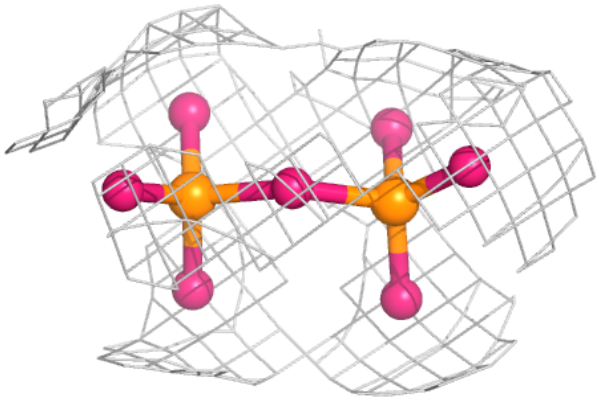


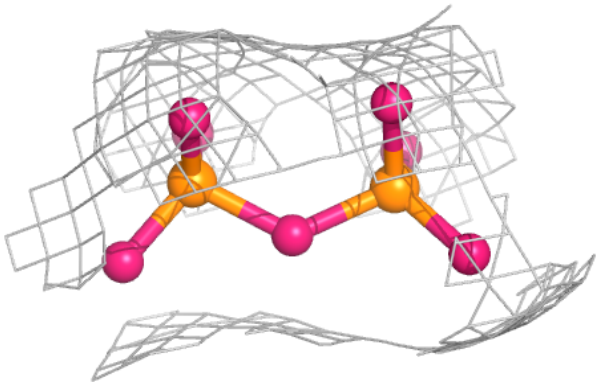


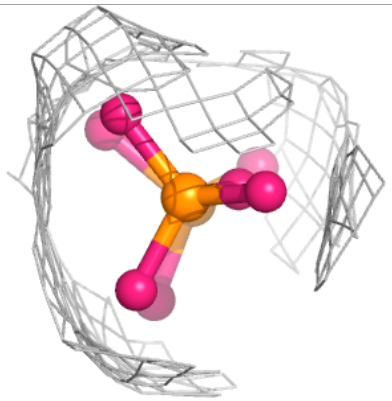


Electron density around ADP J 404:

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

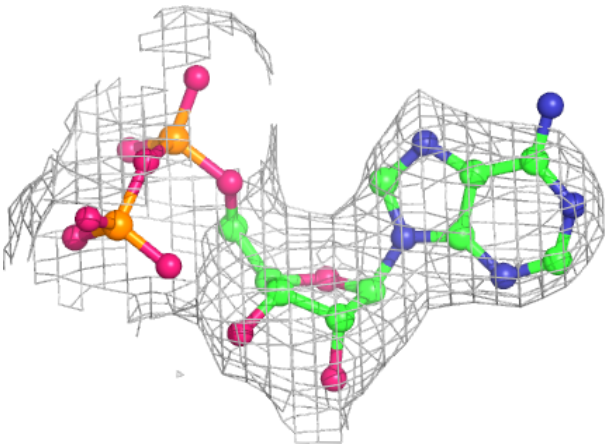


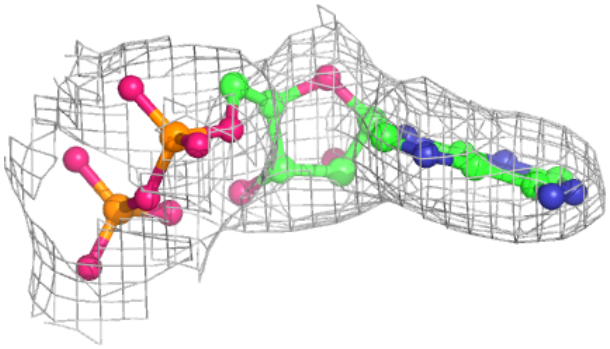


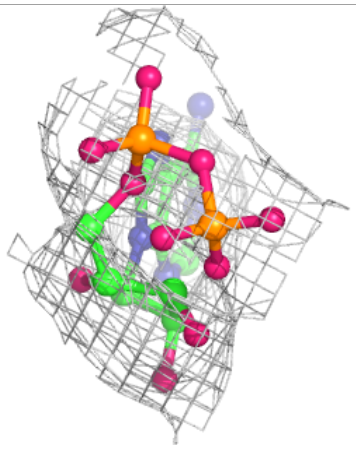


Electron density around ADP N 404:

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

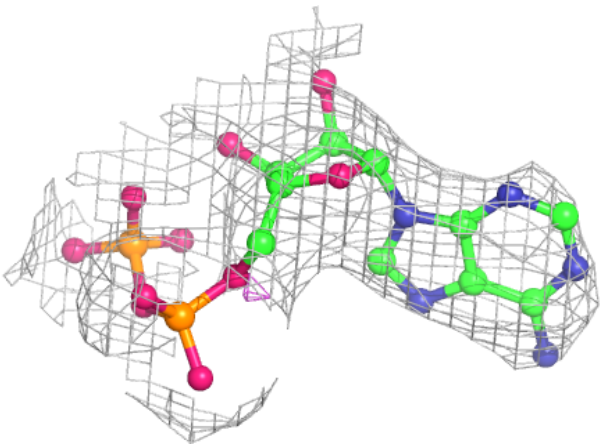


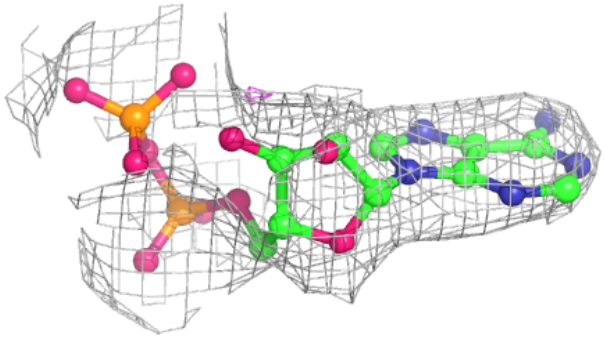


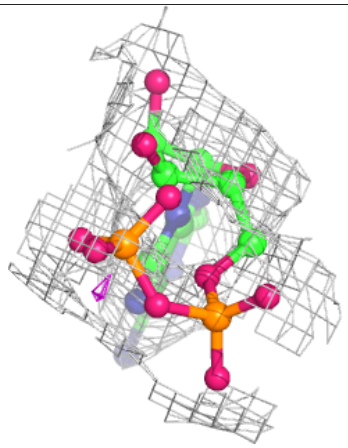


Electron density around ADP B 404:

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

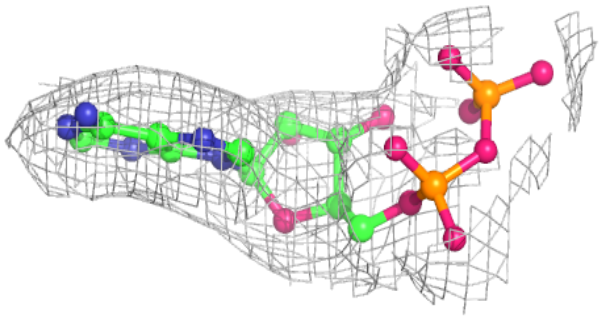


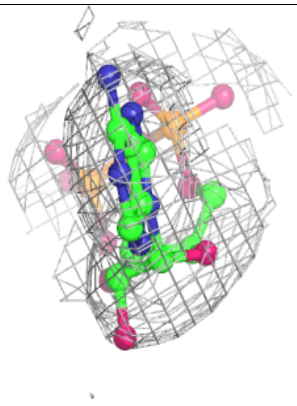




Electron density around ADP R 404:

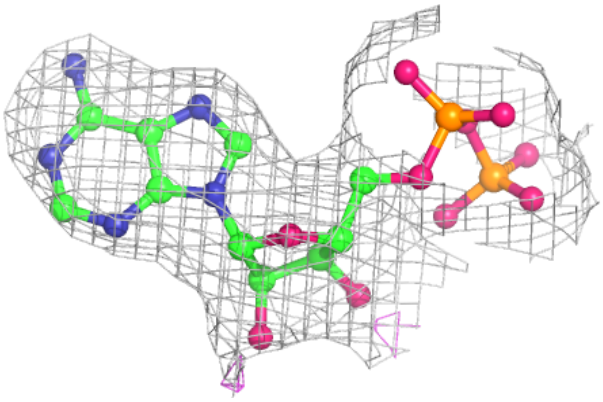
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

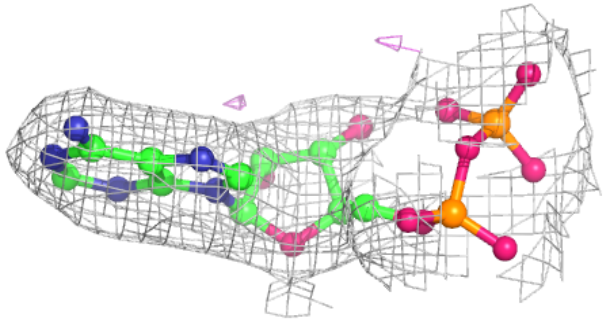


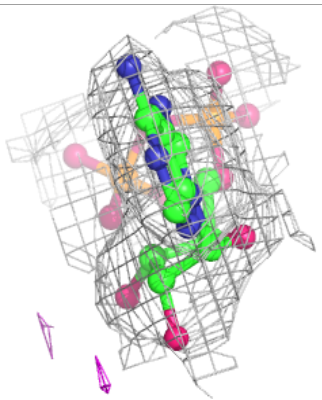


Electron density around ADP L 404:

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

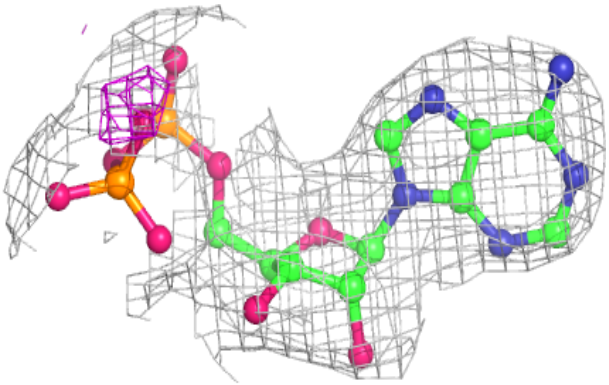


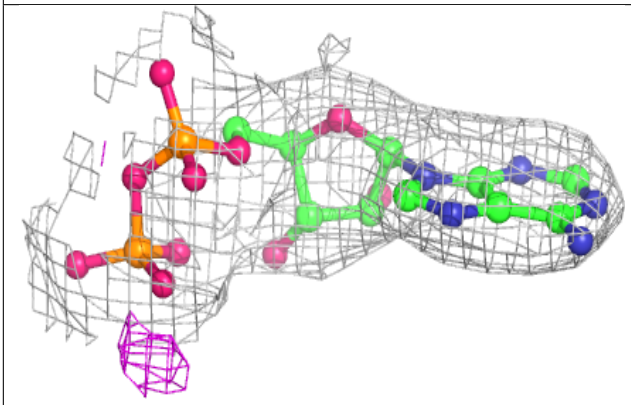


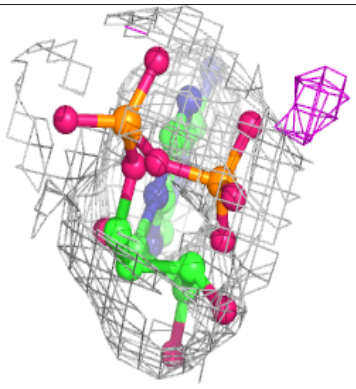


Electron density around ADP D 404:

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

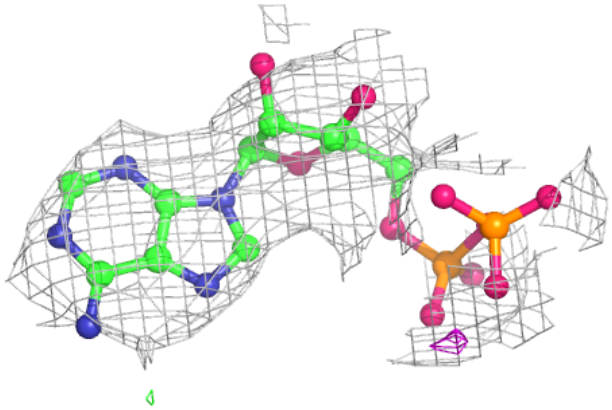


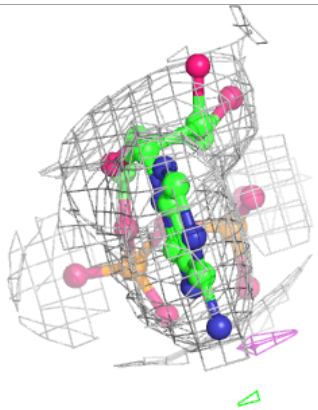




Electron density around ADP T 404:

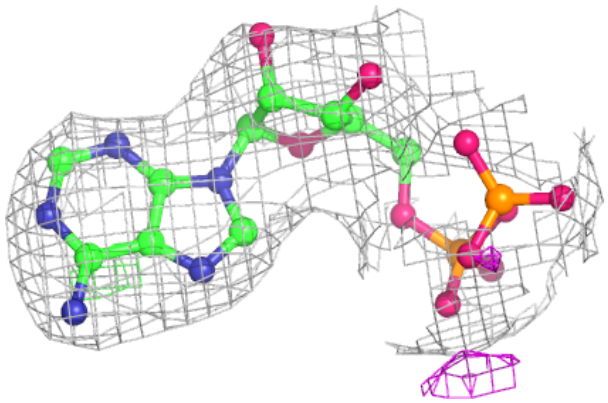
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

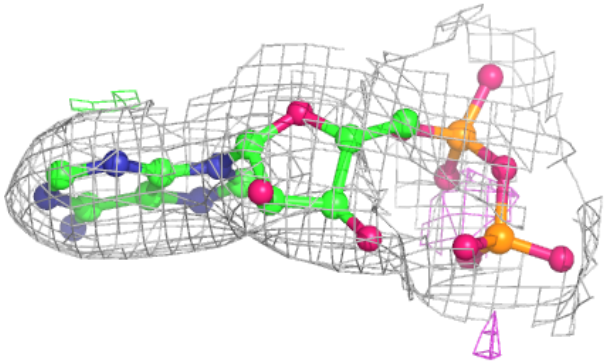


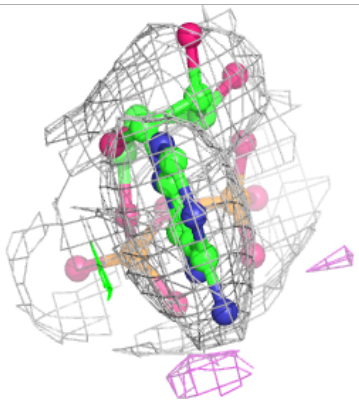


Electron density around ADP P 404:

$2mF_o$-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 (i)

There are no such residues in this entry.