wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2023 – 03:13 AM EDT

PDB ID	:	3LA6
Title	:	Octameric kinase domain of the E. coli tyrosine kinase Wzc with bound ADP
Authors	:	Gruszczyk, J.; Nessler, S.; Gueguen-Chaignon, V.; Vigouroux, A.; Bechet, E.; Grangeasse, C.
Deposited on	:	2010-01-06
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

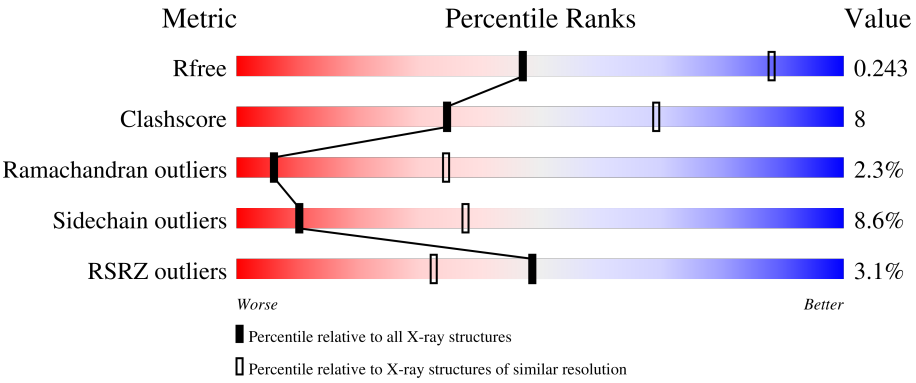
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	286	3% 64% 23% • 9%
1	B	286	4% 69% 18% • 9%
1	C	286	2% 67% 21% • 9%
1	D	286	4% 65% 21% • 10%
1	E	286	2% 69% 18% • 9%

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Mol	Chain	Length	Quality of chain
1	F	286	3% 70% 19% • 10%
1	G	286	5% 65% 22% • 9%
1	H	286	5% 67% 21% • 9%
1	I	286	3% 70% 19% • 9%
1	J	286	2% 66% 22% • 9%
1	K	286	% 68% 19% • 10%
1	L	286	2% 73% 16% • 9%
1	M	286	2% 66% 20% • 10%
1	N	286	3% 67% 21% • 9%
1	O	286	2% 65% 21% • 9%
1	P	286	% 70% 16% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32420 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 Tyrosine-protein kinase wzc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1998	1262	343	383	10			
1	B	260	Total	C	N	O	S	0	0	0
			2004	1265	344	385	10			
1	C	260	Total	C	N	O	S	0	0	0
			2006	1266	345	385	10			
1	D	258	Total	C	N	O	S	0	0	0
			1993	1259	343	381	10			
1	E	260	Total	C	N	O	S	0	0	0
			2013	1272	345	386	10			
1	F	257	Total	C	N	O	S	0	0	0
			1982	1252	340	380	10			
1	G	259	Total	C	N	O	S	0	0	0
			2003	1266	343	384	10			
1	H	260	Total	C	N	O	S	0	0	0
			2004	1265	344	385	10			
1	I	260	Total	C	N	O	S	0	0	0
			2008	1268	345	385	10			
1	J	259	Total	C	N	O	S	0	0	0
			2000	1264	344	382	10			
1	K	258	Total	C	N	O	S	0	0	0
			1993	1259	343	381	10			
1	L	259	Total	C	N	O	S	0	0	0
			1999	1265	343	381	10			
1	M	256	Total	C	N	O	S	0	0	0
			1977	1249	339	379	10			
1	N	260	Total	C	N	O	S	0	0	0
			2008	1268	345	385	10			
1	O	260	Total	C	N	O	S	0	0	0
			2008	1269	344	385	10			
1	P	256	Total	C	N	O	S	0	0	0
			1976	1250	338	378	10			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	MET	-	expression tag	UNP P76387
A	436	ARG	-	expression tag	UNP P76387
A	437	GLY	-	expression tag	UNP P76387
A	438	SER	-	expression tag	UNP P76387
A	439	HIS	-	expression tag	UNP P76387
A	440	HIS	-	expression tag	UNP P76387
A	441	HIS	-	expression tag	UNP P76387
A	442	HIS	-	expression tag	UNP P76387
A	443	HIS	-	expression tag	UNP P76387
A	444	HIS	-	expression tag	UNP P76387
A	445	GLY	-	expression tag	UNP P76387
A	446	SER	-	expression tag	UNP P76387
A	540	MET	LYS	SEE REMARK 999	UNP P76387
B	435	MET	-	expression tag	UNP P76387
B	436	ARG	-	expression tag	UNP P76387
B	437	GLY	-	expression tag	UNP P76387
B	438	SER	-	expression tag	UNP P76387
B	439	HIS	-	expression tag	UNP P76387
B	440	HIS	-	expression tag	UNP P76387
B	441	HIS	-	expression tag	UNP P76387
B	442	HIS	-	expression tag	UNP P76387
B	443	HIS	-	expression tag	UNP P76387
B	444	HIS	-	expression tag	UNP P76387
B	445	GLY	-	expression tag	UNP P76387
B	446	SER	-	expression tag	UNP P76387
B	540	MET	LYS	SEE REMARK 999	UNP P76387
C	435	MET	-	expression tag	UNP P76387
C	436	ARG	-	expression tag	UNP P76387
C	437	GLY	-	expression tag	UNP P76387
C	438	SER	-	expression tag	UNP P76387
C	439	HIS	-	expression tag	UNP P76387
C	440	HIS	-	expression tag	UNP P76387
C	441	HIS	-	expression tag	UNP P76387
C	442	HIS	-	expression tag	UNP P76387
C	443	HIS	-	expression tag	UNP P76387
C	444	HIS	-	expression tag	UNP P76387
C	445	GLY	-	expression tag	UNP P76387
C	446	SER	-	expression tag	UNP P76387
C	540	MET	LYS	SEE REMARK 999	UNP P76387
D	435	MET	-	expression tag	UNP P76387
D	436	ARG	-	expression tag	UNP P76387
D	437	GLY	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
D	438	SER	-	expression tag	UNP P76387
D	439	HIS	-	expression tag	UNP P76387
D	440	HIS	-	expression tag	UNP P76387
D	441	HIS	-	expression tag	UNP P76387
D	442	HIS	-	expression tag	UNP P76387
D	443	HIS	-	expression tag	UNP P76387
D	444	HIS	-	expression tag	UNP P76387
D	445	GLY	-	expression tag	UNP P76387
D	446	SER	-	expression tag	UNP P76387
D	540	MET	LYS	SEE REMARK 999	UNP P76387
E	435	MET	-	expression tag	UNP P76387
E	436	ARG	-	expression tag	UNP P76387
E	437	GLY	-	expression tag	UNP P76387
E	438	SER	-	expression tag	UNP P76387
E	439	HIS	-	expression tag	UNP P76387
E	440	HIS	-	expression tag	UNP P76387
E	441	HIS	-	expression tag	UNP P76387
E	442	HIS	-	expression tag	UNP P76387
E	443	HIS	-	expression tag	UNP P76387
E	444	HIS	-	expression tag	UNP P76387
E	445	GLY	-	expression tag	UNP P76387
E	446	SER	-	expression tag	UNP P76387
E	540	MET	LYS	SEE REMARK 999	UNP P76387
F	435	MET	-	expression tag	UNP P76387
F	436	ARG	-	expression tag	UNP P76387
F	437	GLY	-	expression tag	UNP P76387
F	438	SER	-	expression tag	UNP P76387
F	439	HIS	-	expression tag	UNP P76387
F	440	HIS	-	expression tag	UNP P76387
F	441	HIS	-	expression tag	UNP P76387
F	442	HIS	-	expression tag	UNP P76387
F	443	HIS	-	expression tag	UNP P76387
F	444	HIS	-	expression tag	UNP P76387
F	445	GLY	-	expression tag	UNP P76387
F	446	SER	-	expression tag	UNP P76387
F	540	MET	LYS	SEE REMARK 999	UNP P76387
G	435	MET	-	expression tag	UNP P76387
G	436	ARG	-	expression tag	UNP P76387
G	437	GLY	-	expression tag	UNP P76387
G	438	SER	-	expression tag	UNP P76387
G	439	HIS	-	expression tag	UNP P76387
G	440	HIS	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
G	441	HIS	-	expression tag	UNP P76387
G	442	HIS	-	expression tag	UNP P76387
G	443	HIS	-	expression tag	UNP P76387
G	444	HIS	-	expression tag	UNP P76387
G	445	GLY	-	expression tag	UNP P76387
G	446	SER	-	expression tag	UNP P76387
G	540	MET	LYS	SEE REMARK 999	UNP P76387
H	435	MET	-	expression tag	UNP P76387
H	436	ARG	-	expression tag	UNP P76387
H	437	GLY	-	expression tag	UNP P76387
H	438	SER	-	expression tag	UNP P76387
H	439	HIS	-	expression tag	UNP P76387
H	440	HIS	-	expression tag	UNP P76387
H	441	HIS	-	expression tag	UNP P76387
H	442	HIS	-	expression tag	UNP P76387
H	443	HIS	-	expression tag	UNP P76387
H	444	HIS	-	expression tag	UNP P76387
H	445	GLY	-	expression tag	UNP P76387
H	446	SER	-	expression tag	UNP P76387
H	540	MET	LYS	SEE REMARK 999	UNP P76387
I	435	MET	-	expression tag	UNP P76387
I	436	ARG	-	expression tag	UNP P76387
I	437	GLY	-	expression tag	UNP P76387
I	438	SER	-	expression tag	UNP P76387
I	439	HIS	-	expression tag	UNP P76387
I	440	HIS	-	expression tag	UNP P76387
I	441	HIS	-	expression tag	UNP P76387
I	442	HIS	-	expression tag	UNP P76387
I	443	HIS	-	expression tag	UNP P76387
I	444	HIS	-	expression tag	UNP P76387
I	445	GLY	-	expression tag	UNP P76387
I	446	SER	-	expression tag	UNP P76387
I	540	MET	LYS	SEE REMARK 999	UNP P76387
J	435	MET	-	expression tag	UNP P76387
J	436	ARG	-	expression tag	UNP P76387
J	437	GLY	-	expression tag	UNP P76387
J	438	SER	-	expression tag	UNP P76387
J	439	HIS	-	expression tag	UNP P76387
J	440	HIS	-	expression tag	UNP P76387
J	441	HIS	-	expression tag	UNP P76387
J	442	HIS	-	expression tag	UNP P76387
J	443	HIS	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
J	444	HIS	-	expression tag	UNP P76387
J	445	GLY	-	expression tag	UNP P76387
J	446	SER	-	expression tag	UNP P76387
J	540	MET	LYS	SEE REMARK 999	UNP P76387
K	435	MET	-	expression tag	UNP P76387
K	436	ARG	-	expression tag	UNP P76387
K	437	GLY	-	expression tag	UNP P76387
K	438	SER	-	expression tag	UNP P76387
K	439	HIS	-	expression tag	UNP P76387
K	440	HIS	-	expression tag	UNP P76387
K	441	HIS	-	expression tag	UNP P76387
K	442	HIS	-	expression tag	UNP P76387
K	443	HIS	-	expression tag	UNP P76387
K	444	HIS	-	expression tag	UNP P76387
K	445	GLY	-	expression tag	UNP P76387
K	446	SER	-	expression tag	UNP P76387
K	540	MET	LYS	SEE REMARK 999	UNP P76387
L	435	MET	-	expression tag	UNP P76387
L	436	ARG	-	expression tag	UNP P76387
L	437	GLY	-	expression tag	UNP P76387
L	438	SER	-	expression tag	UNP P76387
L	439	HIS	-	expression tag	UNP P76387
L	440	HIS	-	expression tag	UNP P76387
L	441	HIS	-	expression tag	UNP P76387
L	442	HIS	-	expression tag	UNP P76387
L	443	HIS	-	expression tag	UNP P76387
L	444	HIS	-	expression tag	UNP P76387
L	445	GLY	-	expression tag	UNP P76387
L	446	SER	-	expression tag	UNP P76387
L	540	MET	LYS	SEE REMARK 999	UNP P76387
M	435	MET	-	expression tag	UNP P76387
M	436	ARG	-	expression tag	UNP P76387
M	437	GLY	-	expression tag	UNP P76387
M	438	SER	-	expression tag	UNP P76387
M	439	HIS	-	expression tag	UNP P76387
M	440	HIS	-	expression tag	UNP P76387
M	441	HIS	-	expression tag	UNP P76387
M	442	HIS	-	expression tag	UNP P76387
M	443	HIS	-	expression tag	UNP P76387
M	444	HIS	-	expression tag	UNP P76387
M	445	GLY	-	expression tag	UNP P76387
M	446	SER	-	expression tag	UNP P76387

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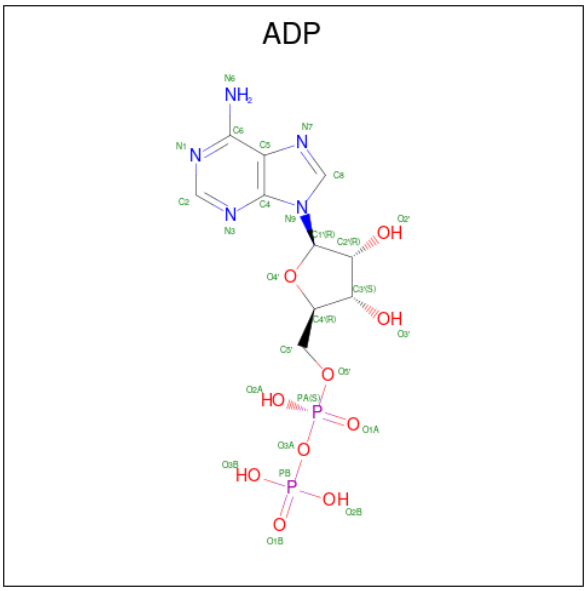
Chain	Residue	Modelled	Actual	Comment	Reference
M	540	MET	LYS	SEE REMARK 999	UNP P76387
N	435	MET	-	expression tag	UNP P76387
N	436	ARG	-	expression tag	UNP P76387
N	437	GLY	-	expression tag	UNP P76387
N	438	SER	-	expression tag	UNP P76387
N	439	HIS	-	expression tag	UNP P76387
N	440	HIS	-	expression tag	UNP P76387
N	441	HIS	-	expression tag	UNP P76387
N	442	HIS	-	expression tag	UNP P76387
N	443	HIS	-	expression tag	UNP P76387
N	444	HIS	-	expression tag	UNP P76387
N	445	GLY	-	expression tag	UNP P76387
N	446	SER	-	expression tag	UNP P76387
N	540	MET	LYS	SEE REMARK 999	UNP P76387
O	435	MET	-	expression tag	UNP P76387
O	436	ARG	-	expression tag	UNP P76387
O	437	GLY	-	expression tag	UNP P76387
O	438	SER	-	expression tag	UNP P76387
O	439	HIS	-	expression tag	UNP P76387
O	440	HIS	-	expression tag	UNP P76387
O	441	HIS	-	expression tag	UNP P76387
O	442	HIS	-	expression tag	UNP P76387
O	443	HIS	-	expression tag	UNP P76387
O	444	HIS	-	expression tag	UNP P76387
O	445	GLY	-	expression tag	UNP P76387
O	446	SER	-	expression tag	UNP P76387
O	540	MET	LYS	SEE REMARK 999	UNP P76387
P	435	MET	-	expression tag	UNP P76387
P	436	ARG	-	expression tag	UNP P76387
P	437	GLY	-	expression tag	UNP P76387
P	438	SER	-	expression tag	UNP P76387
P	439	HIS	-	expression tag	UNP P76387
P	440	HIS	-	expression tag	UNP P76387
P	441	HIS	-	expression tag	UNP P76387
P	442	HIS	-	expression tag	UNP P76387
P	443	HIS	-	expression tag	UNP P76387
P	444	HIS	-	expression tag	UNP P76387
P	445	GLY	-	expression tag	UNP P76387
P	446	SER	-	expression tag	UNP P76387
P	540	MET	LYS	SEE REMARK 999	UNP P76387

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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		
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		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

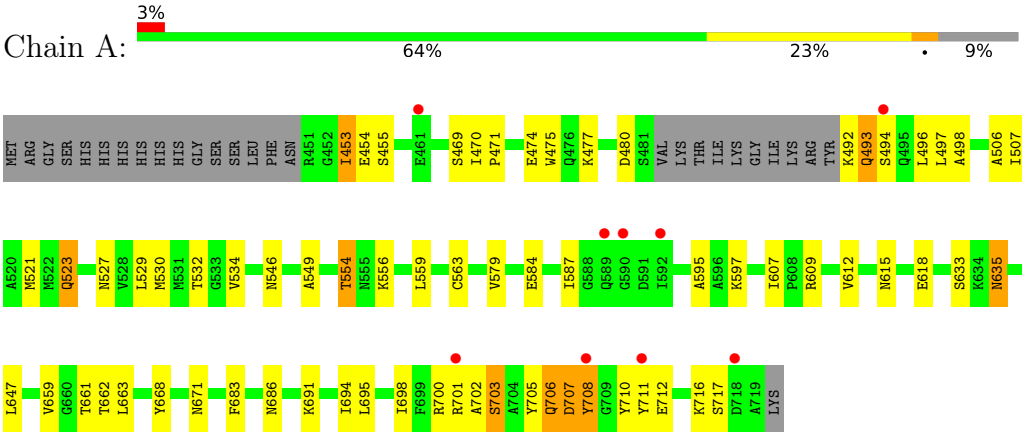
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	L	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	N	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		
3	P	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

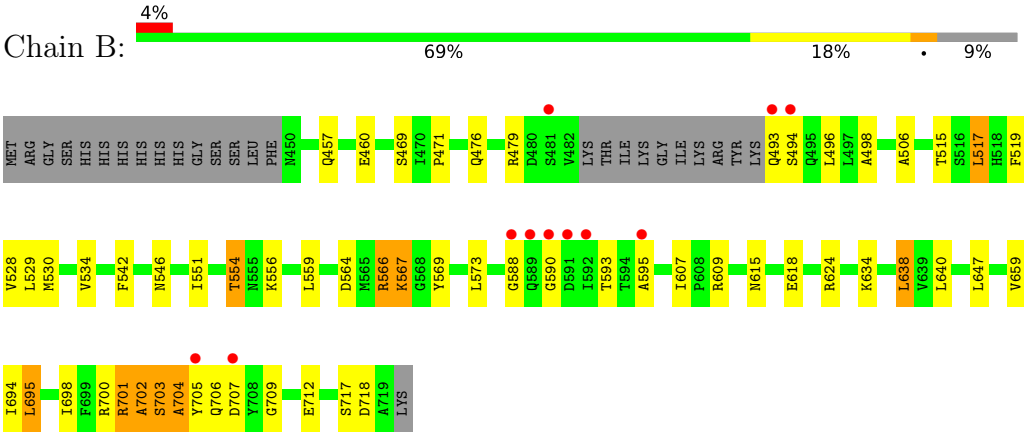
• Molecule 1: Tyrosine-protein kinase wzc

Chain A:



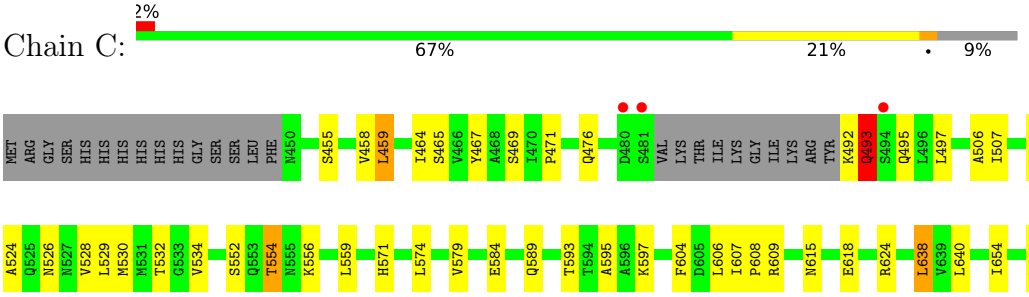
• Molecule 1: Tyrosine-protein kinase wzc

Chain B:

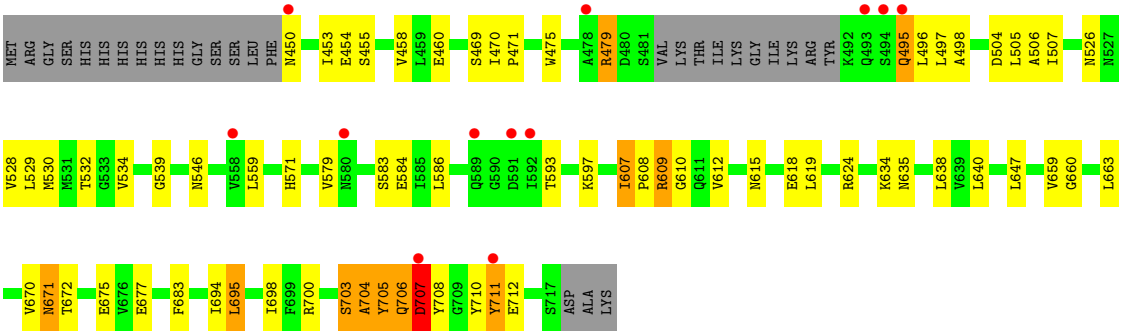


• Molecule 1: Tyrosine-protein kinase wzc

Chain C:

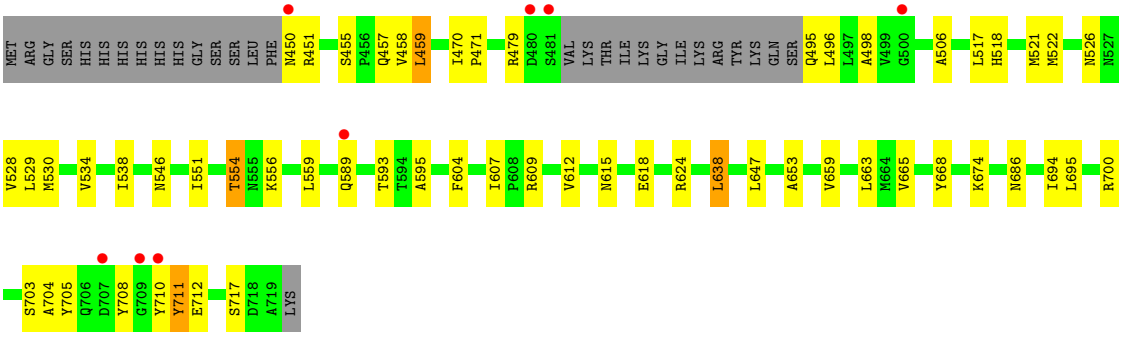


• Molecule 1: Tyrosine-protein kinase wzc

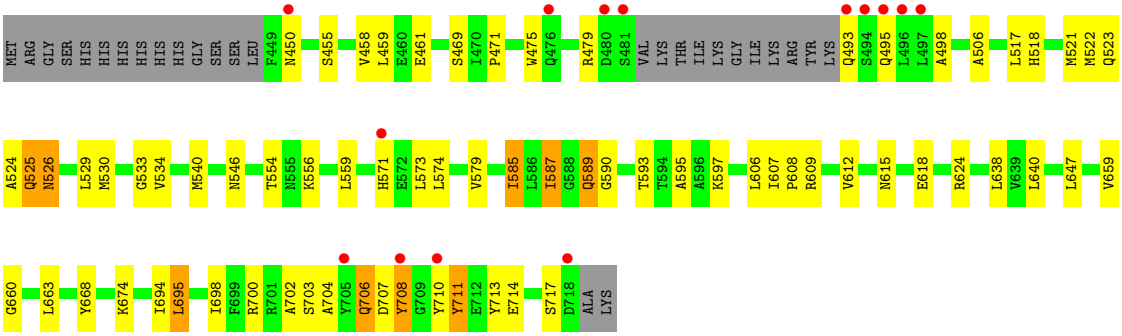


• Molecule 1: Tyrosine-protein kinase wzc

• Molecule 1: Tyrosine-protein kinase wzc

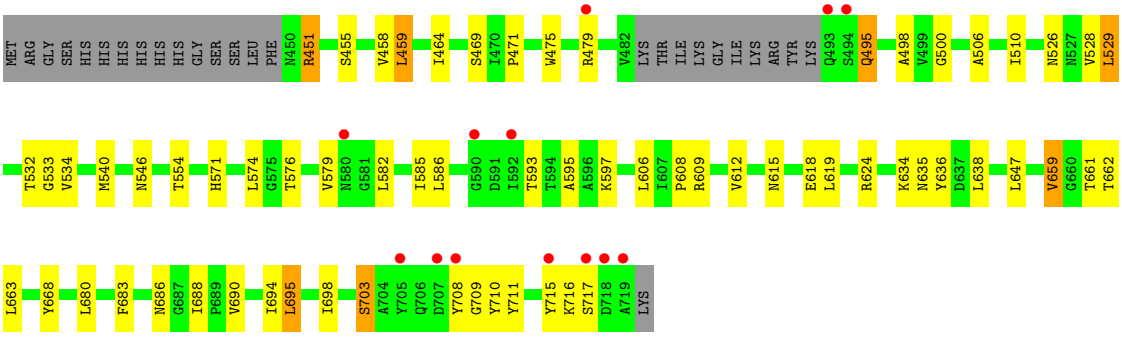


• Molecule 1: Tyrosine-protein kinase wzc



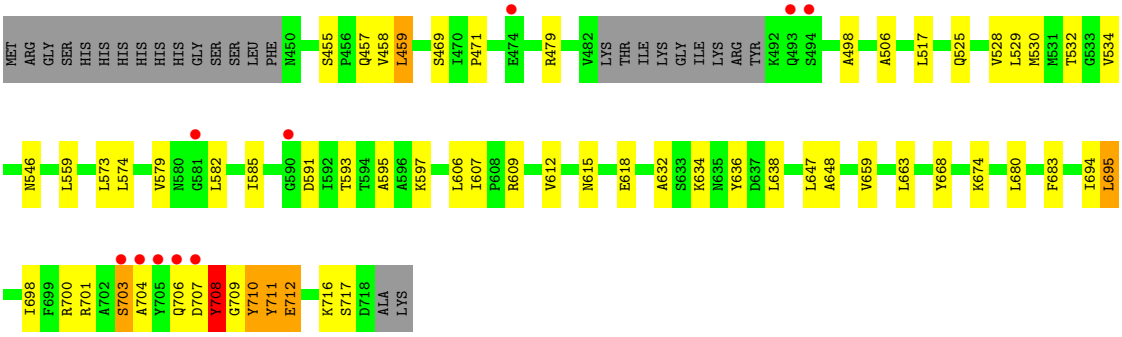
• Molecule 1: Tyrosine-protein kinase wzc

Chain H:



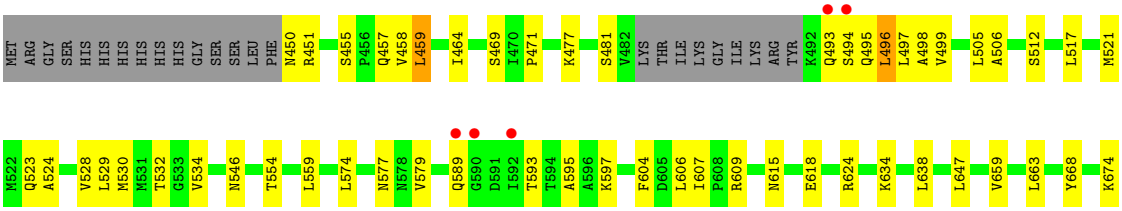
• Molecule 1: Tyrosine-protein kinase wzc

Chain I:



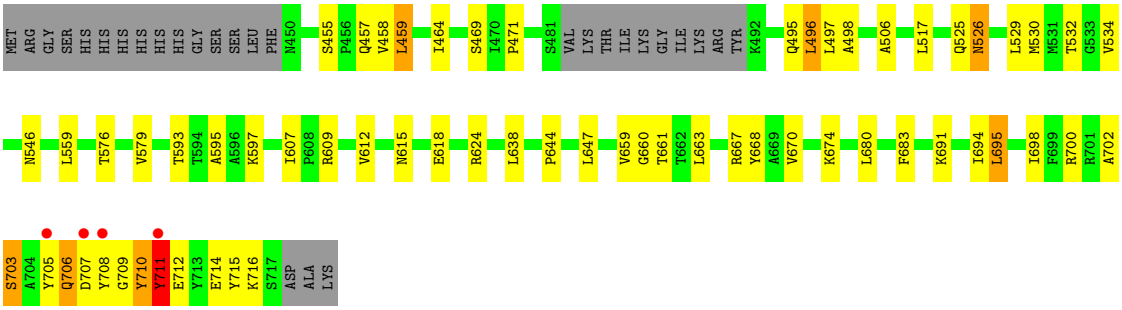
• Molecule 1: Tyrosine-protein kinase wzc

Chain J:



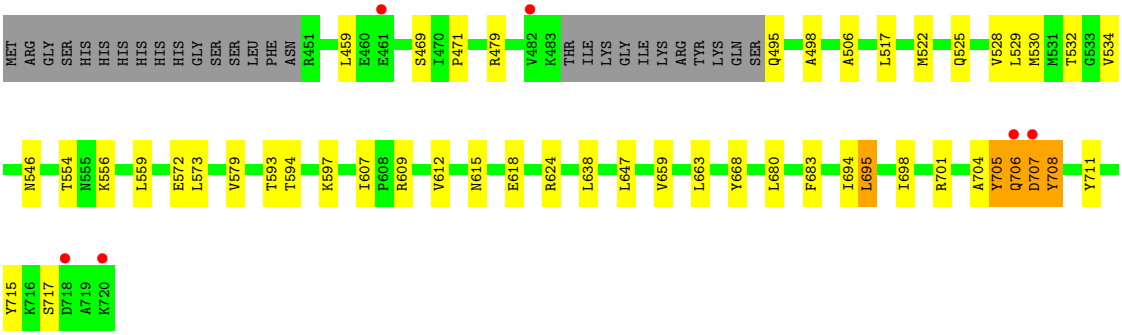
• Molecule 1: Tyrosine-protein kinase wzc

Chain K:



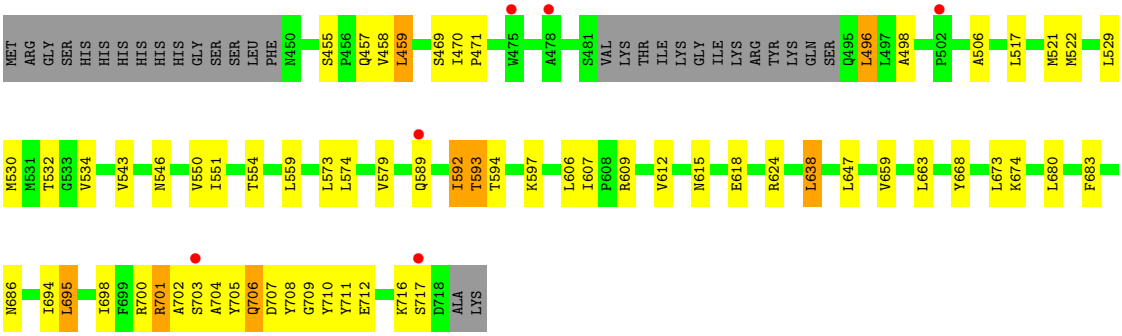
• Molecule 1: Tyrosine-protein kinase wzc

Chain L:



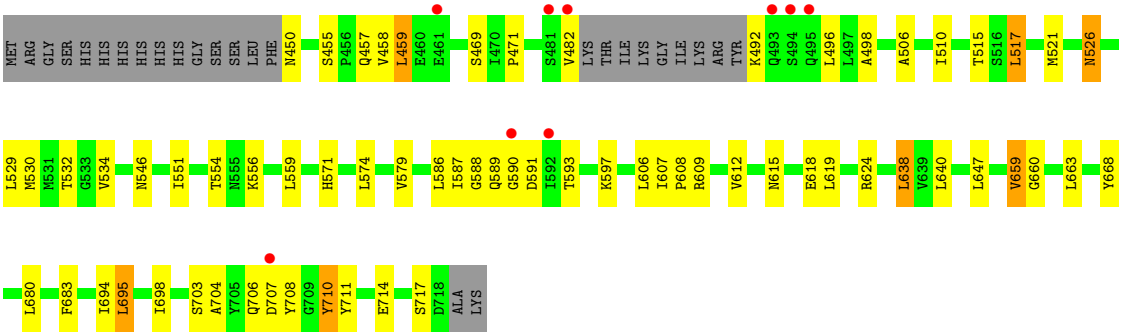
• Molecule 1: Tyrosine-protein kinase wzc

Chain M:



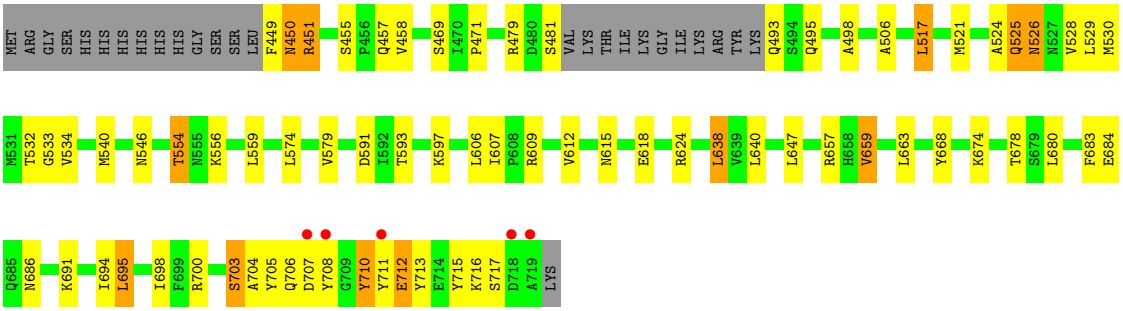
• Molecule 1: Tyrosine-protein kinase wzc

Chain N:



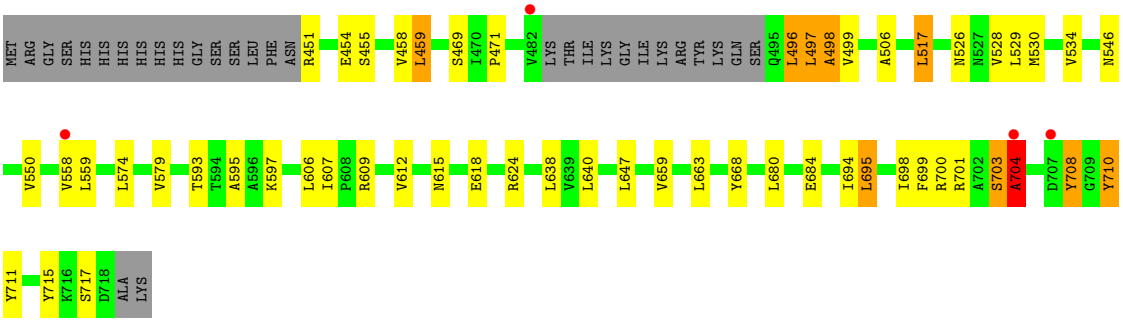
• Molecule 1: Tyrosine-protein kinase wzc

Chain O:



• Molecule 1: Tyrosine-protein kinase wzc

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	245.16Å 137.78Å 158.96Å 90.00° 92.99° 90.00°	Depositor
Resolution (Å)	49.74 – 3.20 49.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.74-3.20) 96.3 (49.74-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.19Å)	Xtriage
Refinement program	TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.186 , 0.223 0.202 , 0.243	Depositor DCC
R_{free} test set	833 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	85.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 81.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.003 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.004 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.006 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.006 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.012 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32420	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.52	0/2032	0.77	1/2759 (0.0%)
1	B	0.51	0/2038	0.76	1/2769 (0.0%)
1	C	0.52	0/2040	0.76	0/2770
1	D	0.50	0/2027	0.77	1/2752 (0.0%)
1	E	0.52	0/2048	0.75	0/2781
1	F	0.50	0/2016	0.75	0/2739
1	G	0.47	0/2038	0.71	0/2768
1	H	0.51	0/2038	0.76	0/2769
1	I	0.49	0/2042	0.74	0/2773
1	J	0.51	0/2034	0.76	0/2762
1	K	0.53	0/2027	0.78	1/2752 (0.0%)
1	L	0.51	0/2033	0.76	0/2760
1	M	0.50	0/2011	0.75	1/2732 (0.0%)
1	N	0.52	0/2042	0.76	0/2773
1	O	0.52	0/2043	0.77	1/2775 (0.0%)
1	P	0.51	0/2010	0.78	2/2731 (0.1%)
All	All	0.51	0/32519	0.76	8/44165 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	712	GLU	C-N-CA	5.81	136.22	121.70
1	M	705	TYR	C-N-CA	5.76	136.11	121.70
1	B	705	TYR	C-N-CA	5.58	135.65	121.70
1	A	705	TYR	C-N-CA	5.51	135.48	121.70
1	K	702	ALA	C-N-CA	5.37	135.12	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1998	0	2015	63	0
1	B	2004	0	2017	35	0
1	C	2006	0	2021	30	0
1	D	1993	0	2012	48	0
1	E	2013	0	2025	30	0
1	F	1982	0	1995	26	0
1	G	2003	0	2012	42	0
1	H	2004	0	2017	32	0
1	I	2008	0	2025	29	0
1	J	2000	0	2021	37	0
1	K	1993	0	2012	33	0
1	L	1999	0	2024	22	0
1	M	1977	0	1990	41	0
1	N	2008	0	2025	50	0
1	O	2008	0	2017	50	0
1	P	1976	0	1993	34	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	2	0
2	D	27	0	12	1	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	1	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	1	0
2	K	27	0	12	0	0
2	L	27	0	12	0	0
2	M	27	0	12	0	0
2	N	27	0	12	1	0
2	O	27	0	12	1	0
2	P	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	32420	0	32413	541	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 8.

The worst 5 of 541 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:454:GLU:CG	1:A:701:ARG:HH22	1.00	1.58
1:A:454:GLU:HG2	1:A:701:ARG:NH2	0.91	1.23
1:N:587:ILE:CG2	1:N:619:LEU:HD22	1.71	1.20
1:N:587:ILE:CG2	1:N:619:LEU:CD2	2.22	1.17
1:A:497:LEU:HG	1:A:507:ILE:HD11	1.26	1.15

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	255/286 (89%)	235 (92%)	14 (6%)	6 (2%)	6 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	256/286 (90%)	233 (91%)	14 (6%)	9 (4%)	3 24
1	C	256/286 (90%)	231 (90%)	20 (8%)	5 (2%)	7 38
1	D	254/286 (89%)	237 (93%)	11 (4%)	6 (2%)	6 34
1	E	256/286 (90%)	234 (91%)	16 (6%)	6 (2%)	6 34
1	F	253/286 (88%)	234 (92%)	13 (5%)	6 (2%)	6 34
1	G	255/286 (89%)	233 (91%)	15 (6%)	7 (3%)	5 30
1	H	256/286 (90%)	231 (90%)	19 (7%)	6 (2%)	6 34
1	I	256/286 (90%)	237 (93%)	14 (6%)	5 (2%)	7 38
1	J	255/286 (89%)	232 (91%)	19 (8%)	4 (2%)	9 43
1	K	254/286 (89%)	232 (91%)	13 (5%)	9 (4%)	3 24
1	L	255/286 (89%)	238 (93%)	15 (6%)	2 (1%)	19 58
1	M	252/286 (88%)	228 (90%)	18 (7%)	6 (2%)	6 34
1	N	256/286 (90%)	236 (92%)	16 (6%)	4 (2%)	9 43
1	O	256/286 (90%)	234 (91%)	16 (6%)	6 (2%)	6 34
1	P	252/286 (88%)	231 (92%)	14 (6%)	7 (3%)	5 29
All	All	4077/4576 (89%)	3736 (92%)	247 (6%)	94 (2%)	6 34

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	TYR
1	A	708	TYR
1	B	496	LEU
1	B	703	SER
1	B	704	ALA

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	220/244 (90%)	203 (92%)	17 (8%)	13 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	221/244 (91%)	202 (91%)	19 (9%)	10 38
1	C	221/244 (91%)	199 (90%)	22 (10%)	7 30
1	D	220/244 (90%)	202 (92%)	18 (8%)	11 41
1	E	222/244 (91%)	202 (91%)	20 (9%)	9 34
1	F	218/244 (89%)	201 (92%)	17 (8%)	12 43
1	G	221/244 (91%)	205 (93%)	16 (7%)	14 47
1	H	221/244 (91%)	202 (91%)	19 (9%)	10 38
1	I	222/244 (91%)	203 (91%)	19 (9%)	10 38
1	J	221/244 (91%)	198 (90%)	23 (10%)	7 28
1	K	220/244 (90%)	202 (92%)	18 (8%)	11 41
1	L	220/244 (90%)	199 (90%)	21 (10%)	8 32
1	M	218/244 (89%)	201 (92%)	17 (8%)	12 43
1	N	222/244 (91%)	205 (92%)	17 (8%)	13 44
1	O	221/244 (91%)	199 (90%)	22 (10%)	7 30
1	P	218/244 (89%)	200 (92%)	18 (8%)	11 40
All	All	3526/3904 (90%)	3223 (91%)	303 (9%)	10 38

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	522	MET
1	P	454	GLU
1	M	624	ARG
1	N	710	TYR
1	P	708	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	495	GLN
1	N	546	ASN
1	O	546	ASN
1	F	476	GLN
1	F	457	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	ADP	P	1000	3	24,29,29	1.49	4 (16%)	29,45,45	1.01	2 (6%)
2	ADP	F	1000	3	24,29,29	1.52	4 (16%)	29,45,45	1.10	3 (10%)
2	ADP	L	1000	3	24,29,29	1.64	5 (20%)	29,45,45	0.97	2 (6%)
2	ADP	C	1000	3	24,29,29	1.44	4 (16%)	29,45,45	1.01	2 (6%)
2	ADP	M	1000	3	24,29,29	1.35	4 (16%)	29,45,45	1.06	2 (6%)
2	ADP	O	1000	3	24,29,29	1.72	3 (12%)	29,45,45	1.17	2 (6%)
2	ADP	A	1000	3	24,29,29	1.36	3 (12%)	29,45,45	1.22	3 (10%)
2	ADP	K	1000	3	24,29,29	1.46	4 (16%)	29,45,45	1.03	3 (10%)
2	ADP	J	1000	3	24,29,29	1.36	4 (16%)	29,45,45	1.08	3 (10%)
2	ADP	G	1000	3	24,29,29	1.71	5 (20%)	29,45,45	1.54	6 (20%)
2	ADP	H	1000	3	24,29,29	1.34	3 (12%)	29,45,45	1.12	1 (3%)
2	ADP	N	1000	3	24,29,29	1.54	4 (16%)	29,45,45	1.34	3 (10%)
2	ADP	E	1000	3	24,29,29	1.31	3 (12%)	29,45,45	1.18	2 (6%)
2	ADP	D	1000	3	24,29,29	1.63	5 (20%)	29,45,45	1.13	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	I	1000	3	24,29,29	1.38	3 (12%)	29,45,45	0.99	2 (6%)
2	ADP	B	1000	3	24,29,29	1.49	3 (12%)	29,45,45	0.98	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	P	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	F	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	L	1000	3	-	2/12/32/32	0/3/3/3
2	ADP	C	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	M	1000	3	-	2/12/32/32	0/3/3/3
2	ADP	O	1000	3	-	2/12/32/32	0/3/3/3
2	ADP	A	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	K	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	J	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	G	1000	3	-	5/12/32/32	0/3/3/3
2	ADP	H	1000	3	-	2/12/32/32	0/3/3/3
2	ADP	N	1000	3	-	1/12/32/32	0/3/3/3
2	ADP	E	1000	3	-	2/12/32/32	0/3/3/3
2	ADP	D	1000	3	-	7/12/32/32	0/3/3/3
2	ADP	I	1000	3	-	0/12/32/32	0/3/3/3
2	ADP	B	1000	3	-	0/12/32/32	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1000	ADP	C2-N1	4.72	1.42	1.33
2	K	1000	ADP	C2-N3	4.37	1.39	1.32
2	O	1000	ADP	C2-N3	4.33	1.39	1.32
2	D	1000	ADP	O4'-C1'	4.29	1.47	1.41
2	N	1000	ADP	O4'-C1'	4.23	1.47	1.41

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1000	ADP	O3B-PB-O3A	4.13	118.49	104.64
2	H	1000	ADP	O3B-PB-O3A	3.89	117.69	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1000	ADP	O3B-PB-O3A	3.77	117.28	104.64
2	E	1000	ADP	O3B-PB-O3A	3.67	116.94	104.64
2	M	1000	ADP	O3B-PB-O3A	3.59	116.68	104.64

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1000	ADP	PA-O3A-PB-O3B
2	E	1000	ADP	PA-O3A-PB-O2B
2	E	1000	ADP	PA-O3A-PB-O3B
2	G	1000	ADP	PA-O3A-PB-O2B
2	G	1000	ADP	PA-O3A-PB-O3B

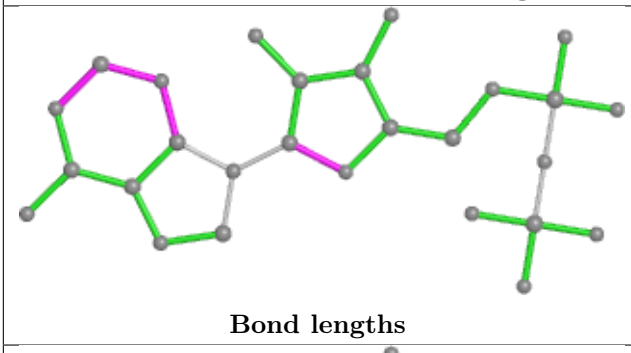
There are no ring outliers.

7 monomers are involved in 8 short contacts:

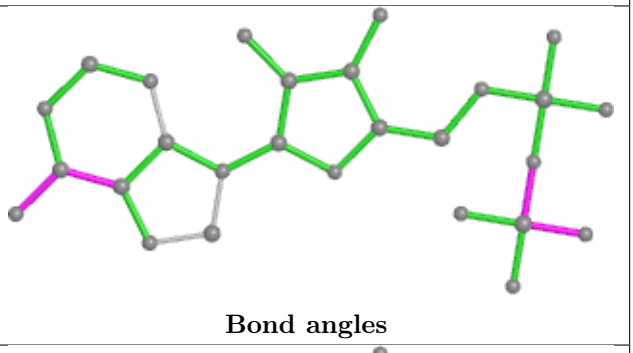
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	ADP	2	0
2	O	1000	ADP	1	0
2	J	1000	ADP	1	0
2	G	1000	ADP	1	0
2	N	1000	ADP	1	0
2	D	1000	ADP	1	0
2	B	1000	ADP	1	0

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 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.

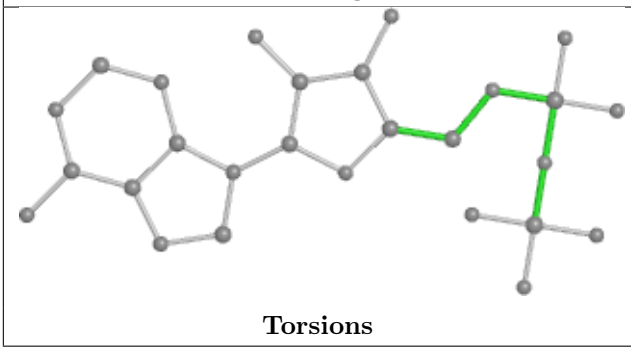
Ligand ADP P 1000



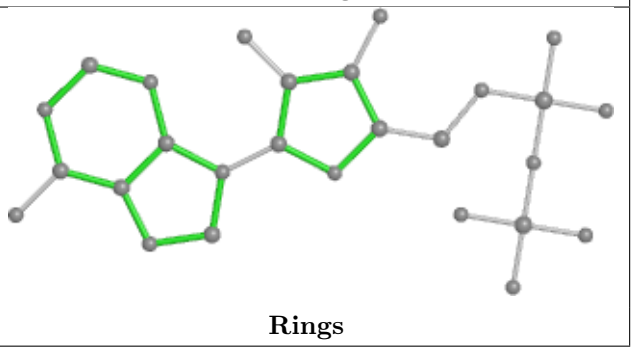
Bond lengths



Bond angles

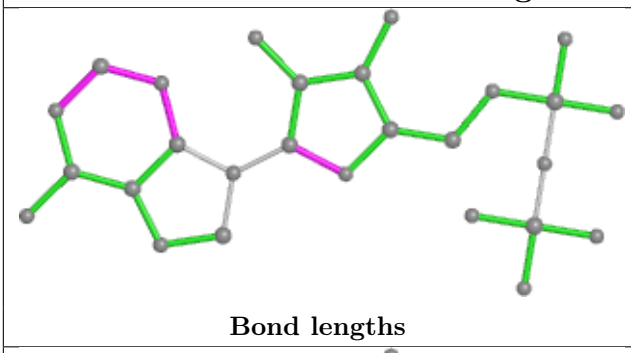


Torsions

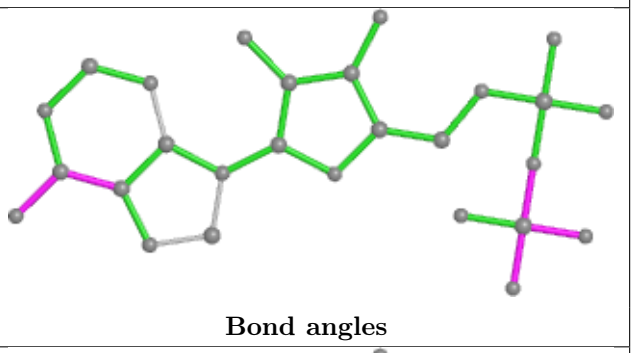


Rings

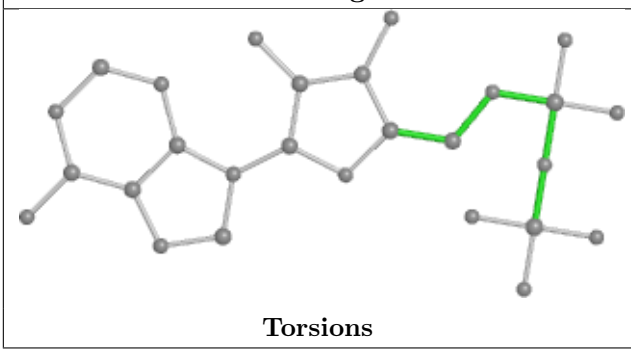
Ligand ADP F 1000



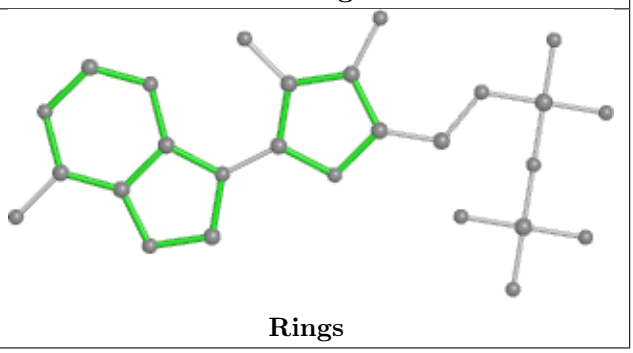
Bond lengths



Bond angles

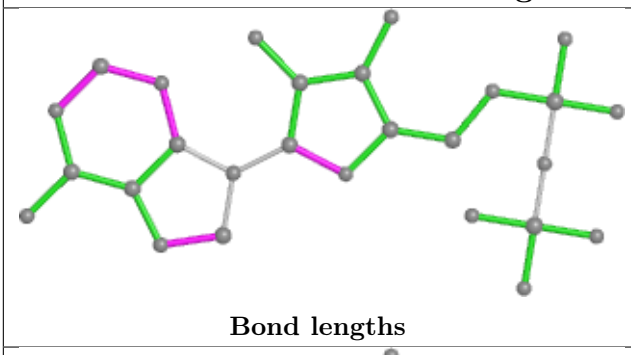


Torsions

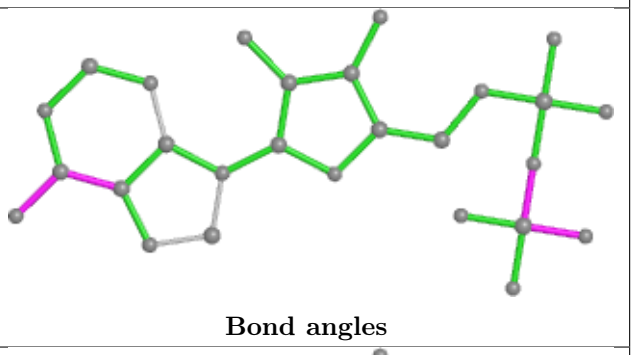


Rings

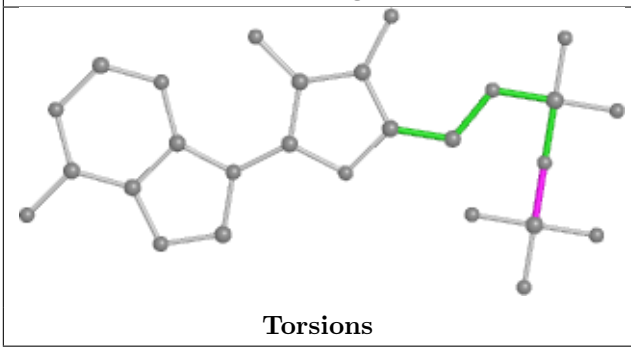
Ligand ADP L 1000



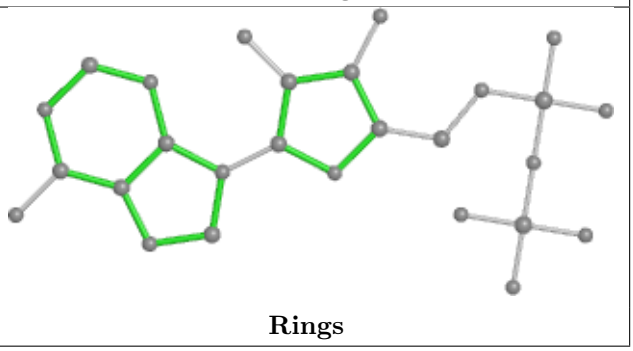
Bond lengths



Bond angles

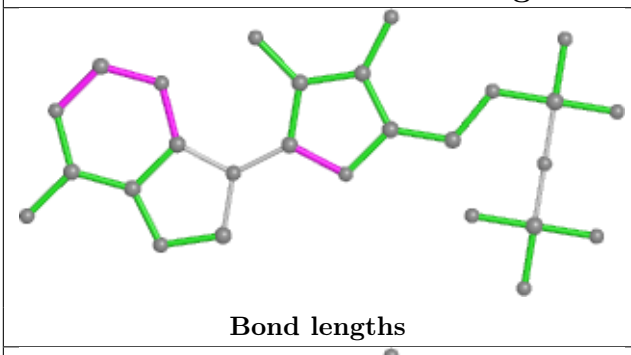


Torsions

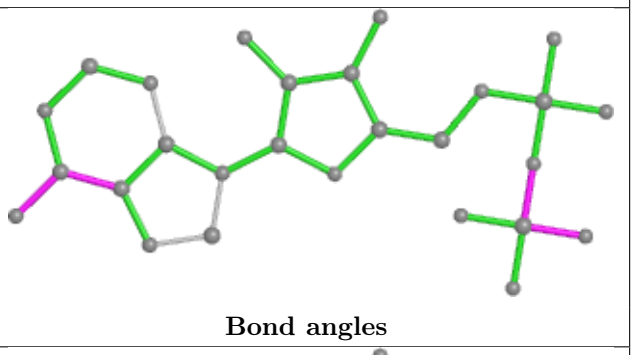


Rings

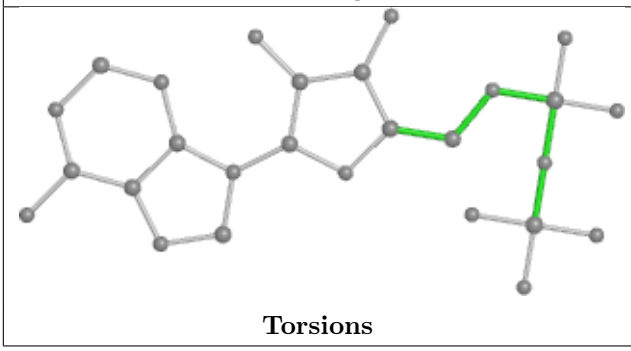
Ligand ADP C 1000



Bond lengths



Bond angles



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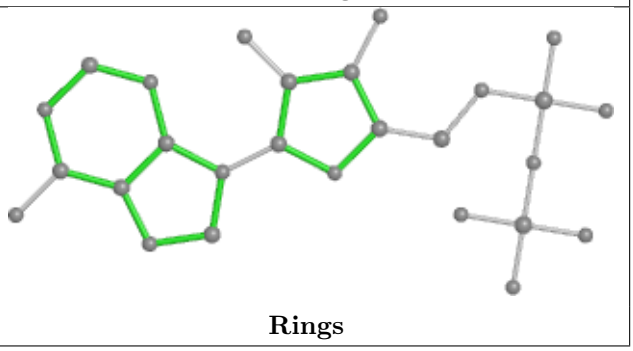
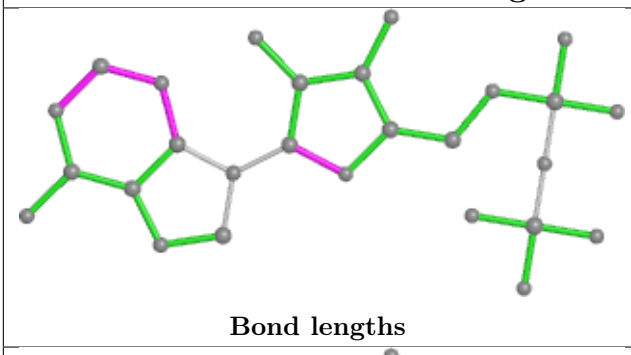


Rings

Ligand ADP M 1000



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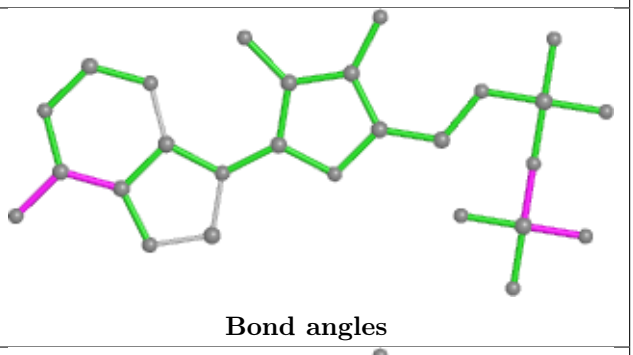
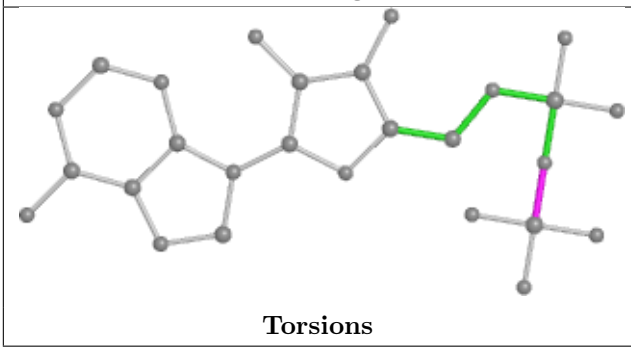


Bond angles



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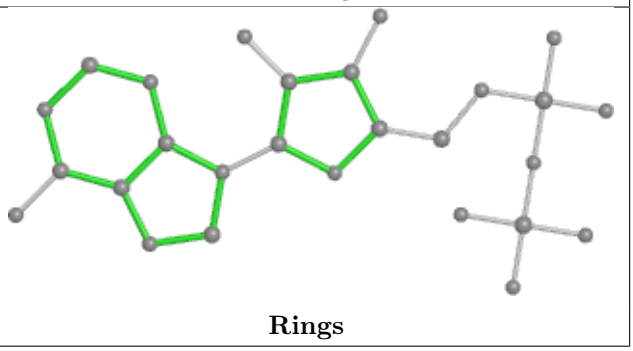

Rings

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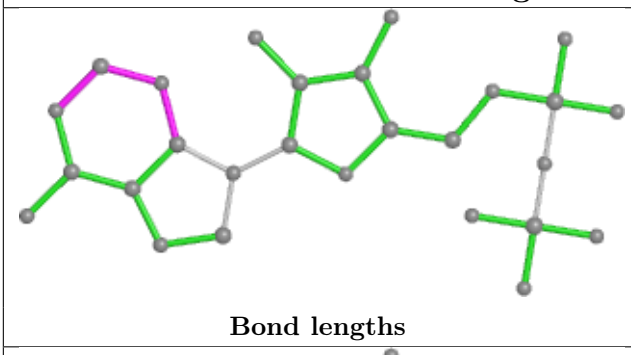

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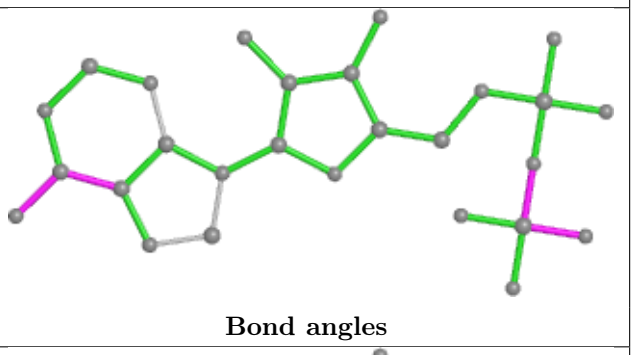
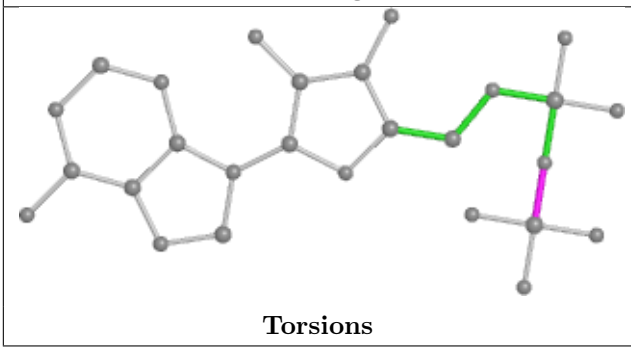


Bond angles



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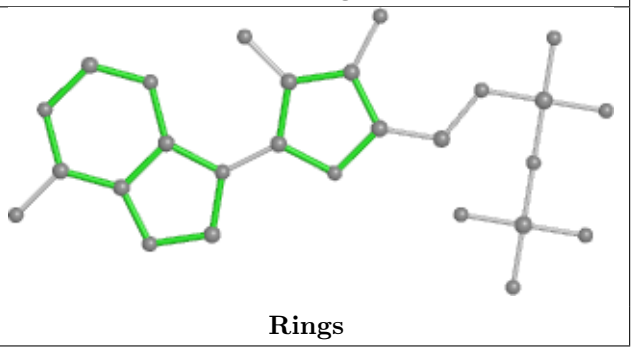

Rings

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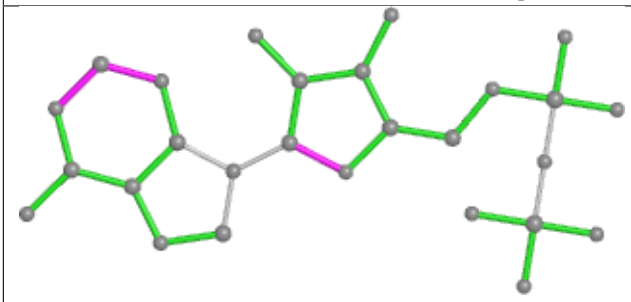

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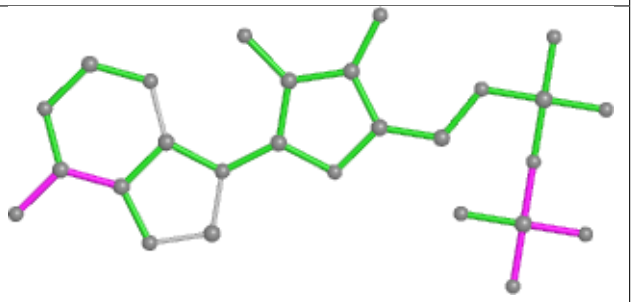

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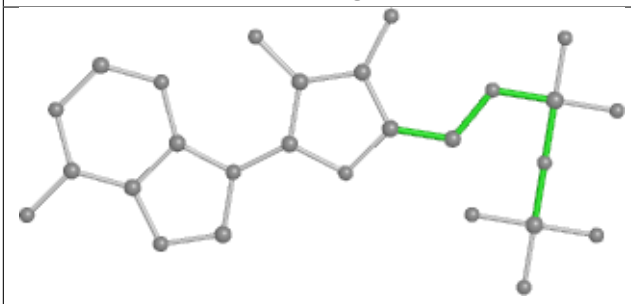

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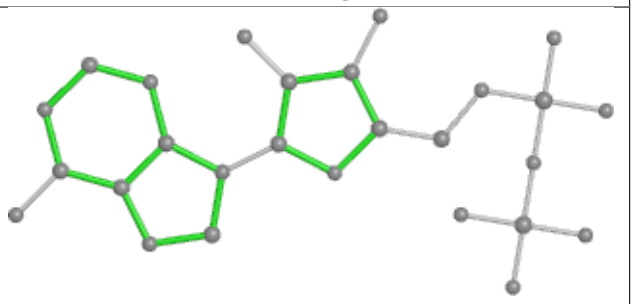

Rings

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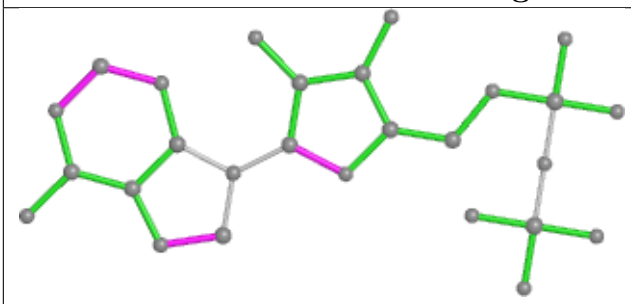

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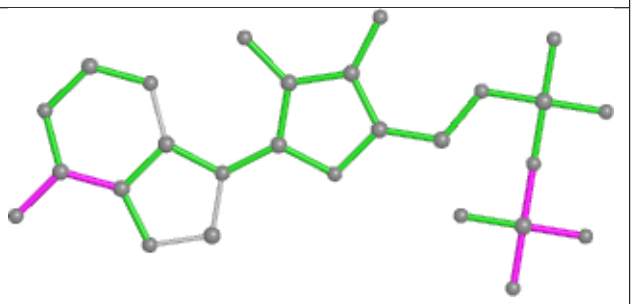

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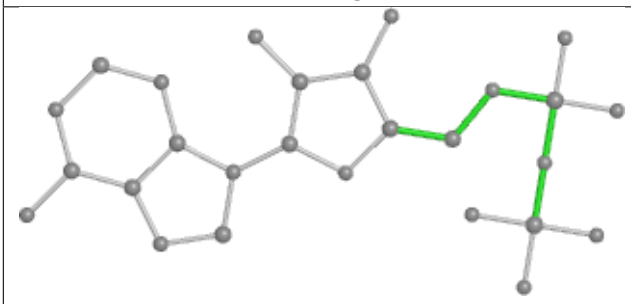
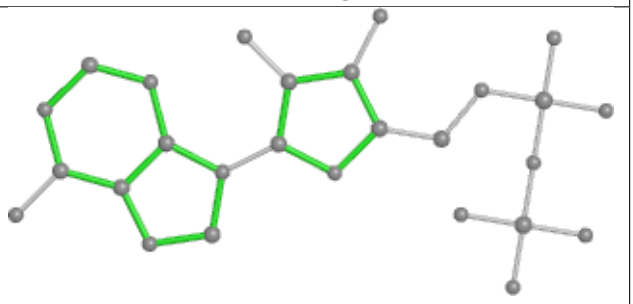
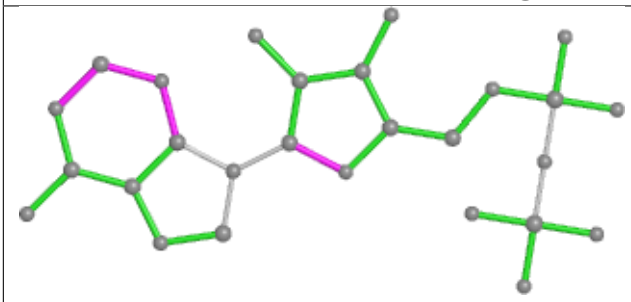


Torsions



Rings

Ligand ADP J 1000



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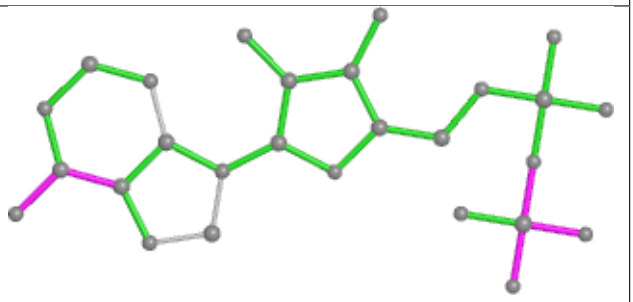
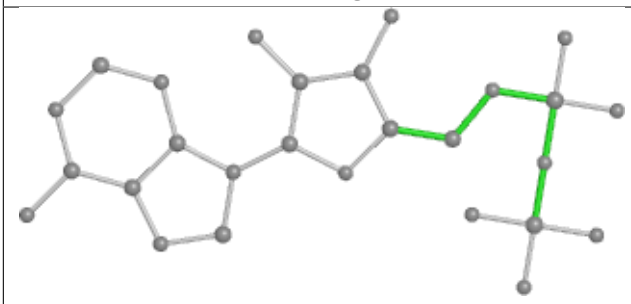


Bond angles



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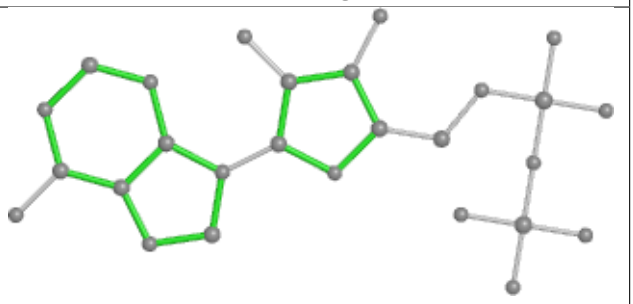
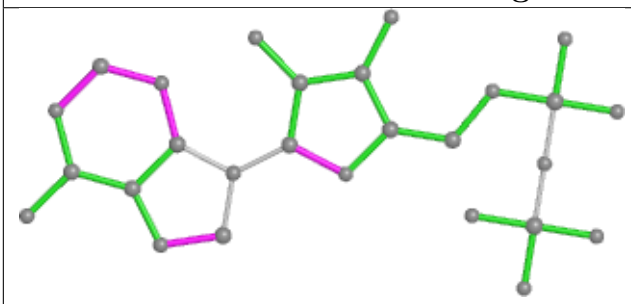


Rings

Ligand ADP G 1000



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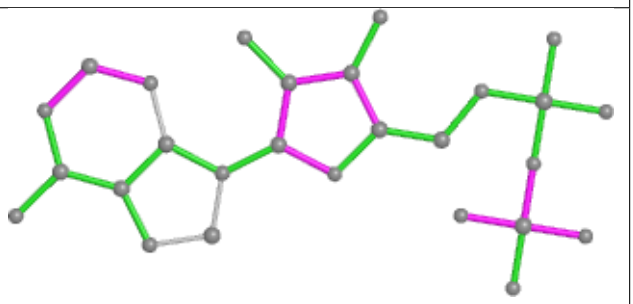
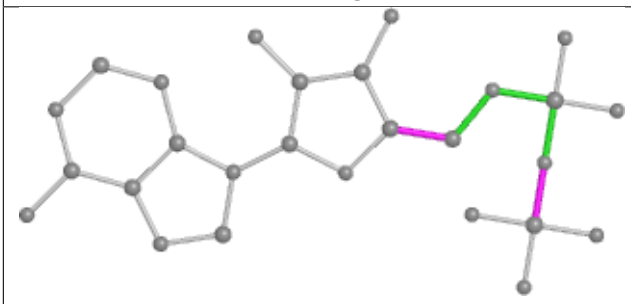


Bond angles



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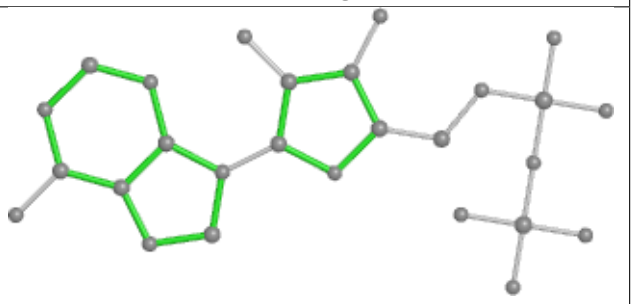
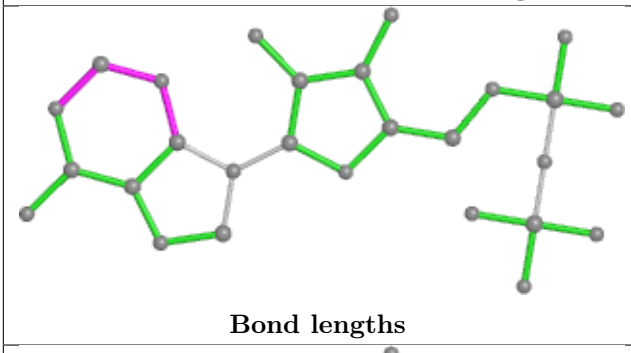
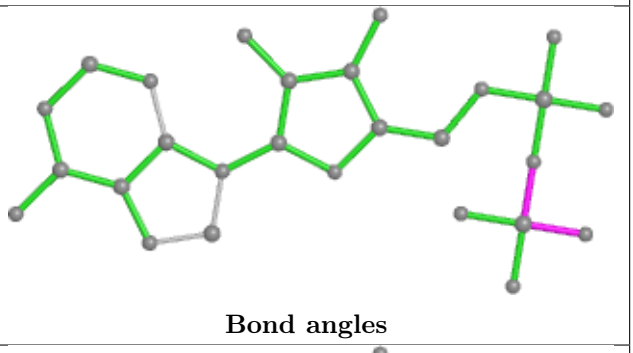


Rings

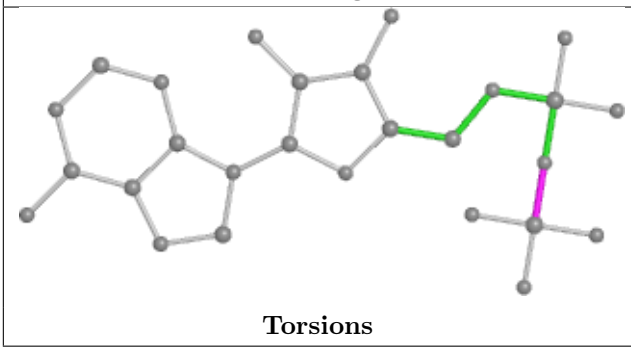
Ligand ADP H 1000



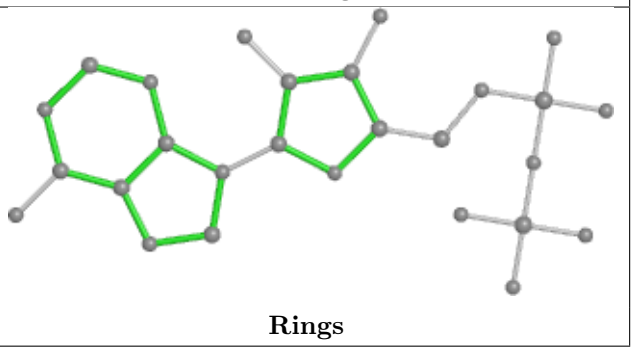
Bond lengths



Bond angles

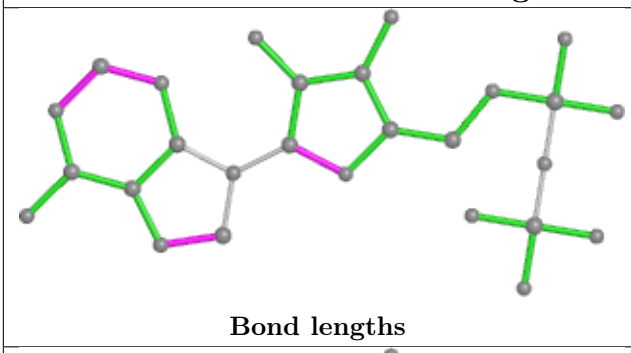


Torsions

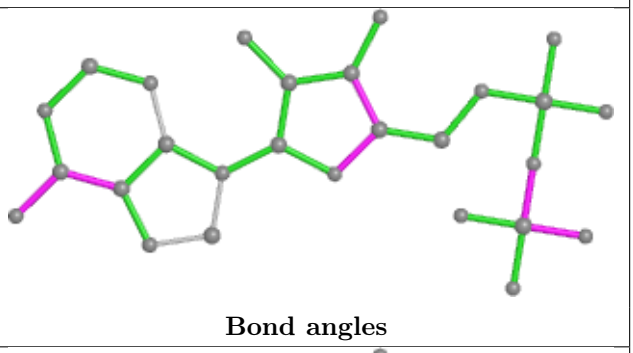


Rings

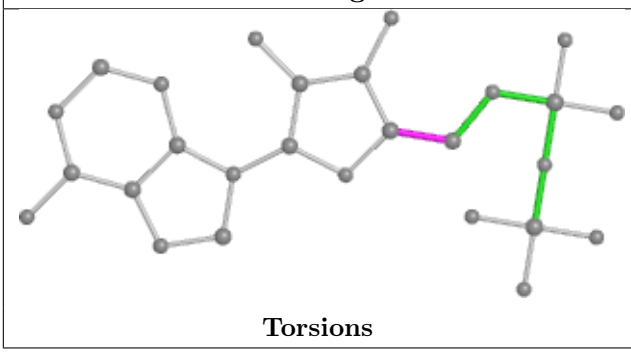
Ligand ADP N 1000



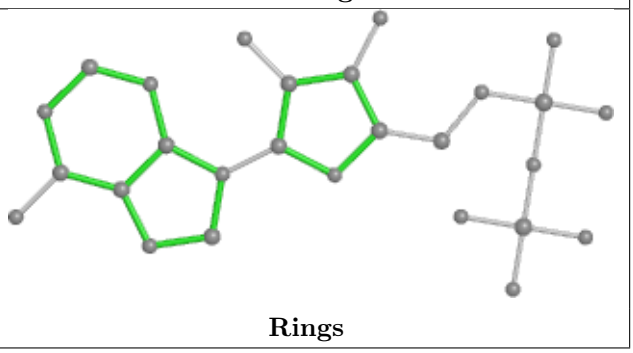
Bond lengths



Bond angles

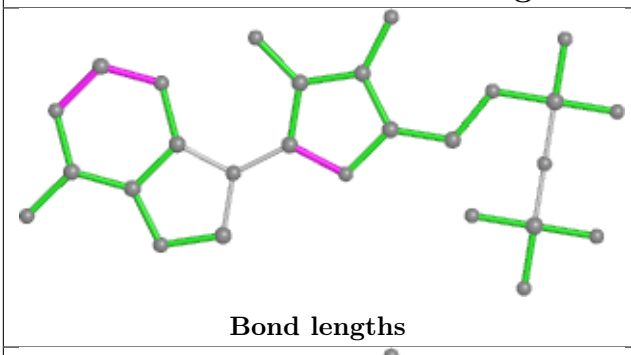


Torsions

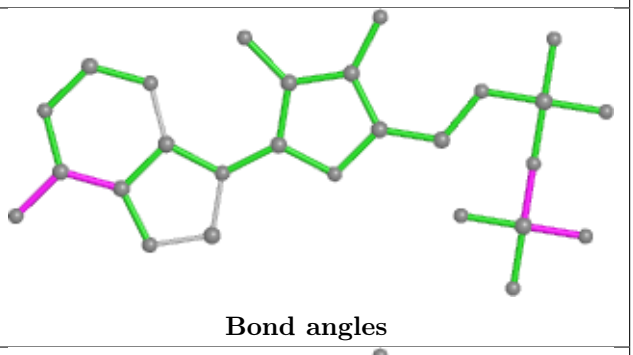


Rings

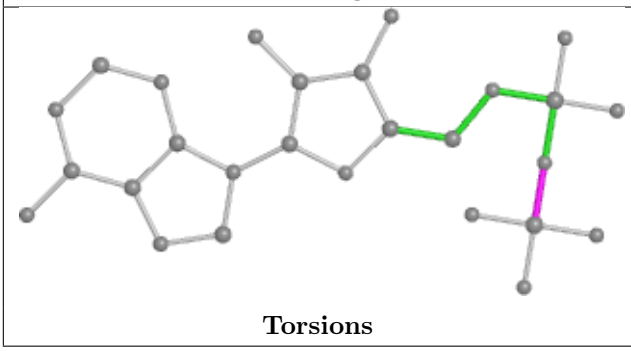
Ligand ADP E 1000



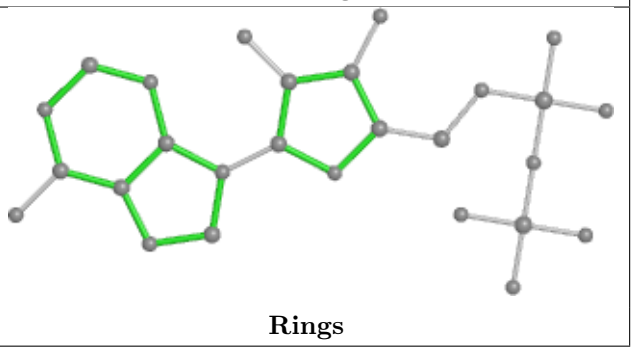
Bond lengths



Bond angles

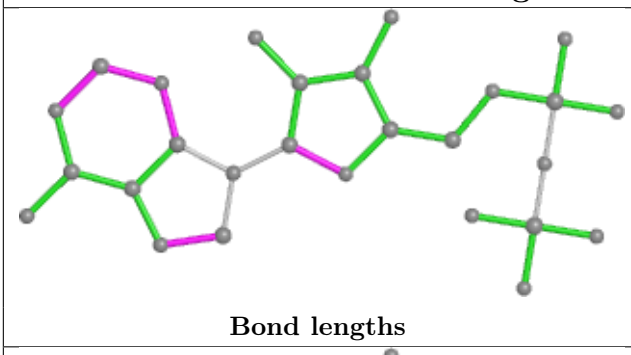


Torsions

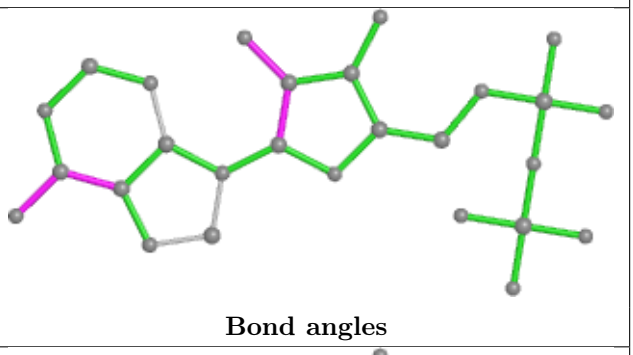


Rings

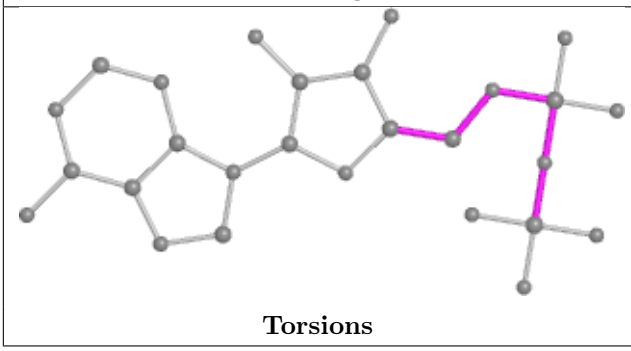
Ligand ADP D 1000



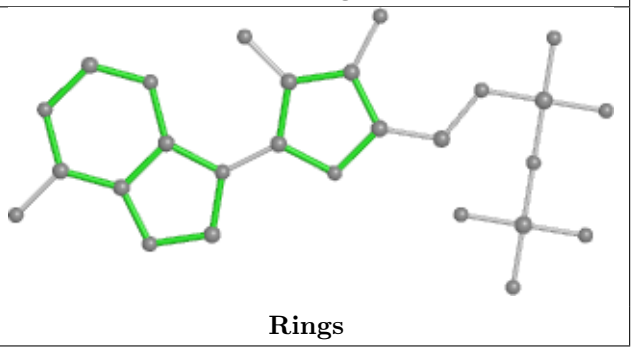
Bond lengths



Bond angles

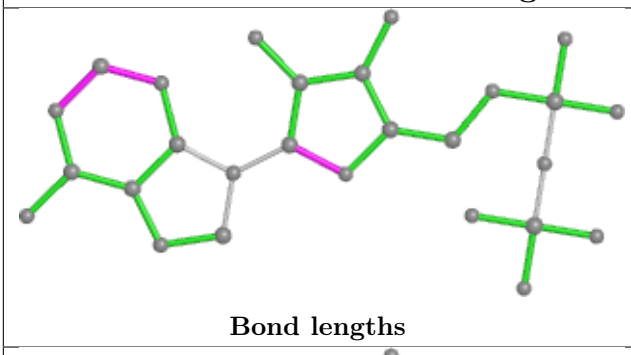


Torsions

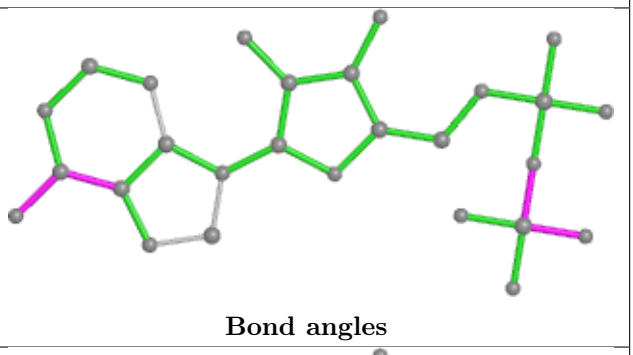


Rings

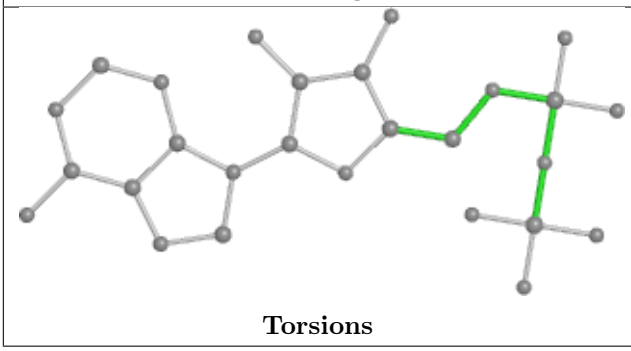
Ligand ADP I 1000



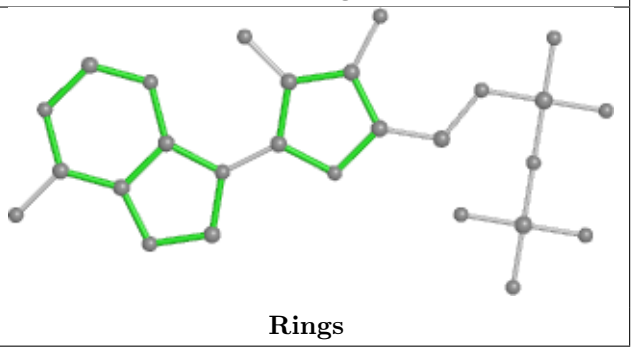
Bond lengths



Bond angles

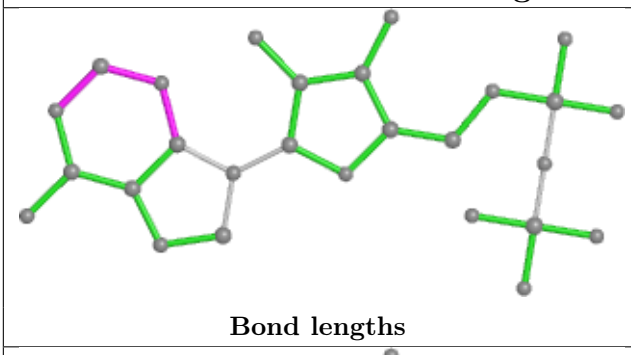


Torsions

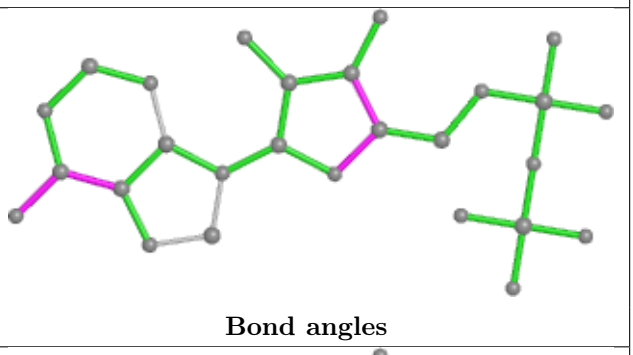


Rings

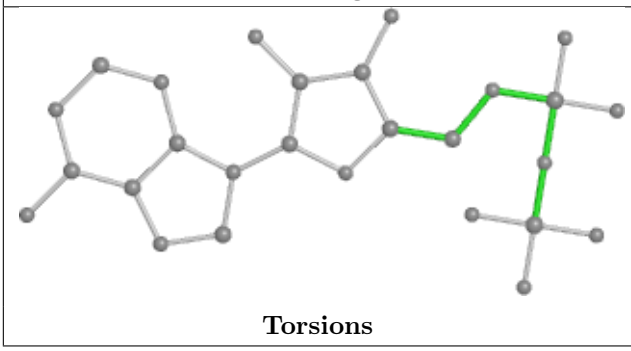
Ligand ADP B 1000



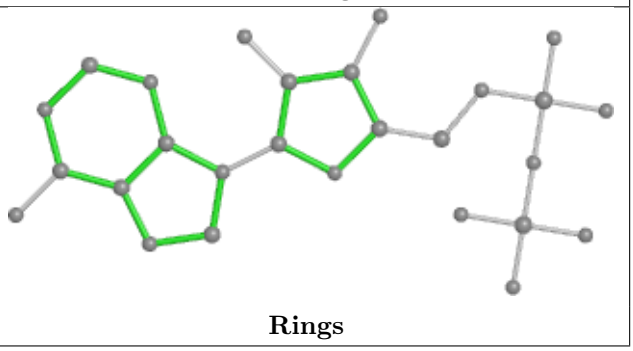
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

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^{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	259/286 (90%)	-0.01	9 (3%)	44	28	48, 72, 112, 127	0
1	B	260/286 (90%)	0.18	11 (4%)	36	23	57, 83, 119, 129	0
1	C	260/286 (90%)	0.02	7 (2%)	54	39	51, 79, 112, 141	0
1	D	258/286 (90%)	0.33	12 (4%)	31	19	62, 90, 120, 148	0
1	E	260/286 (90%)	0.08	6 (2%)	60	47	60, 85, 117, 139	0
1	F	257/286 (89%)	0.05	8 (3%)	49	32	58, 80, 110, 139	0
1	G	259/286 (90%)	0.18	14 (5%)	25	14	67, 91, 120, 143	0
1	H	260/286 (90%)	0.18	13 (5%)	28	16	64, 88, 124, 144	0
1	I	260/286 (90%)	0.14	10 (3%)	40	26	57, 83, 117, 136	0
1	J	259/286 (90%)	0.08	5 (1%)	66	53	57, 80, 115, 133	0
1	K	258/286 (90%)	-0.01	4 (1%)	72	59	54, 73, 112, 147	0
1	L	259/286 (90%)	-0.08	6 (2%)	60	47	51, 72, 112, 140	0
1	M	256/286 (89%)	0.02	6 (2%)	60	47	48, 74, 106, 128	0
1	N	260/286 (90%)	-0.03	9 (3%)	44	28	50, 70, 111, 131	0
1	O	260/286 (90%)	-0.02	5 (1%)	66	53	51, 74, 113, 133	0
1	P	256/286 (89%)	-0.02	4 (1%)	72	59	53, 76, 108, 136	0
All	All	4141/4576 (90%)	0.07	129 (3%)	49	32	48, 80, 116, 148	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	494	SER	5.6
1	J	494	SER	5.4
1	D	707	ASP	5.4
1	B	494	SER	5.1
1	K	707	ASP	4.4

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 monosaccharides 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^{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	CA	H	1001	1/1	0.91	0.16	79,79,79,79	0
2	ADP	I	1000	27/27	0.92	0.21	84,85,87,89	0
3	CA	P	1001	1/1	0.92	0.15	76,76,76,76	0
3	CA	B	1001	1/1	0.93	0.18	73,73,73,73	0
3	CA	C	1001	1/1	0.93	0.18	80,80,80,80	0
3	CA	E	1001	1/1	0.94	0.22	86,86,86,86	0
3	CA	G	1001	1/1	0.94	0.14	89,89,89,89	0
2	ADP	D	1000	27/27	0.94	0.19	79,83,85,87	0
3	CA	I	1001	1/1	0.94	0.13	82,82,82,82	0
3	CA	O	1001	1/1	0.94	0.26	64,64,64,64	0
3	CA	D	1001	1/1	0.94	0.14	94,94,94,94	0
2	ADP	C	1000	27/27	0.95	0.20	72,75,77,79	0
2	ADP	J	1000	27/27	0.95	0.18	74,77,80,82	0
2	ADP	M	1000	27/27	0.95	0.22	72,74,76,78	0
2	ADP	E	1000	27/27	0.95	0.18	74,76,78,79	0
2	ADP	G	1000	27/27	0.95	0.24	83,86,88,90	0
2	ADP	H	1000	27/27	0.95	0.20	81,83,85,88	0
2	ADP	A	1000	27/27	0.96	0.18	53,57,63,64	0
2	ADP	P	1000	27/27	0.96	0.17	66,69,71,72	0
3	CA	A	1001	1/1	0.96	0.33	79,79,79,79	0
2	ADP	F	1000	27/27	0.96	0.18	72,74,76,77	0
3	CA	J	1001	1/1	0.96	0.26	81,81,81,81	0
2	ADP	B	1000	27/27	0.96	0.16	82,83,85,86	0
2	ADP	L	1000	27/27	0.96	0.17	75,76,78,80	0
2	ADP	K	1000	27/27	0.97	0.18	67,69,72,72	0
3	CA	L	1001	1/1	0.97	0.15	71,71,71,71	0
3	CA	M	1001	1/1	0.97	0.23	74,74,74,74	0

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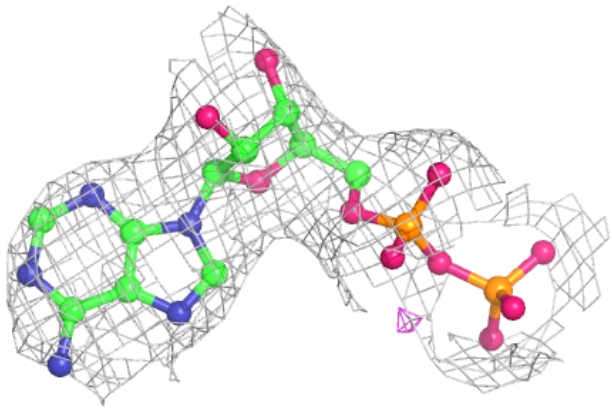
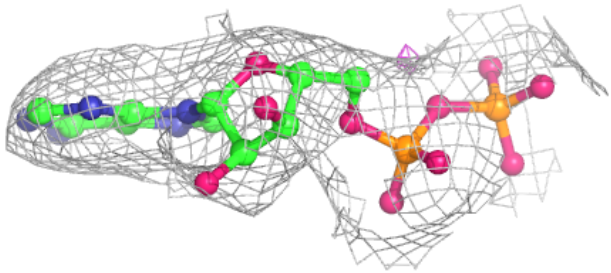
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	N	1001	1/1	0.97	0.26	70,70,70,70	0
2	ADP	N	1000	27/27	0.97	0.18	58,60,62,64	0
2	ADP	O	1000	27/27	0.97	0.16	55,58,61,62	0
3	CA	K	1001	1/1	0.98	0.20	69,69,69,69	0
3	CA	F	1001	1/1	0.98	0.24	83,83,83,83	0

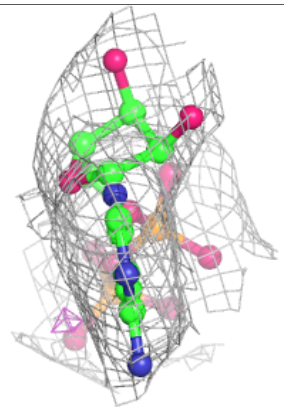
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP I 1000:

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

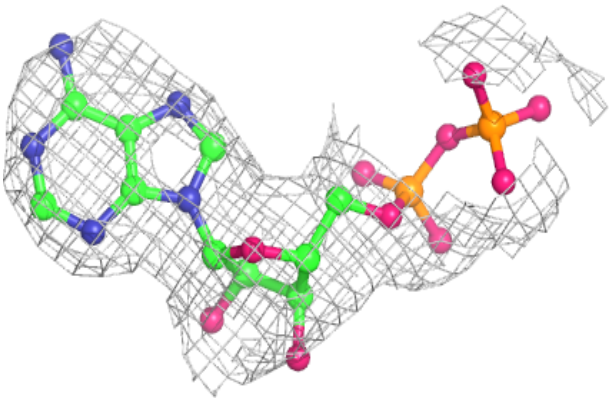


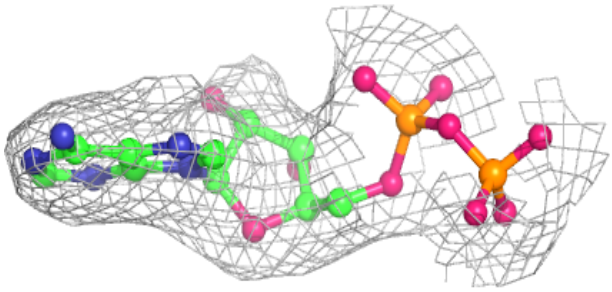


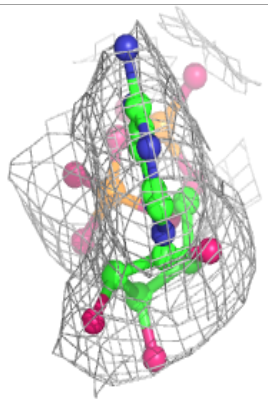


Electron density around ADP D 1000:

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

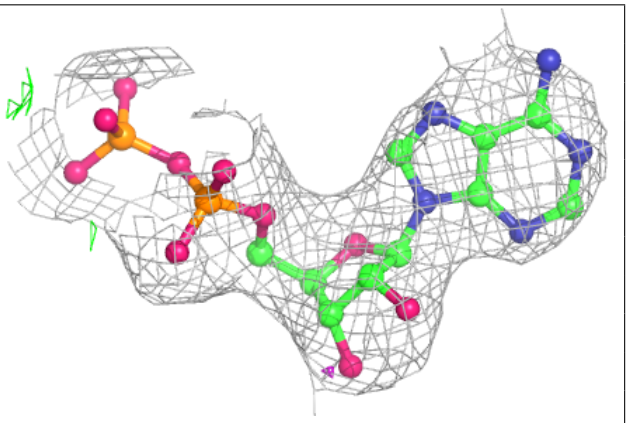


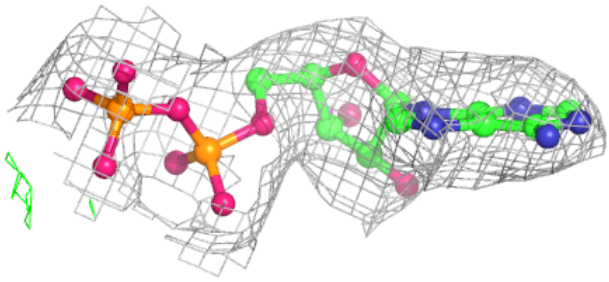


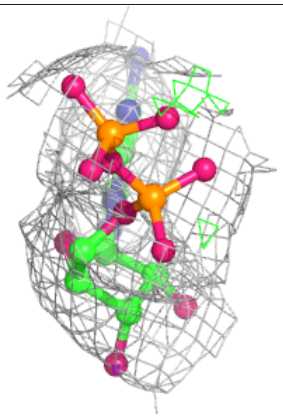


Electron density around ADP C 1000:

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

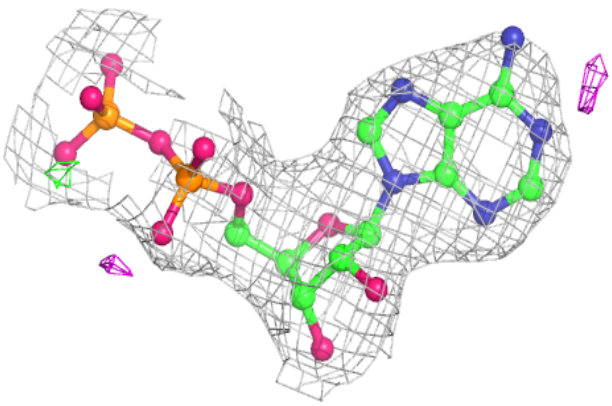


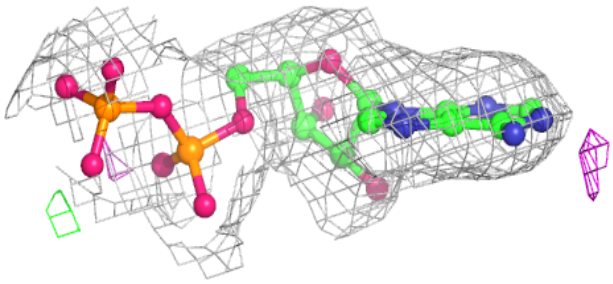


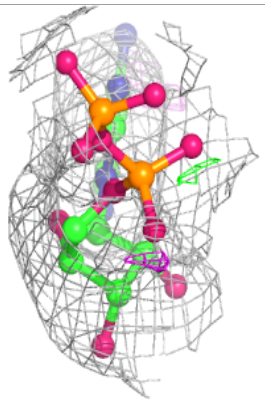


Electron density around ADP J 1000:

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

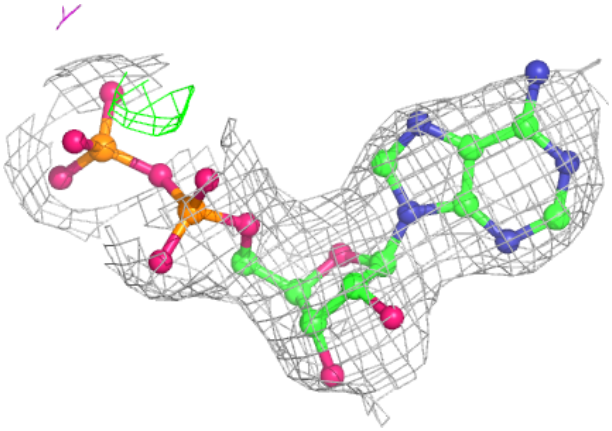


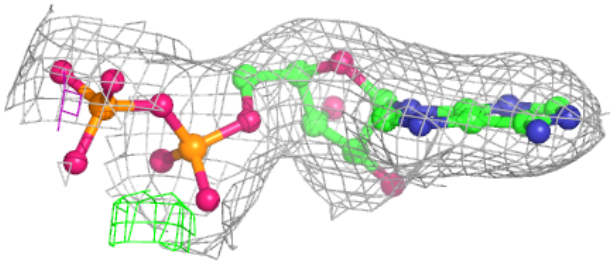


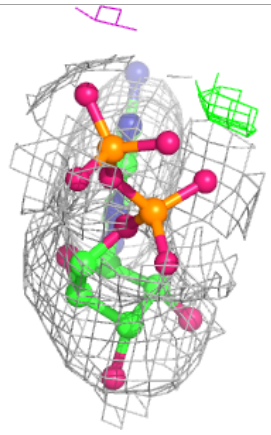


Electron density around ADP M 1000:

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

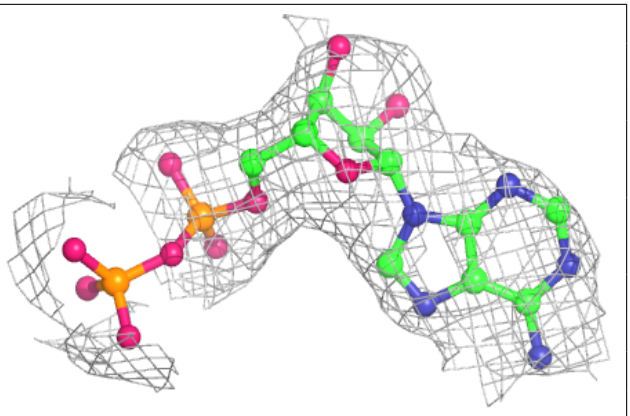


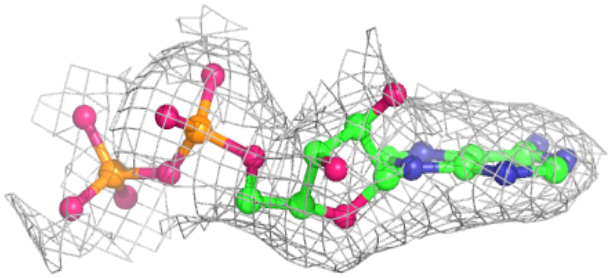


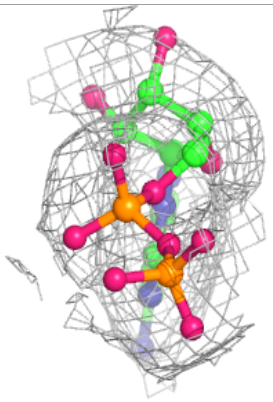


Electron density around ADP E 1000:

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

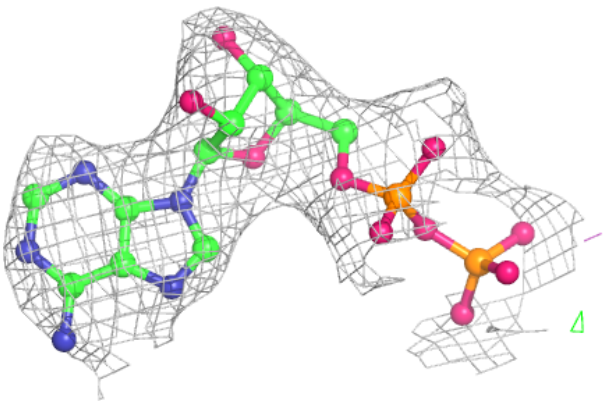


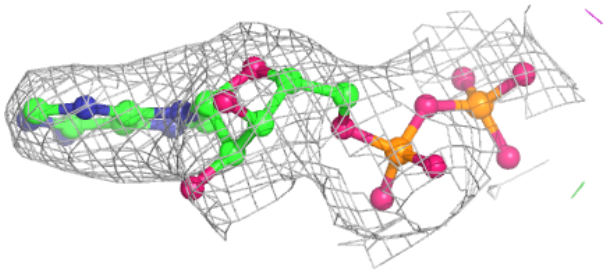


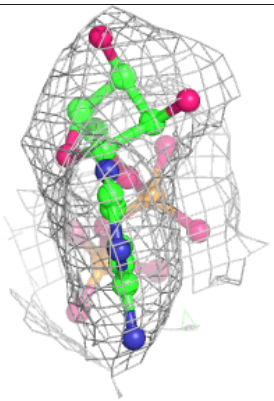


Electron density around ADP G 1000:

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

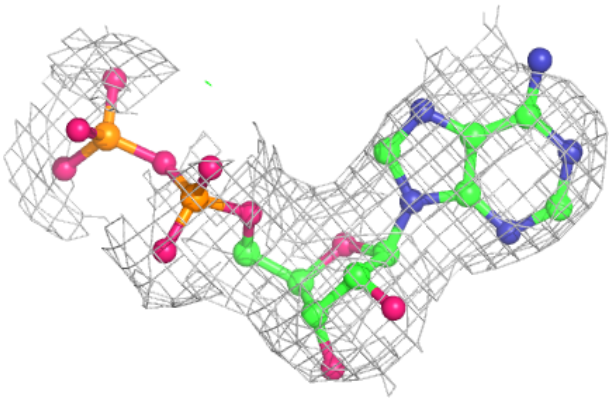


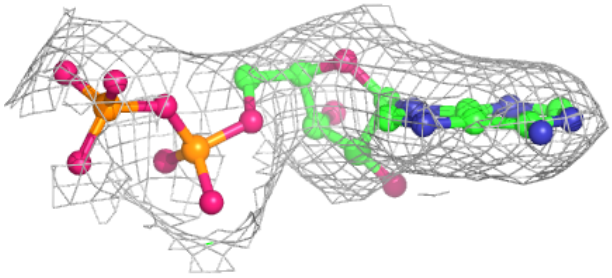


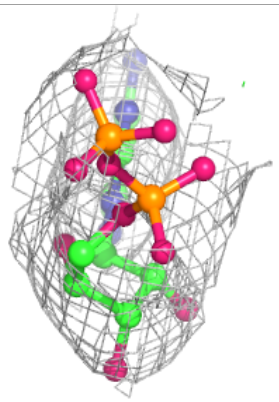


Electron density around ADP H 1000:

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

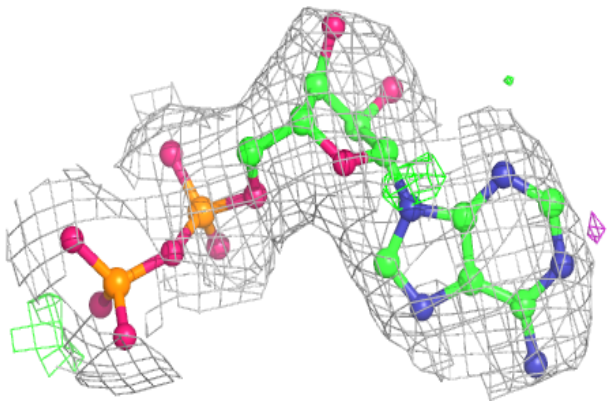


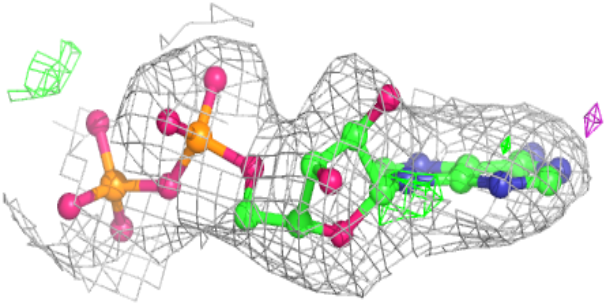


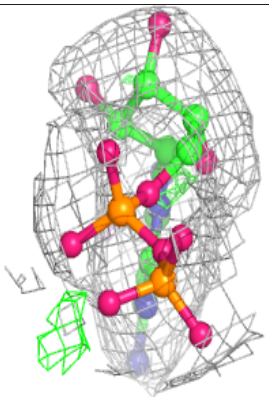


Electron density around ADP A 1000:

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

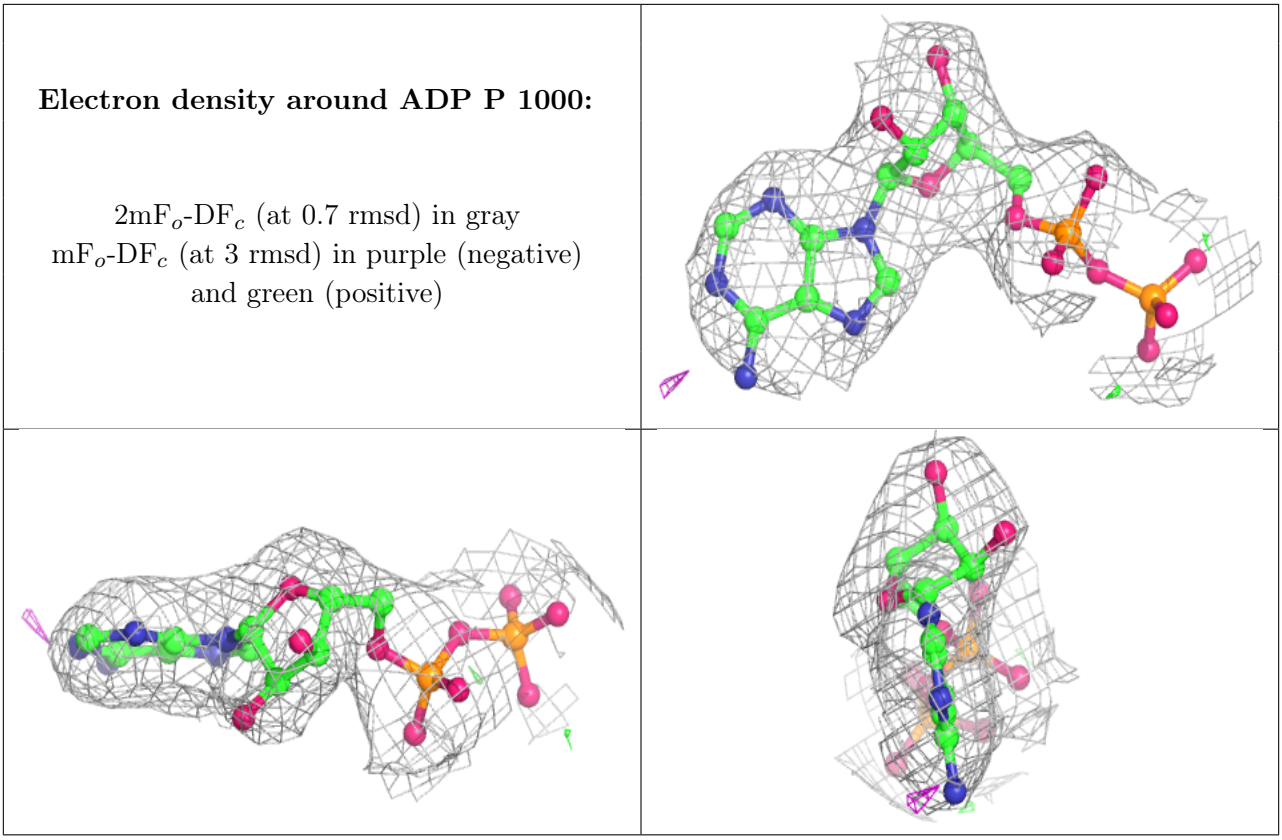






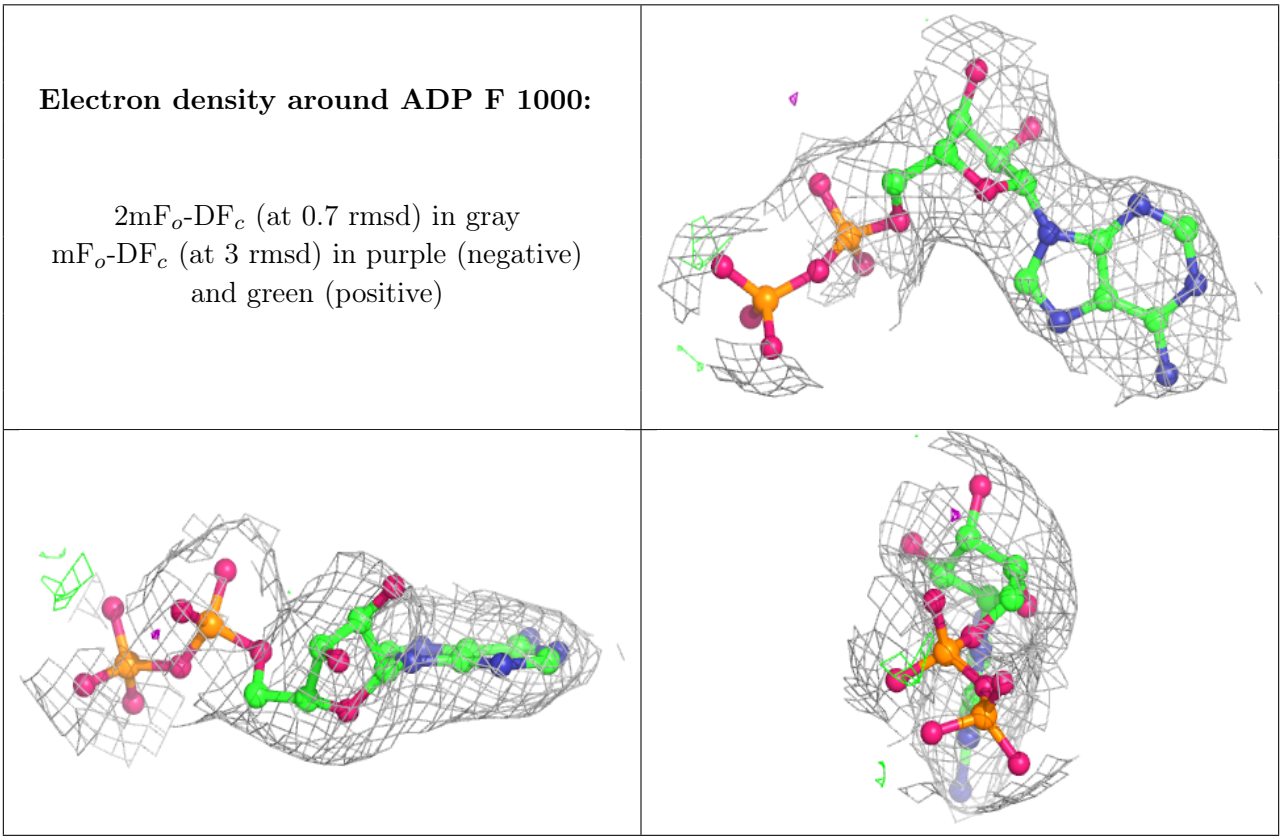
Electron density around ADP P 1000:

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



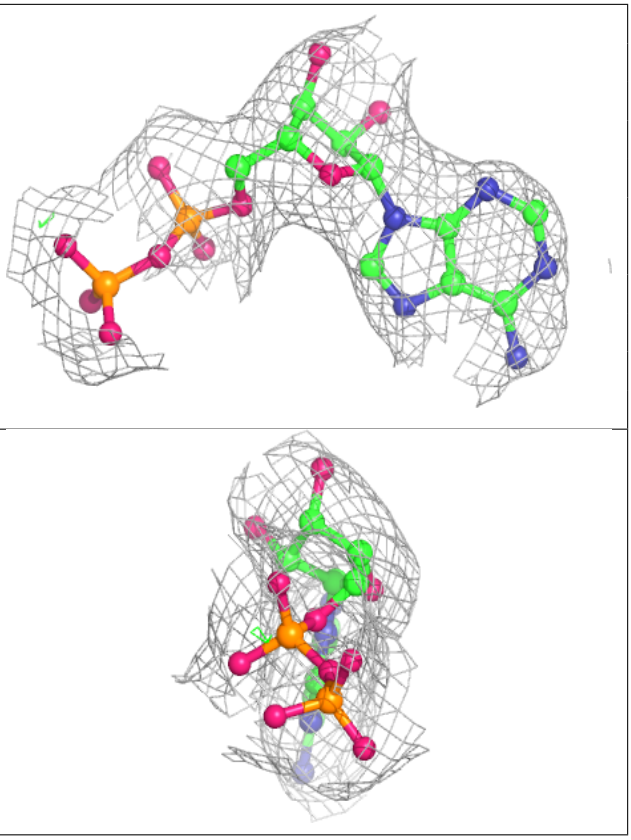
Electron density around ADP F 1000:

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



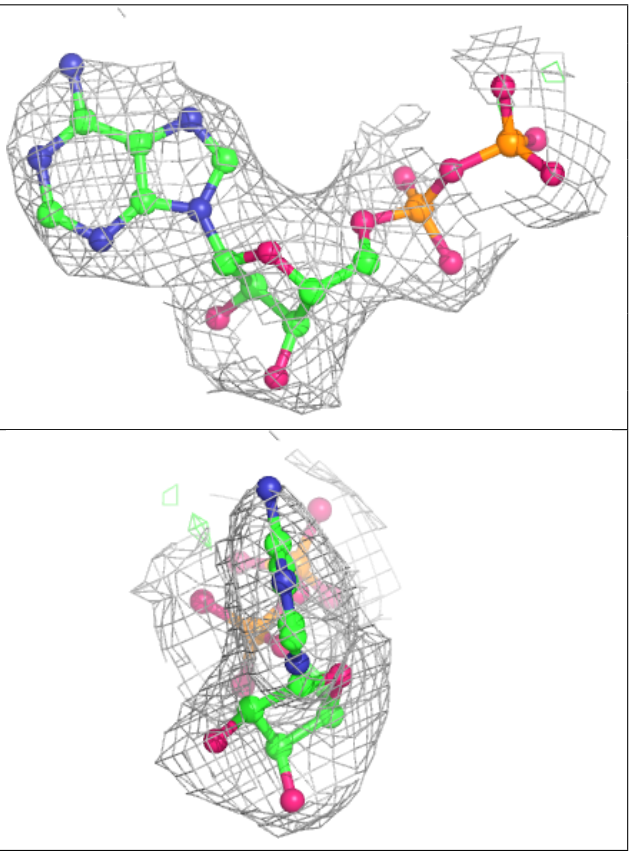
Electron density around ADP B 1000:

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



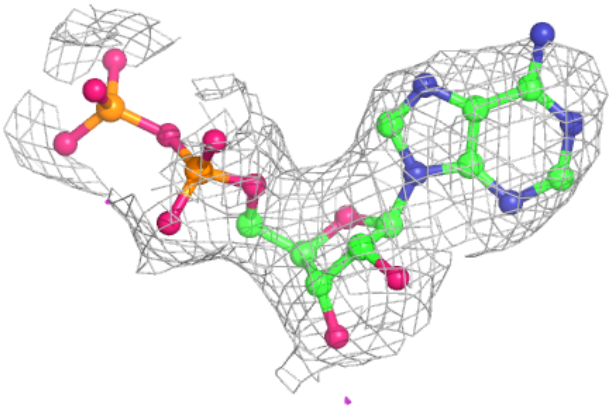
Electron density around ADP L 1000:

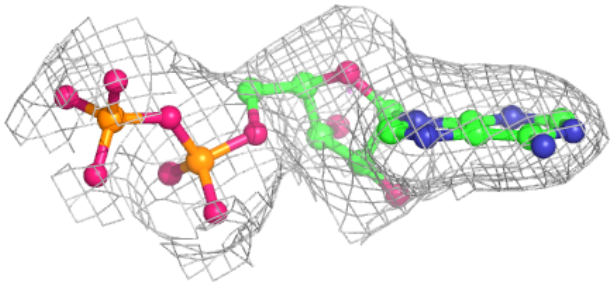
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

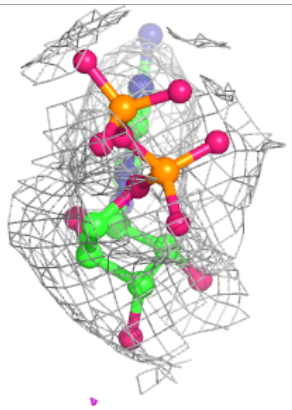


Electron density around ADP K 1000:

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

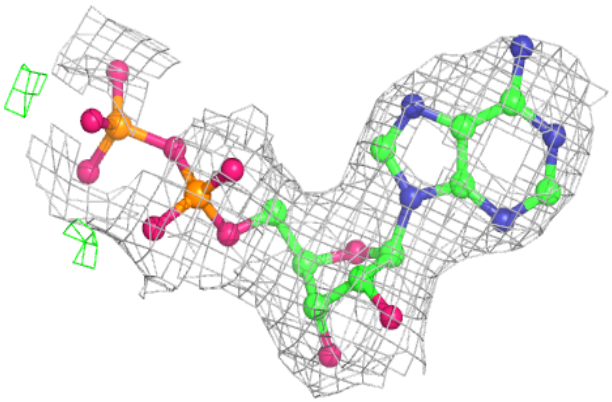


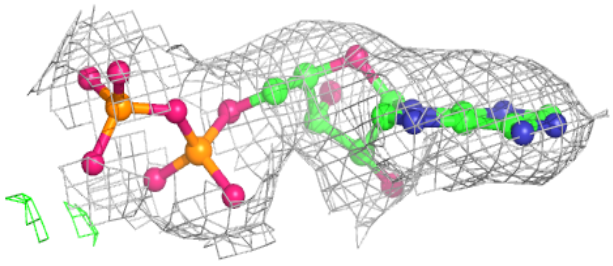


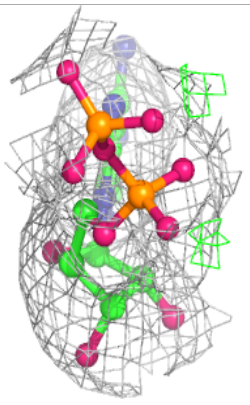


Electron density around ADP N 1000:

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

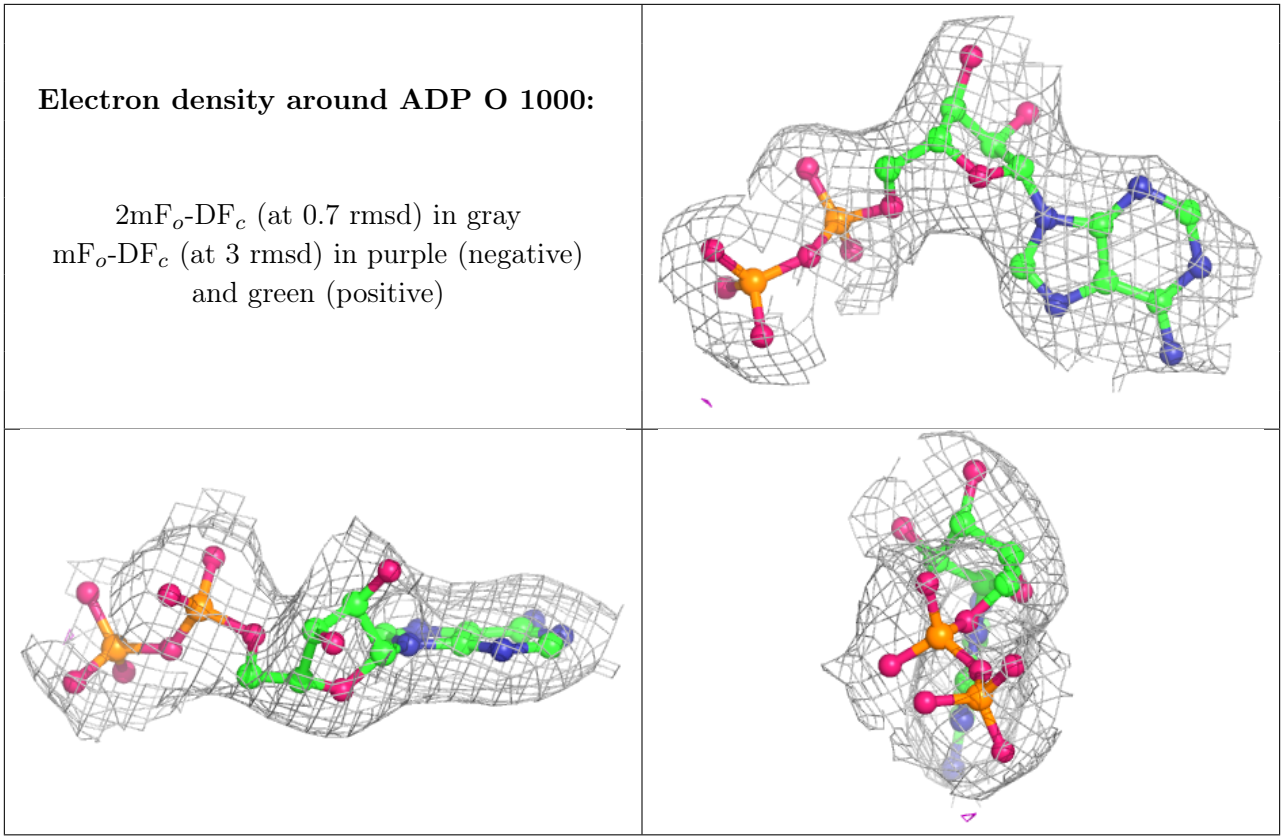






Electron density around ADP O 1000:

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



6.5 Other polymers (i)

There are no such residues in this entry.