wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 02:05 pm BST

PDB ID	:	2IUU
Title	:	P. aeruginosa FtsK motor domain, hexamer
Authors	:	Massey, T.H.; Mercogliano, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on	:	2006-06-07
Resolution	:	2.90 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:

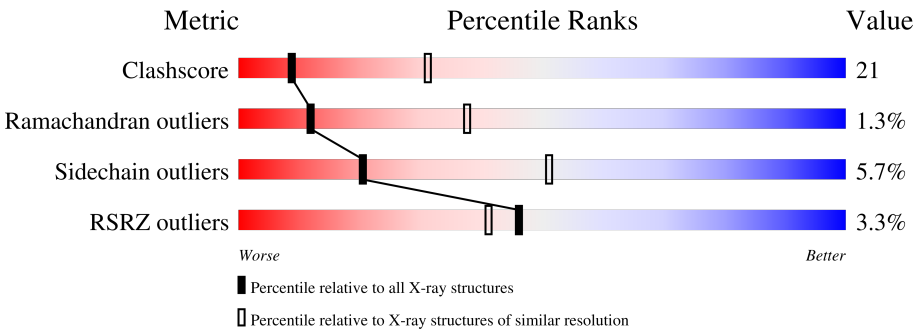
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	491	5%, 52%, 29%, ••, 17%
1	B	491	2%, 51%, 29%, •, 17%
1	C	491	2%, 51%, 29%, ••, 17%
1	D	491	%, 55%, 26%, ••, 17%
1	E	491	3%, 48%, 32%, ••, 17%
1	F	491	4%, 52%, 28%, •, 17%

2 Entry composition (i)

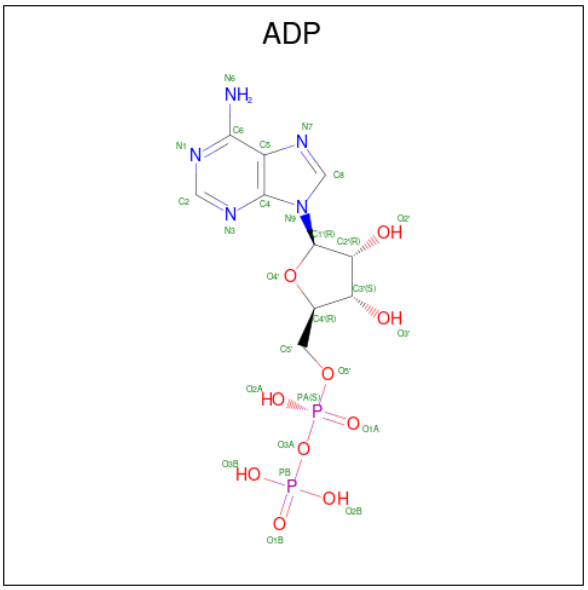
There are 2 unique types of molecules in this entry. The entry contains 18888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3121	1983	540	583	15	0	0	0
1	B	408	3121	1983	540	583	15	0	0	0
1	C	408	3121	1983	540	583	15	0	0	0
1	D	408	3121	1983	540	583	15	0	0	0
1	E	408	3121	1983	540	583	15	0	0	0
1	F	408	3121	1983	540	583	15	0	0	0

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



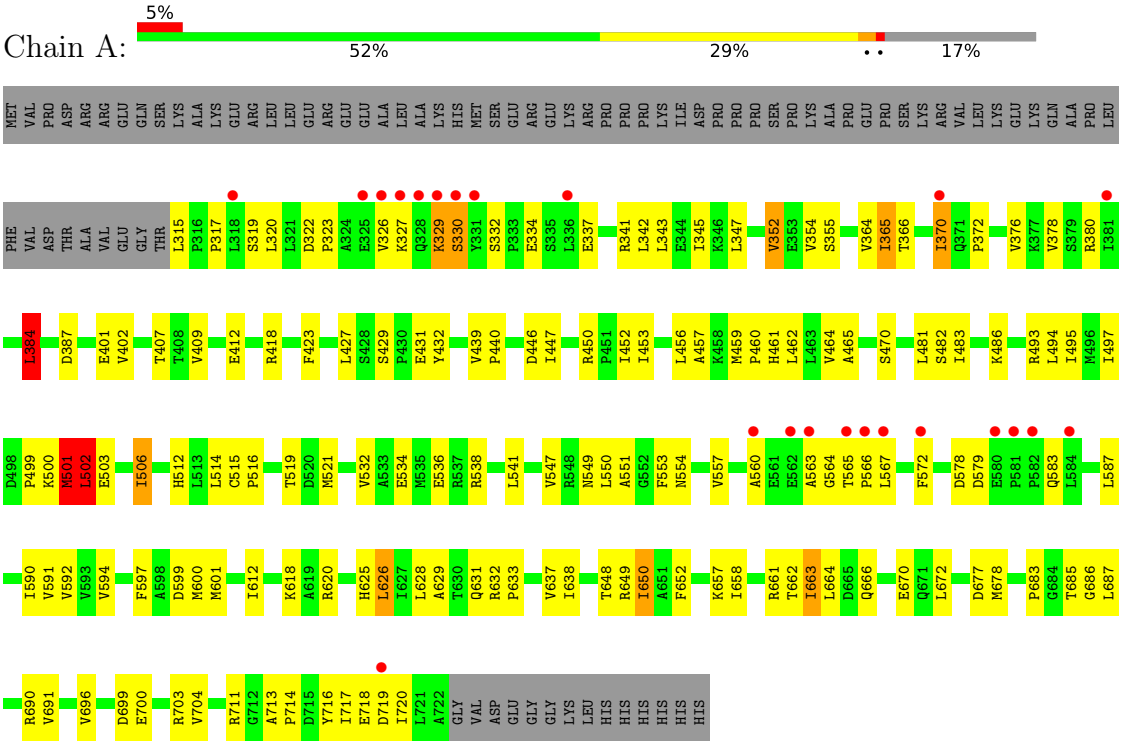
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	27	10	5	10	2	0	0
2	C	1	27	10	5	10	2	0	0
2	D	1	27	10	5	10	2	0	0
2	E	1	27	10	5	10	2	0	0
2	F	1	27	10	5	10	2	0	0

3 Residue-property plots (i)

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

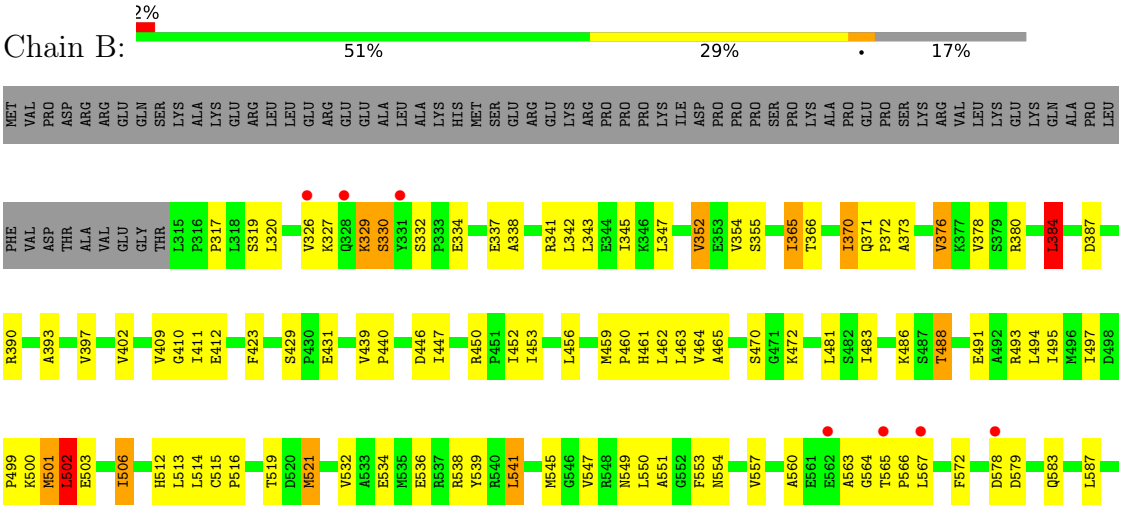
- Molecule 1: DNA TRANSLOCASE FTSK

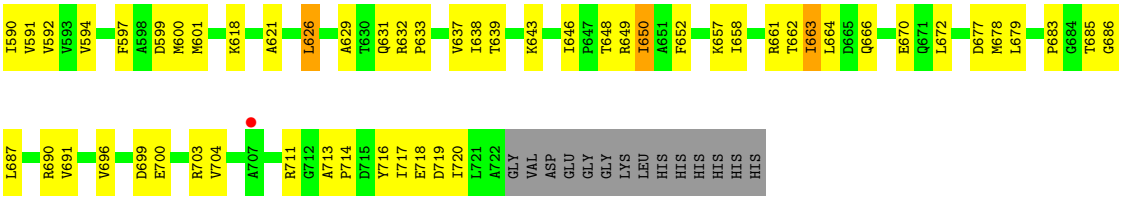
Chain A:



- Molecule 1: DNA TRANSLOCASE FTSK

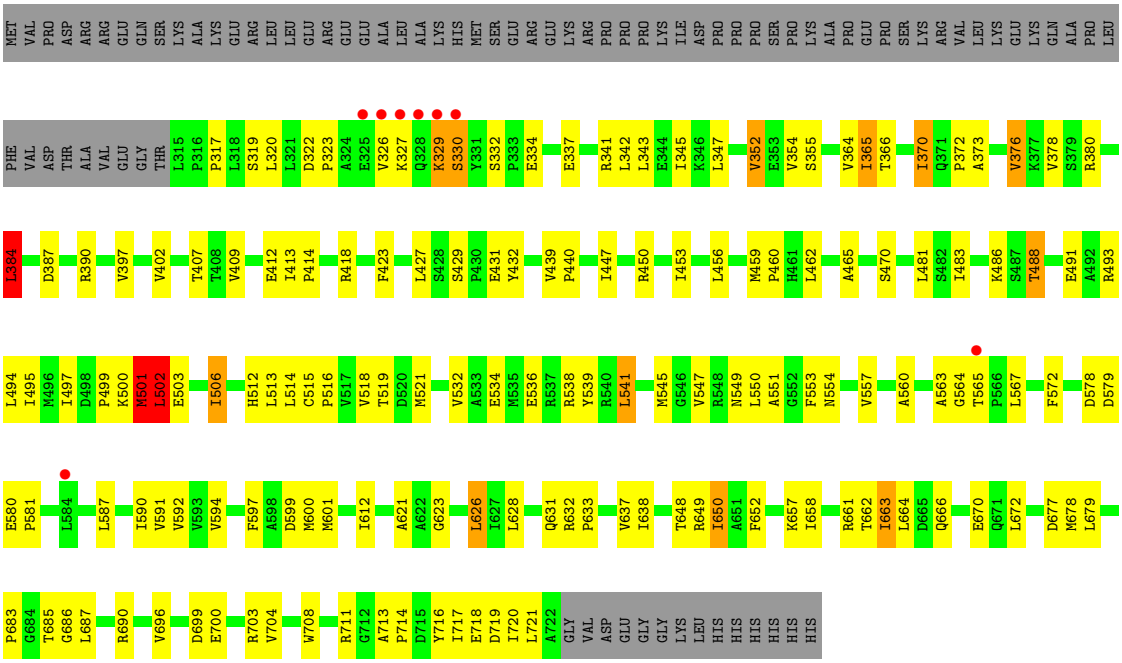
Chain B:





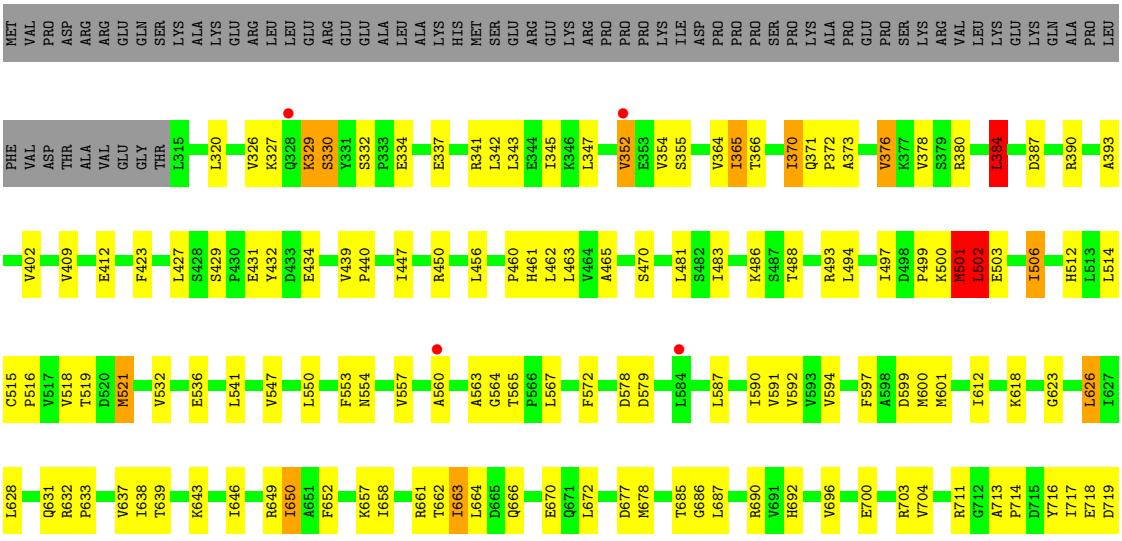
• Molecule 1: DNA TRANSLOCASE FTSK

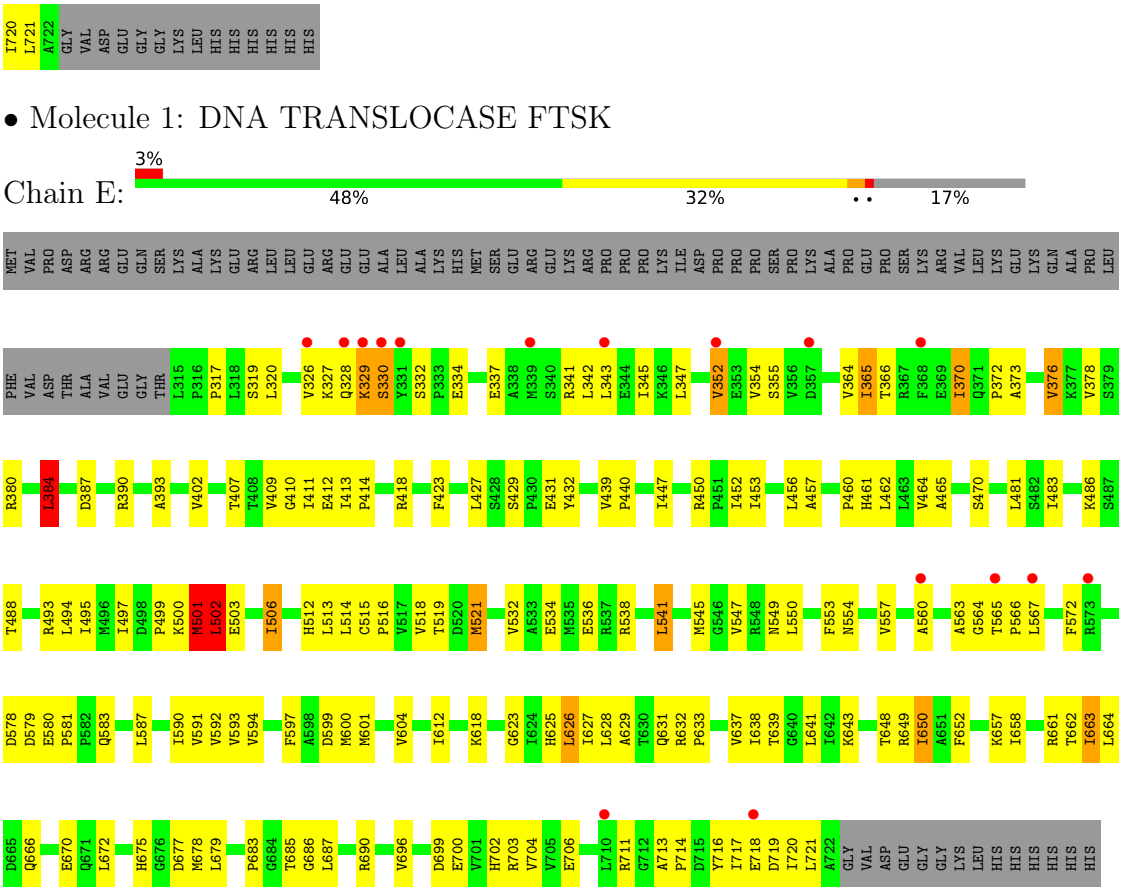
Chain C:



• Molecule 1: DNA TRANSLOCASE FTSK

Chain D:




I720 L721 A722 GLY VAL ASP GLU GLY GLY LYS LEU HIS HIS HIS HIS HIS
• Molecule 1: DNA TRANSLOCASE FTSK
Chain E:
3%
48%
32%
17%
MET VAL PRO ASP ARG ARG GLU GLN SER LYS ALA LYS GLU ARG LEU LEU GLU ARG GLU GLU ALA LEU ALA LYS HIS MET SER GLU ARG GLU LYS ARG PRO PRO PRO LYS ILE ASP PRO PRO PRO SER PRO LYS ALA PRO GLU PRO SER LYS ARG VAL LEU LYS GLU LYS GLN ALA PRO LEU
PHE VAL ASP THR ALA VAL GLU GLY THR L315 P316 P317 L318 S319 L320 V326 K327 Q328 K329 S330 Y331 S332 P333 E334 E337 A338 M339 S340 R341 L342 L343 E344 I345 K346 L347 V352 E353 V354 S355 V356 D357 V364 I365 T366 R367 F368 E369 T370 Q371 P372 A373 V376 K377 V378 S379
R380 L384 D387 R390 A393 V402 T407 T408 V409 G410 I411 E412 I413 P414 R418 F423 L427 S428 S429 P430 E431 Y432 V439 P440 I447 R450 P451 I452 I453 L456 A457 P460 H461 L462 L463 V464 A465 S470 L481 S482 I483 K486 S487
T488 R493 L494 I495 M496 I497 D498 P499 K500 M501 L502 E503 I506 H512 L513 L514 C515 P516 V517 V518 T519 D520 M521 V532 A533 E534 N535 E536 R537 R538 L541 M545 G546 V547 R548 N549 L550 F553 N554 V557 A560 A563 G564 T565 P566 L567 F572 R573
D578 D579 E580 P581 P582 Q583 L587 I590 V591 V592 V593 V594 F597 A598 D599 M600 M601 V604 I612 K618 G623 I624 H625 L626 I627 L628 A629 T630 Q631 R632 P633 V637 I638 T639 G640 L641 I642 K643 T648 R649 I650 A651 F652 K657 I658 R661 T662 I663 L664
D665 Q666 E670 Q671 L672 H675 G676 D677 M678 L679 P683 G684 T685 G686 L687 R690 V696 D699 E700 V701 H702 R703 V704 V705 E706 L710 R711 G712 A713 P714 D715 Y716 I717 E718 D719 I720 L721 A722 GLY VAL ASP GLU GLY GLY LYS LEU HIS HIS HIS HIS HIS HIS
• Molecule 1: DNA TRANSLOCASE FTSK
Chain F:
4%
52%
28%
17%
MET VAL PRO ASP ARG ARG GLU GLN SER LYS ALA LYS GLU ARG LEU LEU GLU ARG GLU GLU ALA LEU ALA LYS HIS MET SER GLU ARG GLU LYS ARG PRO PRO PRO LYS ILE ASP PRO PRO PRO SER PRO LYS ALA PRO GLU PRO SER LYS ARG VAL LEU LYS GLU LYS GLN ALA PRO LEU
PHE VAL ASP THR ALA VAL GLU GLY THR L315 P316 P317 L318 S319 L320 L321 D322 P323 A324 E325 V326 K327 Q328 K329 S330 L336 E337 R341 L342 L343 E344 I345 K346 L347 V352 E353 V354 S355 P361 V364 I365 T366 I370 Q371 P372 A373 V376 K377 V378 S379 R380 N383
L384 D387 R390 A393 V402 T407 T408 V409 E412 R418 Q419 F423 L427 S428 S429 P430 E431 Y432 V439 P440 I447 R450 I453 L456 M459 P460 H461 L462 L463 V464 A465 S470 G471 K472 V476 L481 S482 I483 K486 S487 T488
E491 A492 R493 L494 I495 M496 I497 D498 P499 K500 M501 L502 E503 I506 H512 L513 L514 C515 P516 V517 V518 T519 D520 M521 V532 A533 E534 N535 E536 R537 R538 L541 M545 G546 V547 R548 N549 L550 F553 N554 V557 A560 E561 E562 A563 G564 T565 P566 L567 F572
D578 D579 E580 P581 P582 Q583 L584 L587 I590 V591 V592 V593 V594 F597 A598 D599 M600 M601 K618 L626 I627 L628 A629 T630 Q631 R632 P633 V637 I638 T639 K643 R649 I650 A651 F652 K657 I658 R661 T662 I663 L664 D665 Q666 E670 Q671 L672 D677
M678 L679 T685 G686 L687 R690 V696 E700 V701 H702 R703 V704 L710 R711 G712 A713 P714 D715 Y716 I717 E718 D719 I720 L721 A722 GLY VAL ASP GLU GLY GLY LYS LEU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.01Å 221.76Å 134.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.90 48.11 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (100.00-2.90) 99.7 (48.11-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.259 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18888	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/3177	0.70	3/4312 (0.1%)
1	B	0.42	0/3177	0.70	3/4312 (0.1%)
1	C	0.43	0/3177	0.70	3/4312 (0.1%)
1	D	0.44	0/3177	0.71	3/4312 (0.1%)
1	E	0.41	0/3177	0.70	3/4312 (0.1%)
1	F	0.44	0/3177	0.70	1/4312 (0.0%)
All	All	0.43	0/19062	0.70	16/25872 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	384	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	502	LEU	CA-CB-CG	5.82	128.69	115.30
1	E	502	LEU	CA-CB-CG	5.81	128.67	115.30
1	C	384	LEU	CA-CB-CG	5.75	128.53	115.30

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	3121	0	3238	132	0
1	B	3121	0	3238	140	1
1	C	3121	0	3238	134	0
1	D	3121	0	3238	124	1
1	E	3121	0	3238	148	0
1	F	3121	0	3238	133	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
All	All	18888	0	19500	788	1

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 21.

The worst 5 of 788 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:D:502:LEU:HD13	1:D:503:GLU:HG2	1.53	0.91
1:E:502:LEU:HD13	1:E:503:GLU:HG2	1.49	0.91
1:F:502:LEU:HD13	1:F:503:GLU:HG2	1.51	0.90
1:B:502:LEU:HD13	1:B:503:GLU:HG2	1.54	0.88
1:A:502:LEU:HD13	1:A:503:GLU:HG2	1.55	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ALA:O	1:D:434:GLU:OE2[4_554]	2.00	0.20

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	406/491 (83%)	373 (92%)	27 (7%)	6 (2%)	10	34
1	B	406/491 (83%)	376 (93%)	25 (6%)	5 (1%)	13	40
1	C	406/491 (83%)	377 (93%)	24 (6%)	5 (1%)	13	40
1	D	406/491 (83%)	380 (94%)	21 (5%)	5 (1%)	13	40
1	E	406/491 (83%)	375 (92%)	26 (6%)	5 (1%)	13	40
1	F	406/491 (83%)	375 (92%)	26 (6%)	5 (1%)	13	40
All	All	2436/2946 (83%)	2256 (93%)	149 (6%)	31 (1%)	12	37

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	MET
1	B	501	MET
1	C	501	MET
1	D	501	MET
1	E	501	MET

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	346/419 (83%)	328 (95%)	18 (5%)	23	55
1	B	346/419 (83%)	325 (94%)	21 (6%)	18	48
1	C	346/419 (83%)	326 (94%)	20 (6%)	20	50
1	D	346/419 (83%)	326 (94%)	20 (6%)	20	50
1	E	346/419 (83%)	326 (94%)	20 (6%)	20	50
1	F	346/419 (83%)	326 (94%)	20 (6%)	20	50
All	All	2076/2514 (83%)	1957 (94%)	119 (6%)	20	51

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	663	ILE
1	F	502	LEU
1	D	506	ILE
1	F	501	MET
1	F	696	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	666	GLN
1	F	328	GLN
1	F	554	ASN
1	C	383	ASN
1	C	328	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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	E	1723	-	24,29,29	1.03	1 (4%)	29,45,45	1.58	5 (17%)
2	ADP	D	1723	-	24,29,29	0.98	1 (4%)	29,45,45	1.58	5 (17%)
2	ADP	F	1723	-	24,29,29	1.07	1 (4%)	29,45,45	1.59	5 (17%)
2	ADP	C	1723	-	24,29,29	1.00	1 (4%)	29,45,45	1.51	5 (17%)
2	ADP	B	1723	-	24,29,29	0.98	1 (4%)	29,45,45	1.58	5 (17%)
2	ADP	A	1723	-	24,29,29	1.02	1 (4%)	29,45,45	1.57	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	1723	-	-	2/12/32/32	0/3/3/3
2	ADP	D	1723	-	-	3/12/32/32	0/3/3/3
2	ADP	F	1723	-	-	2/12/32/32	0/3/3/3
2	ADP	C	1723	-	-	2/12/32/32	0/3/3/3
2	ADP	B	1723	-	-	3/12/32/32	0/3/3/3
2	ADP	A	1723	-	-	2/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1723	ADP	C2-N1	3.58	1.40	1.33
2	A	1723	ADP	C2-N1	3.48	1.40	1.33
2	E	1723	ADP	C2-N1	3.47	1.40	1.33
2	C	1723	ADP	C2-N1	3.37	1.40	1.33
2	D	1723	ADP	C2-N1	3.32	1.40	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1723	ADP	C5-C6-N6	3.81	126.14	120.35
2	E	1723	ADP	C5-C6-N6	3.71	126.00	120.35
2	A	1723	ADP	C5-C6-N6	3.63	125.87	120.35
2	D	1723	ADP	C5-C6-N6	3.59	125.81	120.35
2	F	1723	ADP	C5-C6-N6	3.58	125.79	120.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

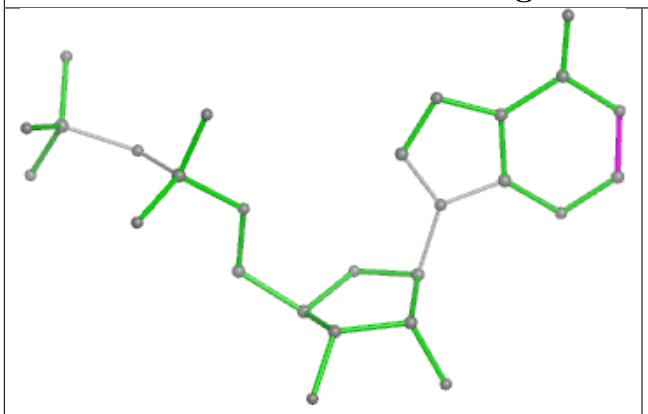
Mol	Chain	Res	Type	Atoms
2	A	1723	ADP	PA-O3A-PB-O3B
2	B	1723	ADP	PA-O3A-PB-O3B
2	C	1723	ADP	PA-O3A-PB-O3B
2	D	1723	ADP	PA-O3A-PB-O3B
2	E	1723	ADP	PA-O3A-PB-O3B

There are no ring outliers.

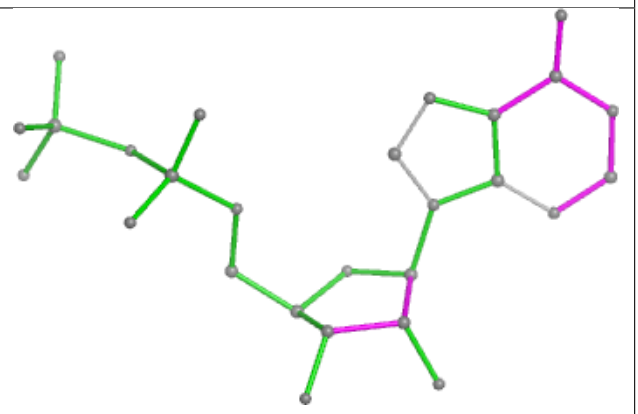
No monomer is involved in short contacts.

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.

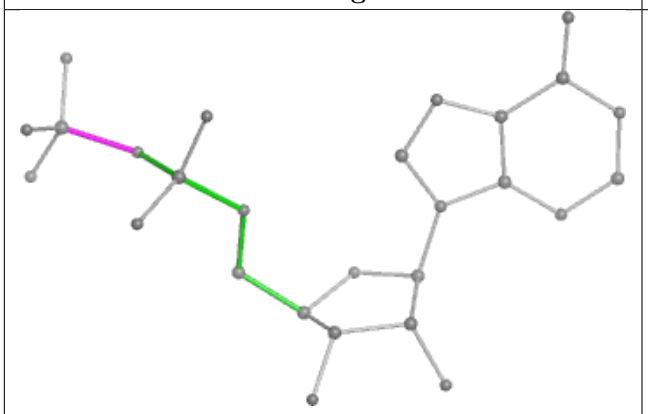
Ligand ADP E 1723



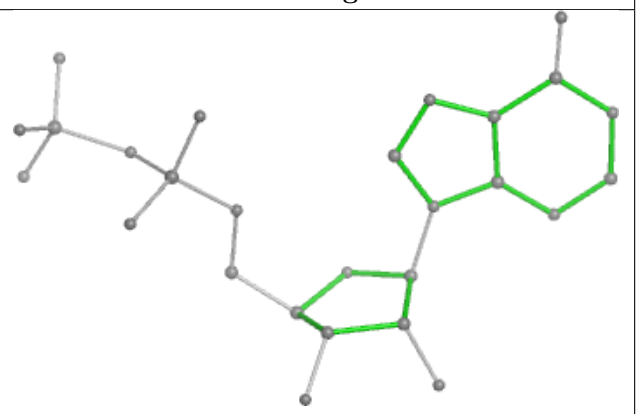
Bond lengths



Bond angles

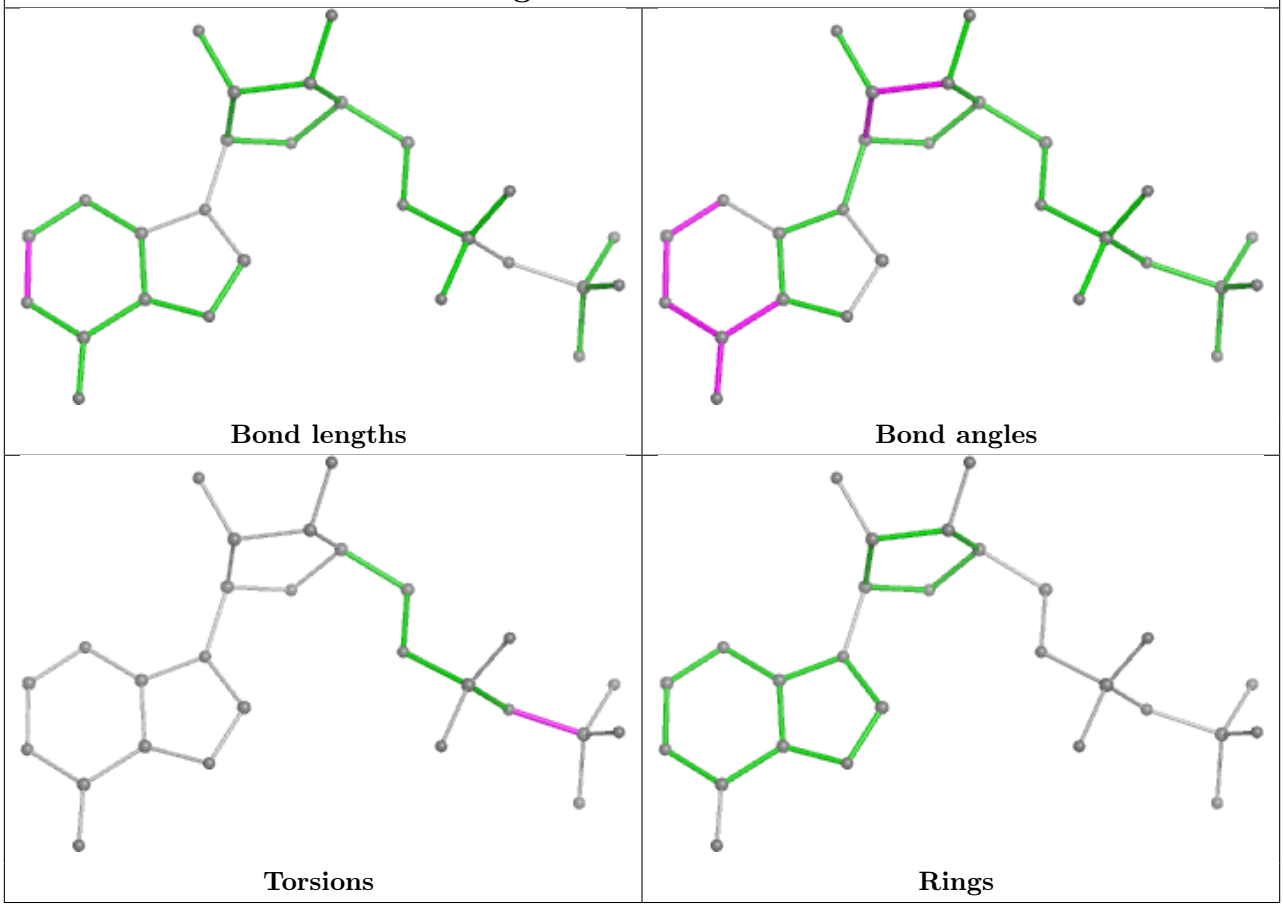


Torsions

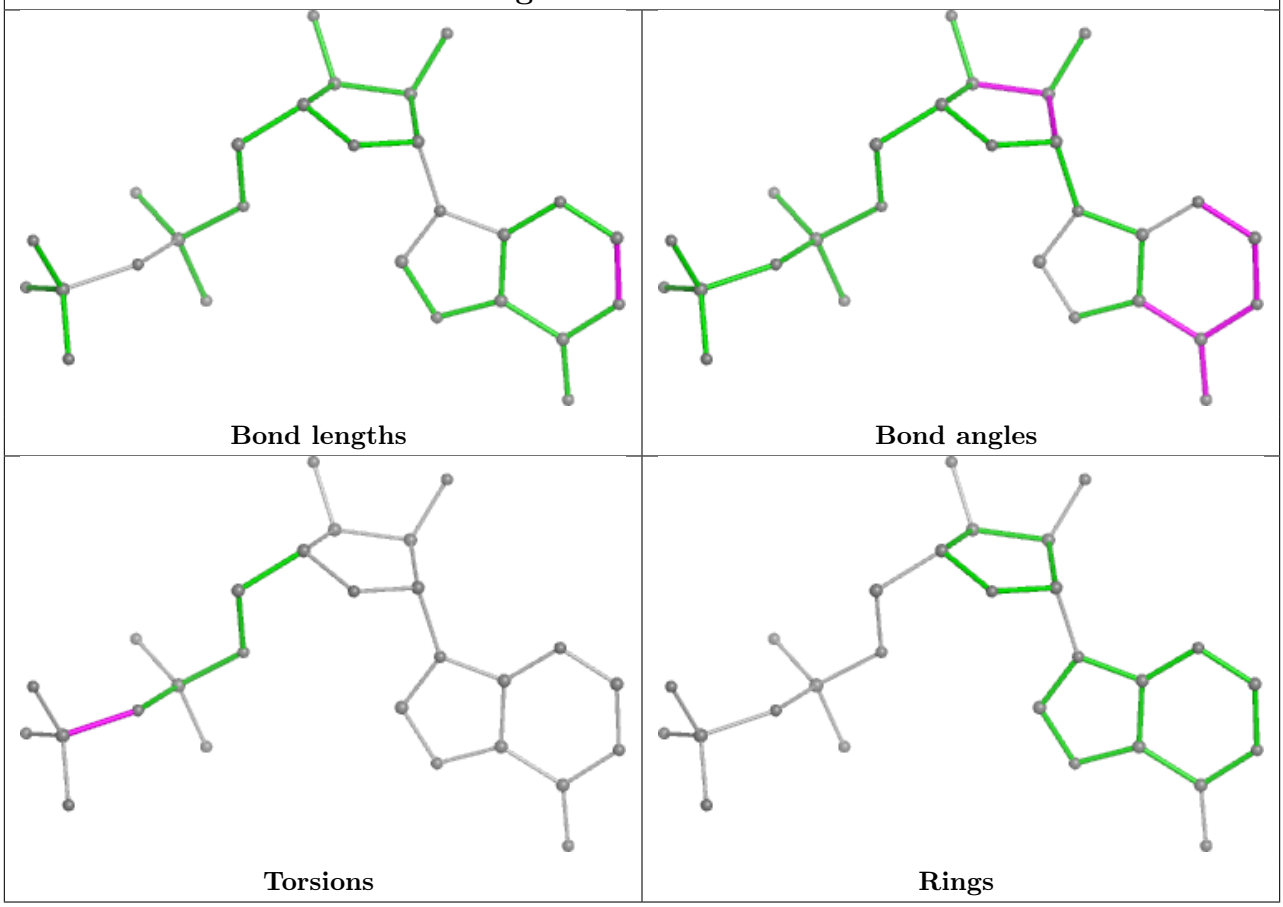


Rings

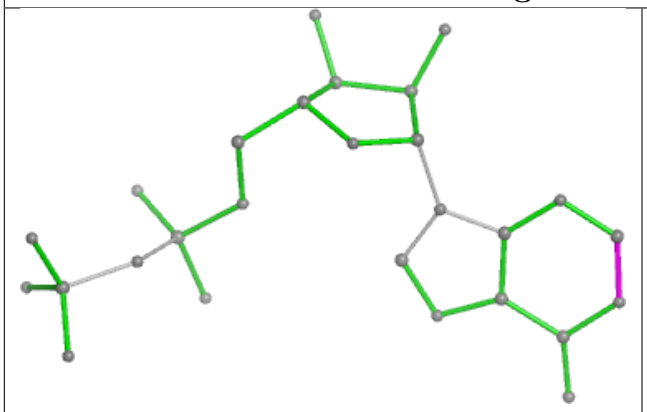
Ligand ADP D 1723



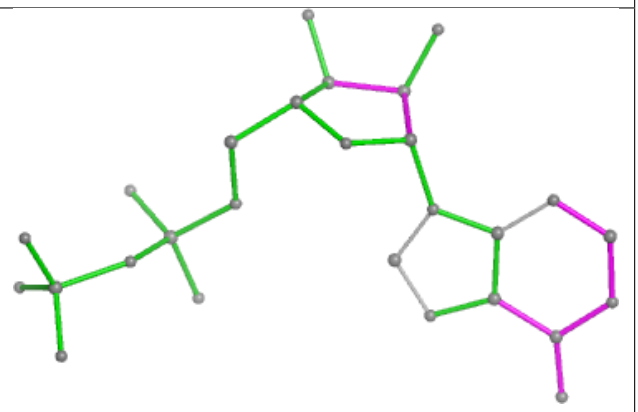
Ligand ADP F 1723



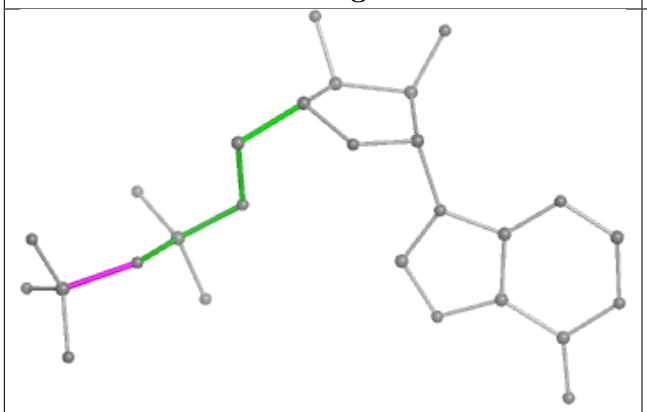
Ligand ADP C 1723



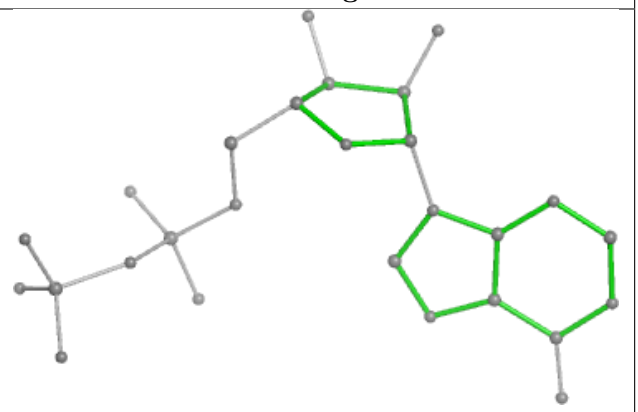
Bond lengths



Bond angles

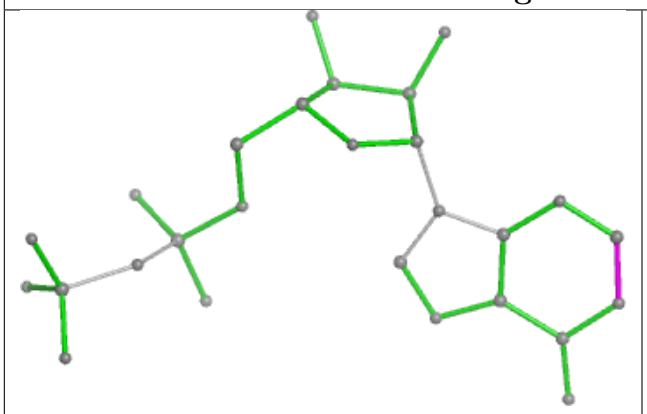


Torsions

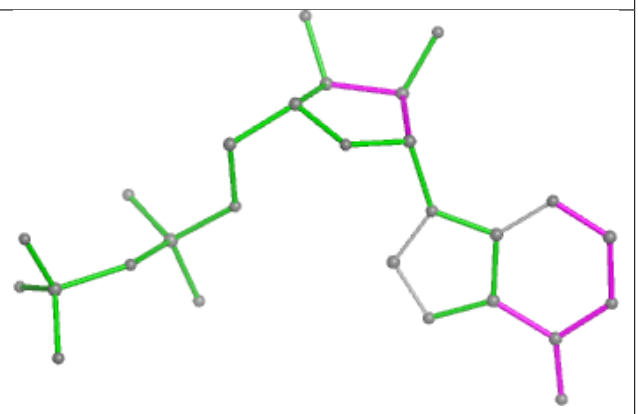


Rings

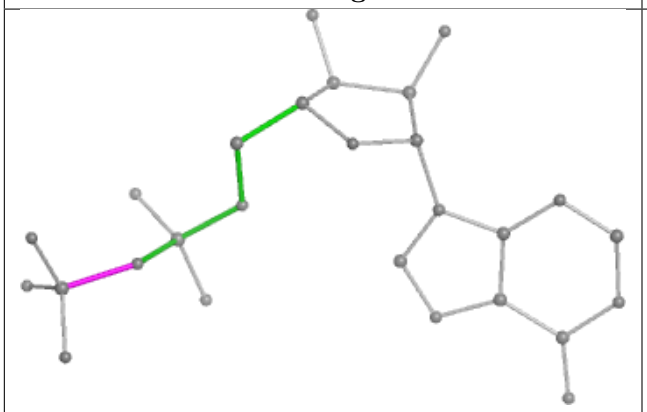
Ligand ADP B 1723



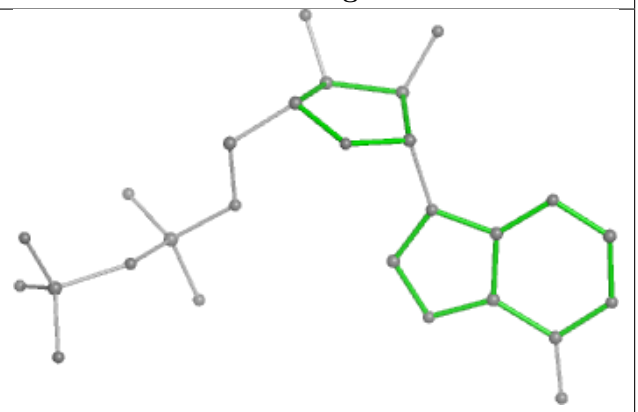
Bond lengths



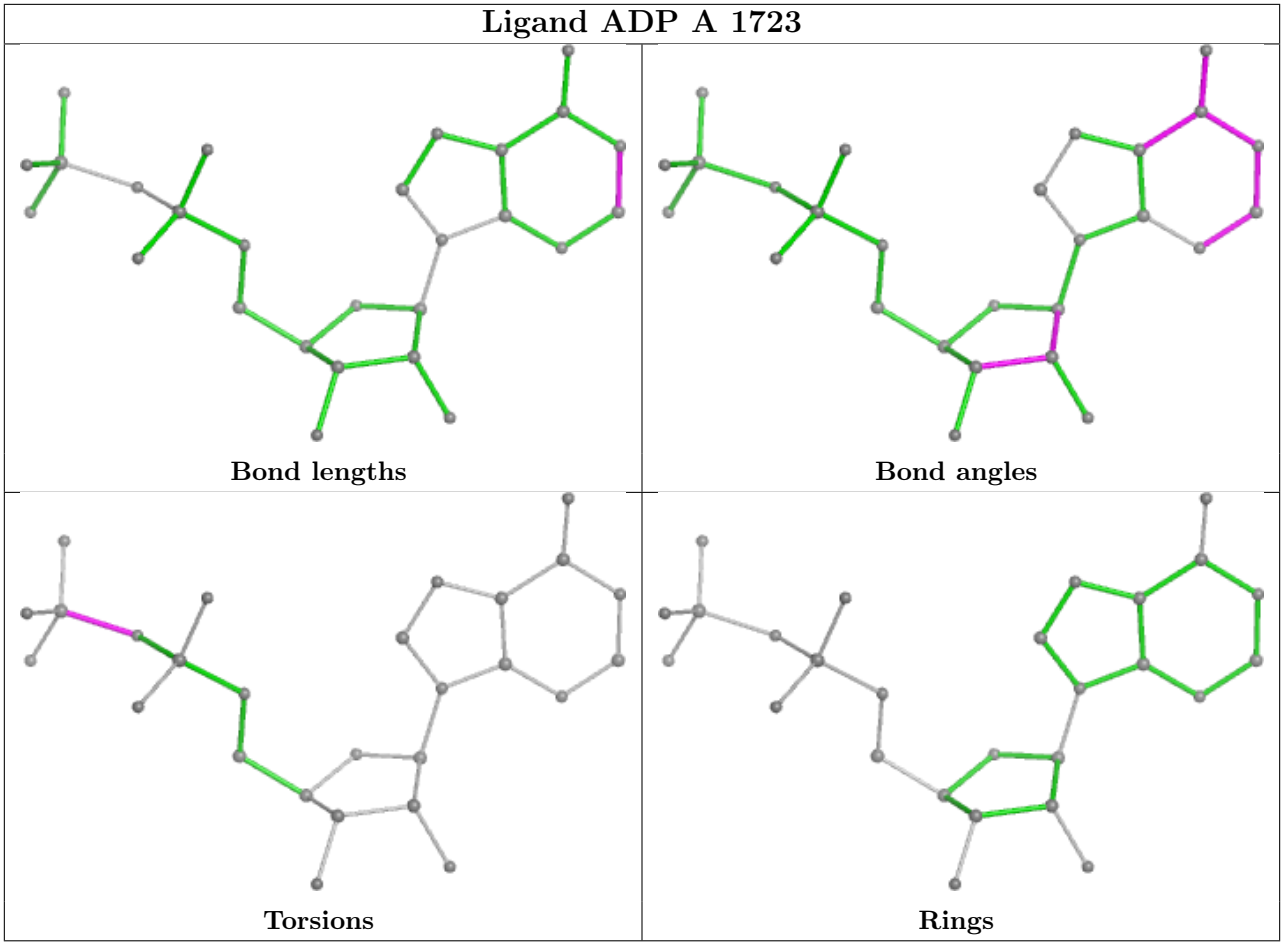
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	408/491 (83%)	0.40	23 (5%)	24	20	48, 72, 110, 136	0
1	B	408/491 (83%)	0.16	8 (1%)	65	63	37, 57, 97, 127	0
1	C	408/491 (83%)	0.11	8 (1%)	65	63	31, 51, 93, 140	0
1	D	408/491 (83%)	0.09	4 (0%)	82	82	32, 49, 85, 131	0
1	E	408/491 (83%)	0.27	16 (3%)	39	35	42, 65, 102, 142	0
1	F	408/491 (83%)	0.33	21 (5%)	28	24	47, 73, 108, 140	0
All	All	2448/2946 (83%)	0.23	80 (3%)	46	41	31, 62, 103, 142	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	328	GLN	8.4
1	E	329	LYS	6.1
1	C	328	GLN	4.3
1	F	326	VAL	4.2
1	C	329	LYS	4.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

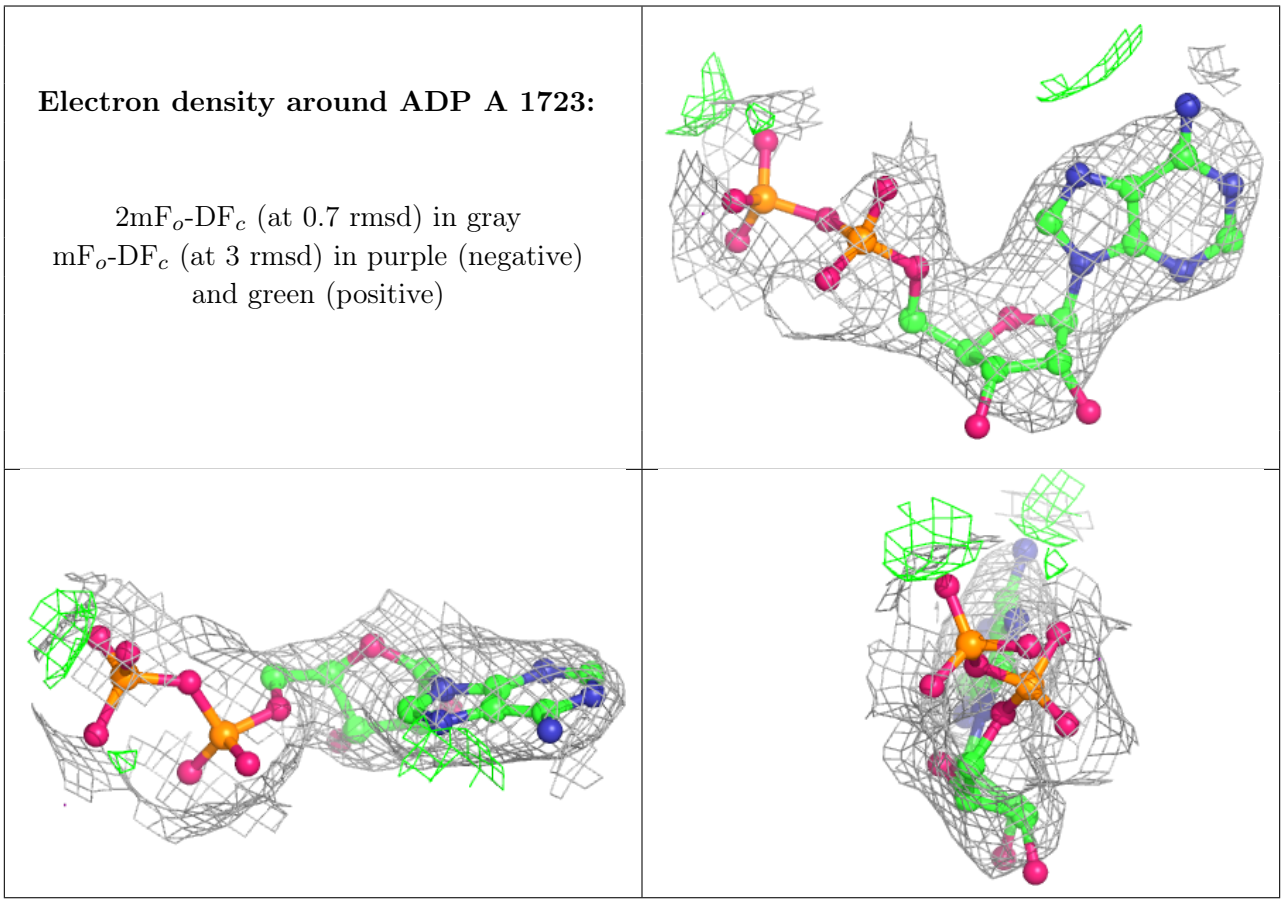
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	1723	27/27	0.85	0.23	93,96,103,104	0
2	ADP	F	1723	27/27	0.86	0.22	87,100,105,105	0
2	ADP	E	1723	27/27	0.90	0.22	87,90,91,91	0
2	ADP	D	1723	27/27	0.92	0.22	62,72,76,81	0
2	ADP	B	1723	27/27	0.92	0.21	75,82,85,88	0
2	ADP	C	1723	27/27	0.92	0.22	67,82,87,88	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.

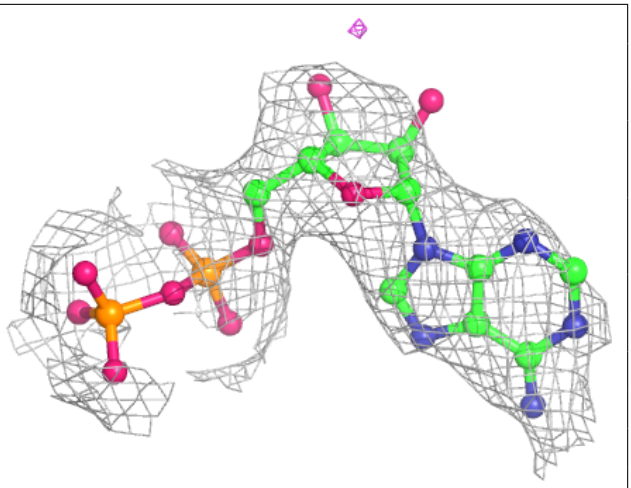
Electron density around ADP A 1723:

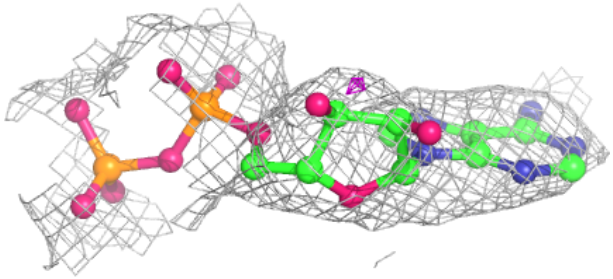
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

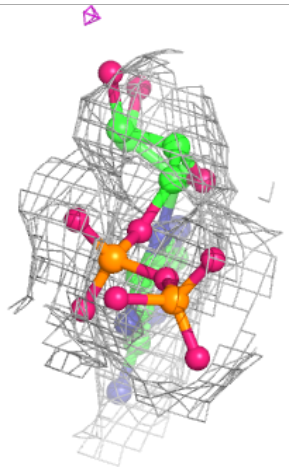


Electron density around ADP F 1723:

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

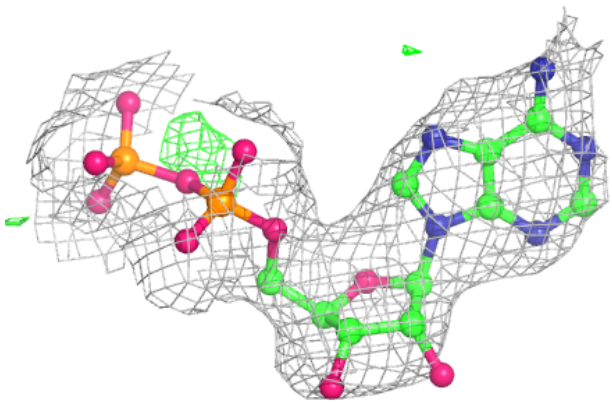


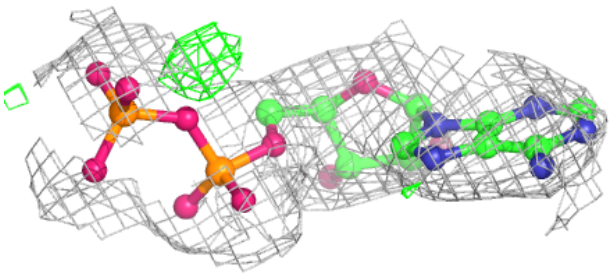


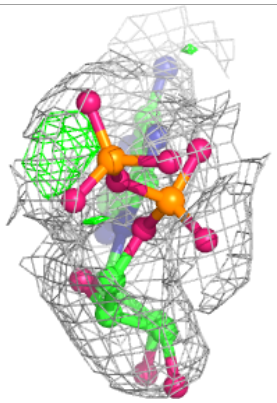


Electron density around ADP E 1723:

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

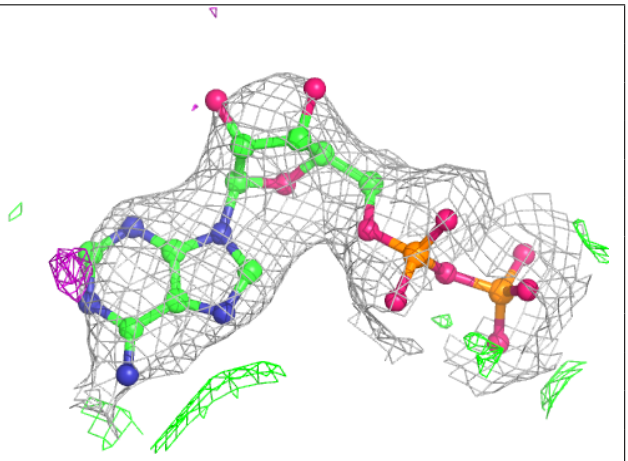


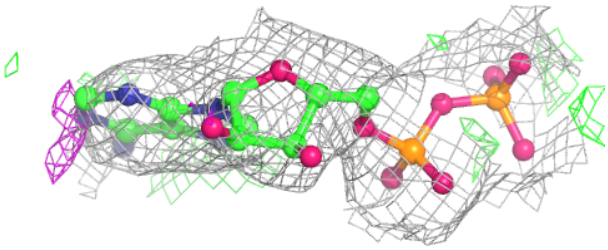


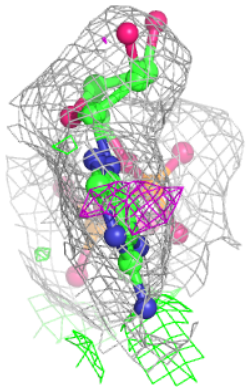


Electron density around ADP D 1723:

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

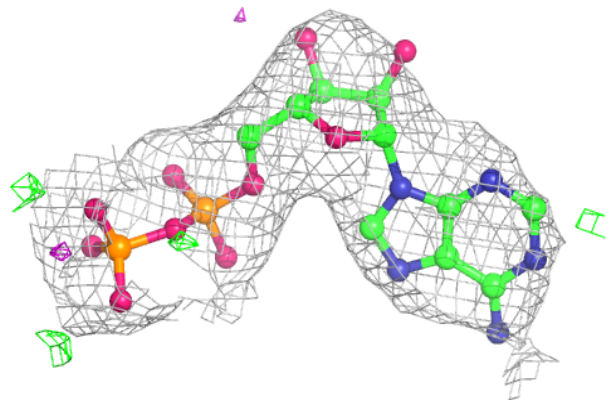


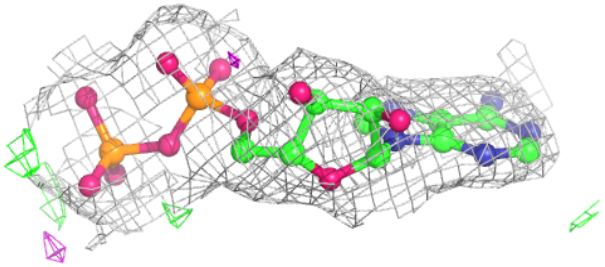




Electron density around ADP B 1723:

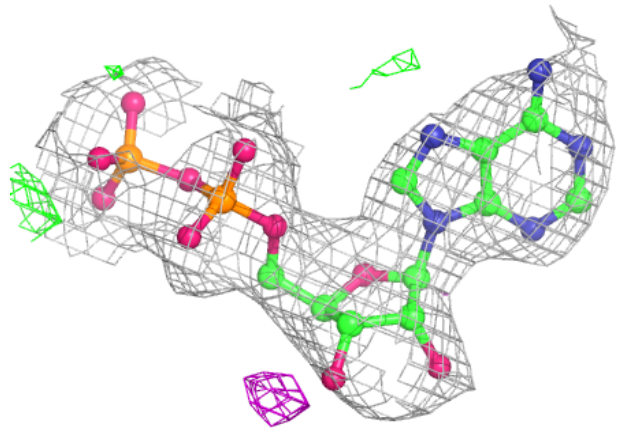
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

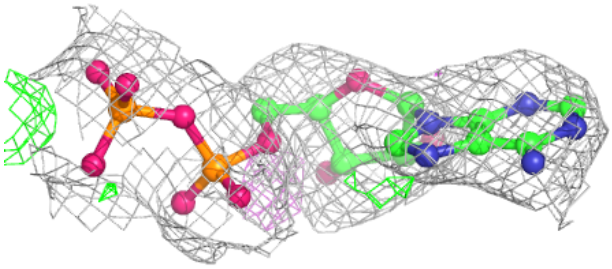


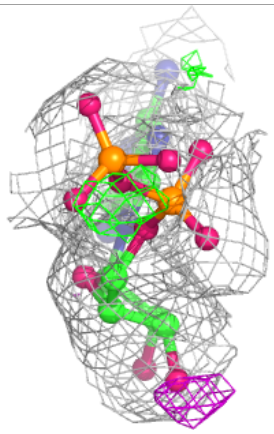


Electron density around ADP C 1723:

$2mF_o$-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.