wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 10:07 pm BST

PDB ID	:	3CF3
Title	:	Structure of P97/vcp in complex with ADP
Authors	:	Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.
Deposited on	:	2008-03-01
Resolution	:	4.25 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 following versions of software and data (see references (i)) were used in the production of this report:

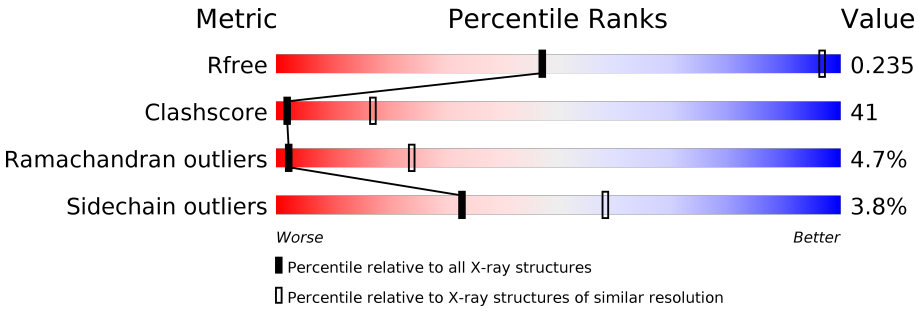
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.25 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	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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%

Mol	Chain	Length	Quality of chain
1	A	806	37% 48% 5% 10%
1	B	806	37% 49% • 10%
1	C	806	37% 47% 5% 10%

2 Entry composition

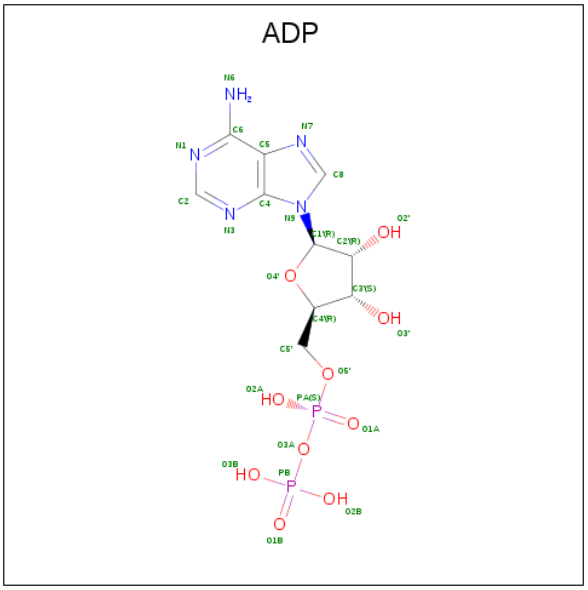
There are 2 unique types of molecules in this entry. The entry contains 17139 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	B	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	C	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			

- 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	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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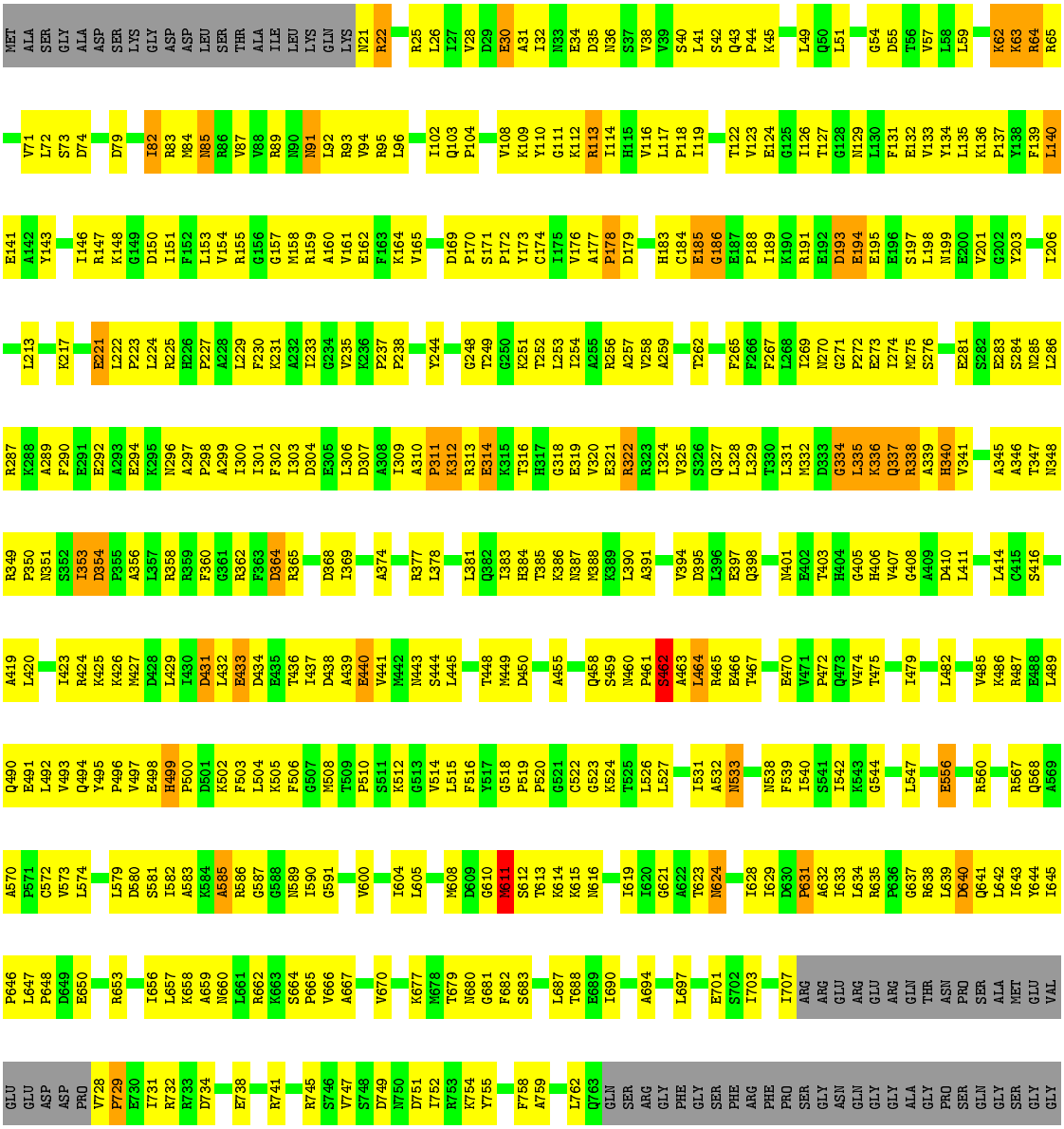
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

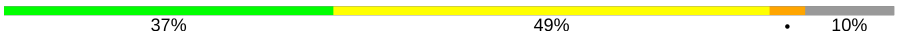
- Molecule 1: Transitional endoplasmic reticulum ATPase

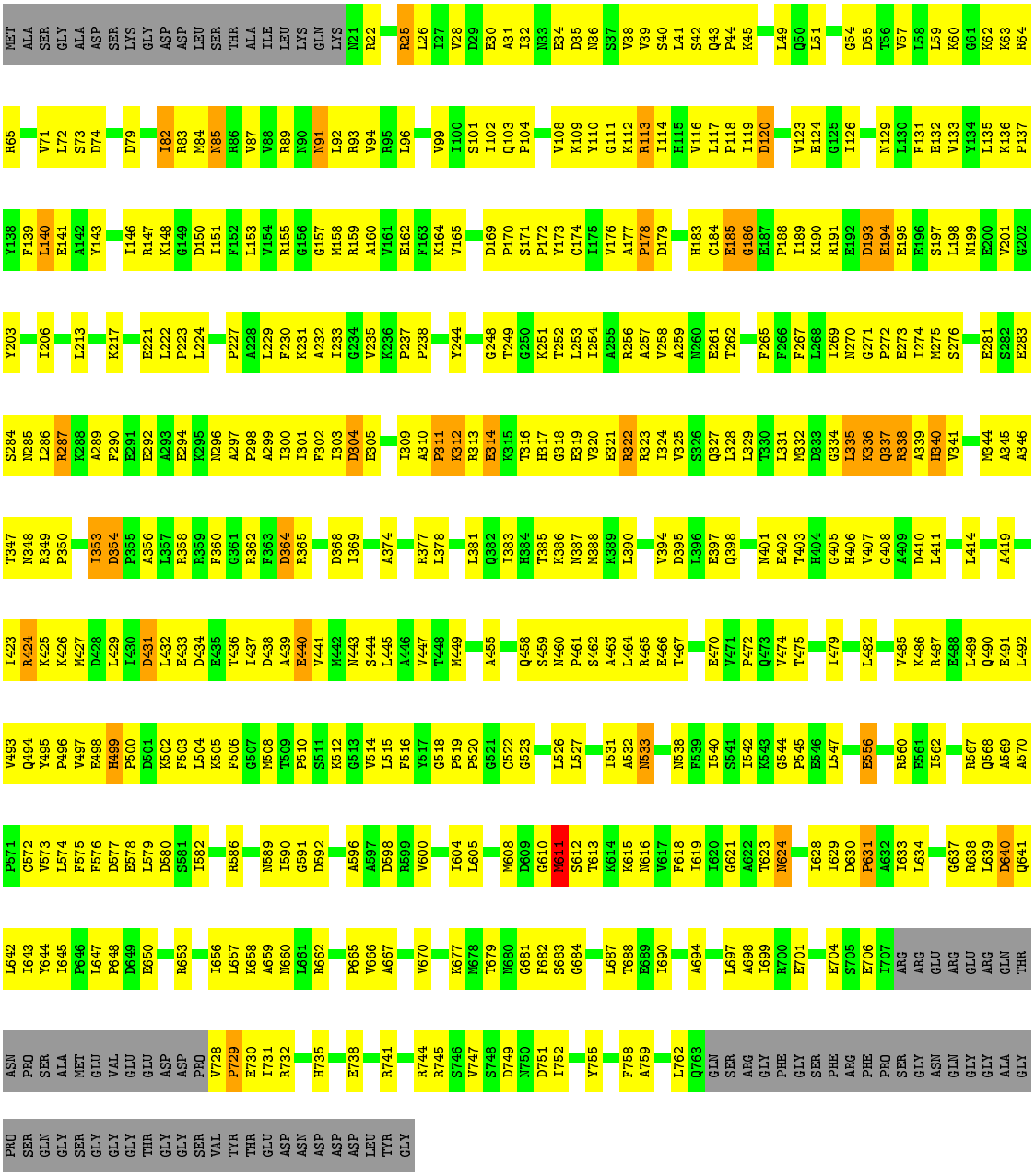
Chain A:



- Molecule 1: Transitional endoplasmic reticulum ATPase

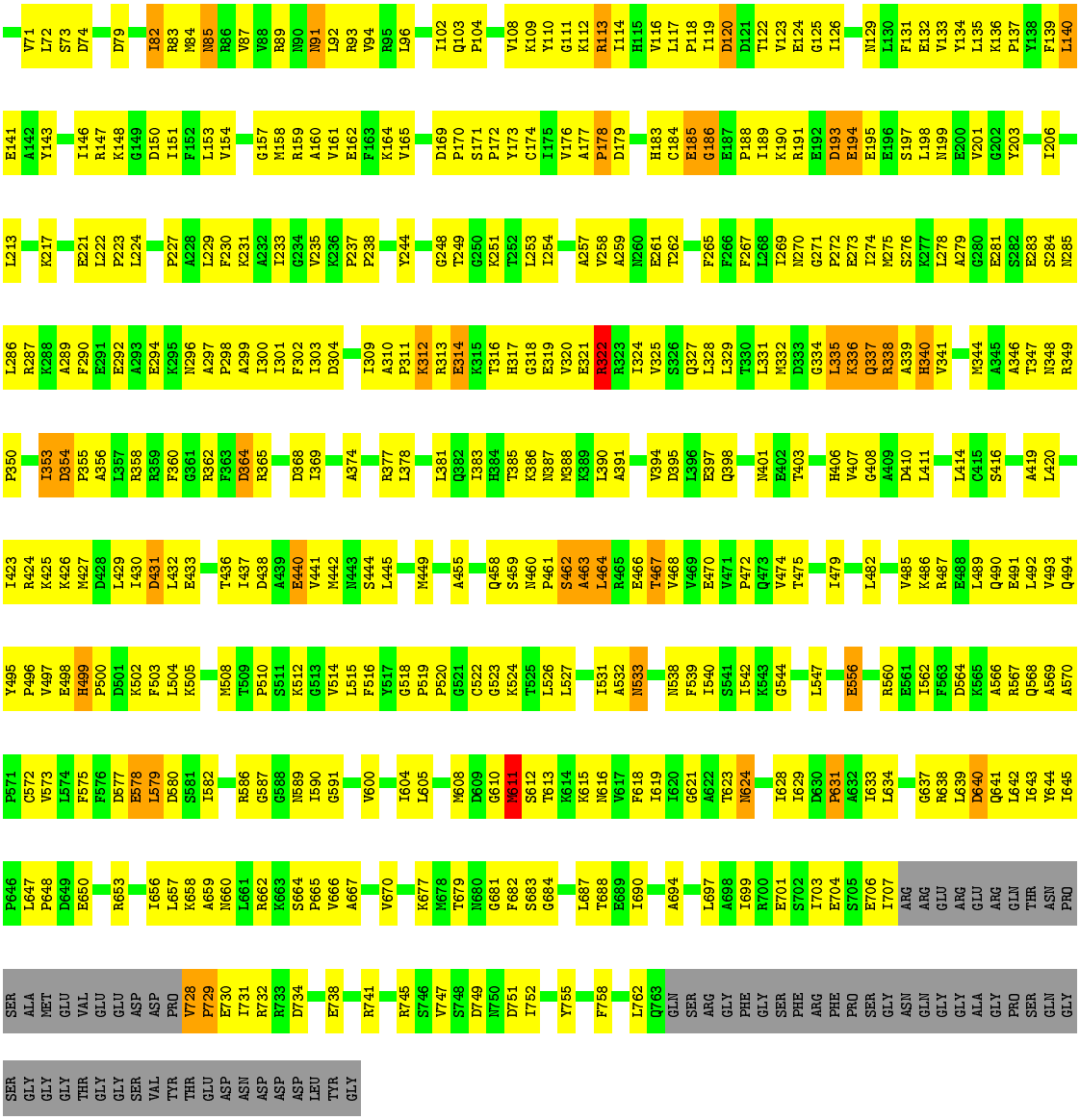
Chain B:





- Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:


V71 L72 S73 D74 D79 I82 R83 M84 N85 R86 V87 V88 R89 N90 N91 L92 R93 V94 R95 L96 I102 Q103 P104 V108 K109 Y110 G111 K112 R113 I114 H115 V116 L117 P118 I119 D120 D121 T122 V123 E124 G125 I126 N129 L130 F131 E132 V133 Y134 L135 K136 P137 Y138 F139 L140
E141 A142 Y143 I146 R147 K148 G149 D150 I151 F152 L153 V154 G157 M158 R159 A160 V161 E162 F163 K164 V165 D169 P170 S171 P172 Y173 C174 I175 V176 A177 P178 D179 H183 C184 E185 G186 E187 P188 I189 K190 R191 E192 D193 E194 E195 E196 S197 L198 N199 E200 V201 G202 Y203 I206
L213 K217 E221 L222 P223 L224 P227 A228 L229 F230 K231 A232 I233 G234 V235 K236 P237 P238 Y244 G248 T249 G250 K251 T252 L253 I254 A257 V258 A259 N260 E261 T262 P265 F266 F267 L268 I269 N270 G271 P272 E273 I274 M275 S276 K277 L278 A279 G280 E281 S282 E283 S284 N285
L286 R287 K288 A289 F290 E291 E292 A293 E294 K295 N296 A297 P298 A299 I300 I301 F302 I303 D304 I309 A310 P311 K312 R313 E314 K315 T316 H317 G318 E319 V320 E321 R322 R323 I324 V325 S326 Q327 L328 L329 T330 L331 M332 D333 G334 L335 K336 Q337 R338 A339 H340 V341 M344 A345 A346 T347 N348 R349
P350 I353 D354 P355 A356 L357 R358 R359 F360 G361 R362 F363 D364 R365 D368 I369 A374 R377 L378 L381 Q382 I383 H384 T385 K386 N387 M388 K389 L390 A391 V394 D395 L396 E397 Q398 N401 E402 T403 H406 V407 G408 A409 D410 L411 L414 C415 S416 A419 L420
I423 R424 K425 K426 M427 D428 L429 I430 D431 L432 E433 T436 I437 D438 A439 E440 V441 M442 N443 S444 L445 M449 A455 Q458 S459 N460 P461 S462 A463 L464 R465 E466 T467 V468 V469 E470 V471 P472 Q473 V474 T475 I479 L482 V485 K486 R487 E488 L489 Q490 E491 L492 V493 Q494
Y495 P496 V497 E498 H499 P500 D501 K502 F503 L504 K505 M508 T509 P510 S511 K512 G513 V514 L515 F516 Y517 G518 P519 P520 G521 C522 G523 K524 T525 L526 L527 I531 A532 N533 N538 F539 I540 S541 I542 K543 G544 L547 E556 R560 E561 I562 P563 D564 K565 A566 R567 Q568 A569 A570
P571 C572 V573 L574 F575 F576 D577 E578 L579 D580 S581 I582 R586 G587 G588 N589 I590 G591 V600 I604 L605 M608 D609 G610 M611 S612 T613 K614 K615 N616 V617 F618 I619 I620 G621 A622 T623 M624 I628 I629 D630 P631 A632 I633 L634 G637 R638 L639 D640 Q641 L642 I643 Y644 I645
P646 L647 P648 D649 E650 R653 I656 I657 K658 A659 N660 L661 R662 K663 S664 P665 V666 A667 V670 K677 M678 T679 W680 G681 F682 S683 G684 L687 T688 E689 I690 A694 L697 A698 I699 R700 E701 S702 I703 E704 S705 E706 I707 ARG ARG GLU ARG GLU ARG GLN THR ASN PRO
SER ALA MET GLU VAL GLU GLU ASP ASP PRO V728 P729 E730 I731 R732 R733 D734 E738 R741 R745 S746 V747 S748 D749 N750 D751 I752 Y755 F758 L762 Q763 GLN SER ARG GLY PHE GLY SER PHE ARG PHE PRO SER GLY ASN GLN GLY GLY ALA GLY PRO SER GLN GLY
SER GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	163.97Å 178.93Å 320.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.25 29.94 – 4.25	Depositor EDS
% Data completeness (in resolution range)	86.4 (40.00-4.25) 92.9 (29.94-4.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 4.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.226 0.210 , 0.235	Depositor DCC
R_{free} test set	4669 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å^2)	143.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 188.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17139	wwPDB-VP
Average B, all atoms (Å^2)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% 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: 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	0.38	0/5751	0.87	9/7767 (0.1%)
1	B	0.37	0/5751	0.87	9/7767 (0.1%)
1	C	0.38	0/5751	0.88	9/7767 (0.1%)
All	All	0.38	0/17253	0.87	27/23301 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	322	ARG	NE-CZ-NH2	-29.67	105.46	120.30
1	A	338	ARG	NE-CZ-NH1	-29.13	105.74	120.30
1	B	287	ARG	NE-CZ-NH2	-28.38	106.11	120.30
1	A	338	ARG	NE-CZ-NH2	27.38	133.99	120.30
1	B	287	ARG	NE-CZ-NH1	27.28	133.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5659	0	5731	495	0
1	B	5659	0	5731	491	0
1	C	5659	0	5731	466	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	54	0	24	6	0
2	B	54	0	24	4	0
2	C	54	0	24	3	0
All	All	17139	0	17265	1421	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 41.

The worst 5 of 1421 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:206:ILE:CD1	1:A:213:LEU:HD11	1.25	1.64
1:B:206:ILE:CD1	1:B:213:LEU:HD11	1.24	1.61
1:C:206:ILE:CD1	1:C:213:LEU:HD11	1.25	1.59
1:A:206:ILE:HD11	1:A:213:LEU:CD1	1.55	1.34
1:C:206:ILE:HD11	1:C:213:LEU:CD1	1.55	1.34

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	719/806 (89%)	566 (79%)	119 (17%)	34 (5%)	2 24
1	B	719/806 (89%)	564 (78%)	123 (17%)	32 (4%)	2 24
1	C	719/806 (89%)	561 (78%)	122 (17%)	36 (5%)	2 23
All	All	2157/2418 (89%)	1691 (78%)	364 (17%)	102 (5%)	2 24

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	85	ASN
1	A	140	LEU
1	A	185	GLU
1	A	312	LYS

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	615/678 (91%)	590 (96%)	25 (4%)	30	56
1	B	615/678 (91%)	593 (96%)	22 (4%)	35	60
1	C	615/678 (91%)	592 (96%)	23 (4%)	34	59
All	All	1845/2034 (91%)	1775 (96%)	70 (4%)	33	58

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	287	ARG
1	B	440	GLU
1	C	579	LEU
1	B	314	GLU
1	B	340	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	ASN
1	B	348	ASN
1	C	616	ASN
1	B	327	GLN
1	B	401	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	B	900	-	24,29,29	1.50	3 (12%)	29,45,45	1.58	3 (10%)
2	ADP	B	807	-	24,29,29	1.71	5 (20%)	29,45,45	1.77	4 (13%)
2	ADP	A	807	-	24,29,29	1.80	7 (29%)	29,45,45	1.91	6 (20%)
2	ADP	C	807	-	24,29,29	1.46	3 (12%)	29,45,45	1.72	3 (10%)
2	ADP	C	900	-	24,29,29	1.73	4 (16%)	29,45,45	1.73	2 (6%)
2	ADP	A	900	-	24,29,29	1.85	7 (29%)	29,45,45	1.71	1 (3%)

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	B	900	-	-	8/12/32/32	0/3/3/3
2	ADP	B	807	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	807	-	-	5/12/32/32	0/3/3/3
2	ADP	C	807	-	-	5/12/32/32	0/3/3/3
2	ADP	C	900	-	-	6/12/32/32	0/3/3/3
2	ADP	A	900	-	-	8/12/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	O4'-C1'	4.59	1.47	1.41
2	C	900	ADP	O4'-C1'	4.49	1.47	1.41
2	B	807	ADP	C2-N3	4.10	1.38	1.32
2	A	900	ADP	C2-N3	3.79	1.38	1.32
2	A	807	ADP	C2-N3	3.69	1.38	1.32

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	807	ADP	N3-C2-N1	-7.54	116.89	128.68
2	C	900	ADP	N3-C2-N1	-7.33	117.22	128.68
2	A	900	ADP	N3-C2-N1	-7.25	117.35	128.68
2	B	807	ADP	N3-C2-N1	-7.19	117.45	128.68
2	C	807	ADP	N3-C2-N1	-7.18	117.45	128.68

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	ADP	C5'-O5'-PA-O1A
2	B	900	ADP	C5'-O5'-PA-O2A
2	B	900	ADP	C5'-O5'-PA-O3A
2	B	807	ADP	C5'-O5'-PA-O1A
2	B	807	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	ADP	1	0
2	B	807	ADP	3	0
2	A	807	ADP	4	0

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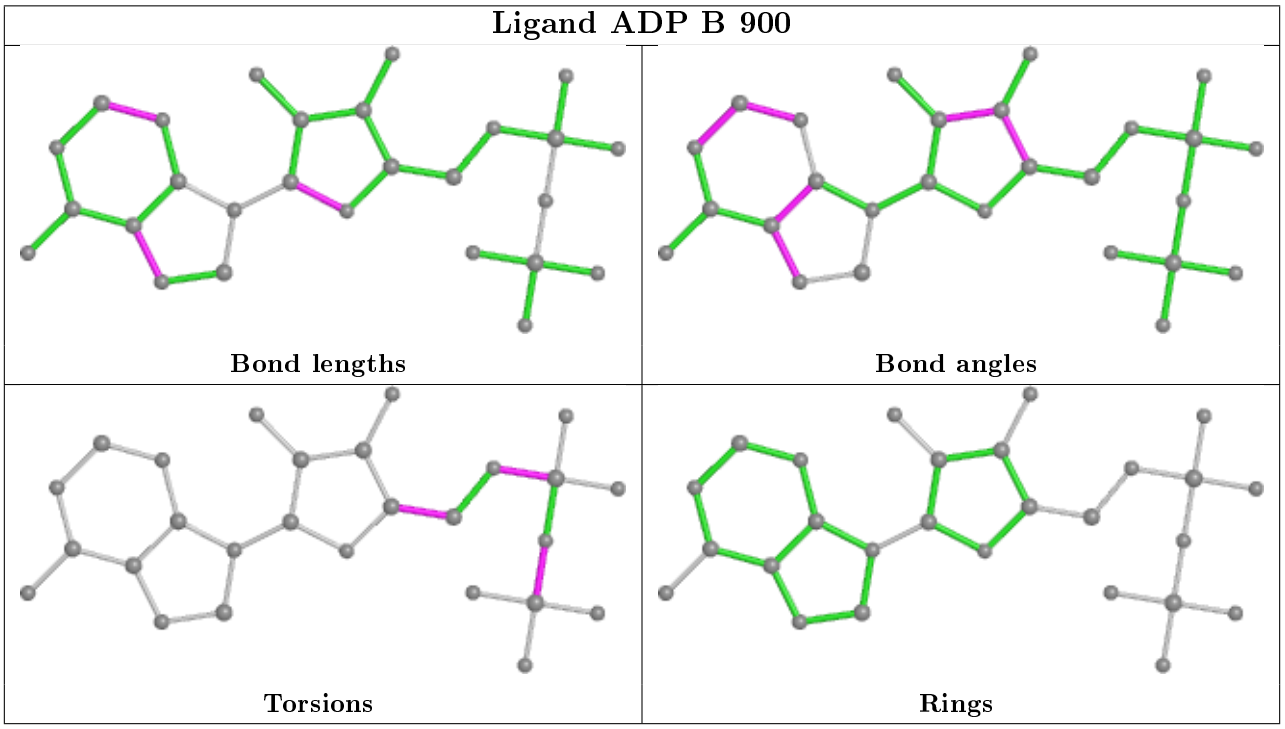
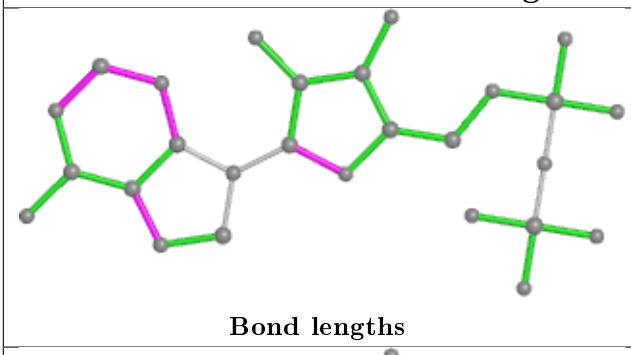
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	807	ADP	1	0
2	C	900	ADP	2	0
2	A	900	ADP	2	0

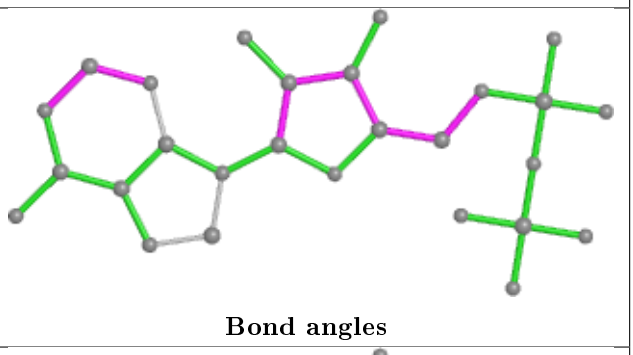
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



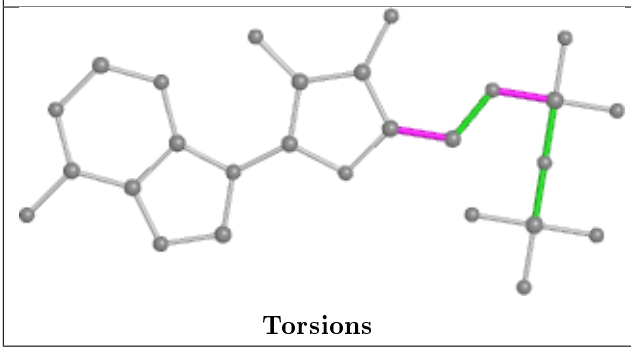
Ligand ADP B 807



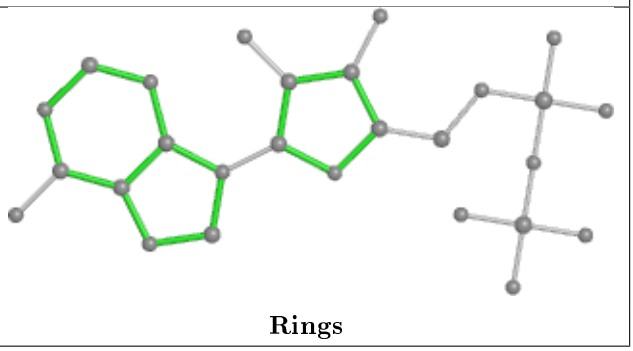
Bond lengths



Bond angles

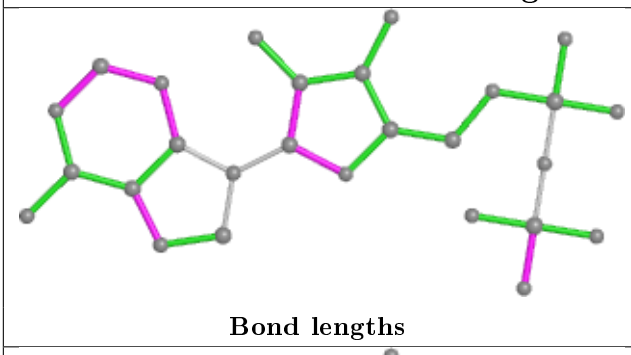


Torsions

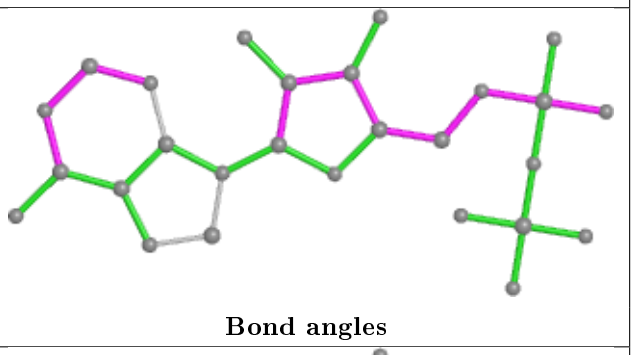


Rings

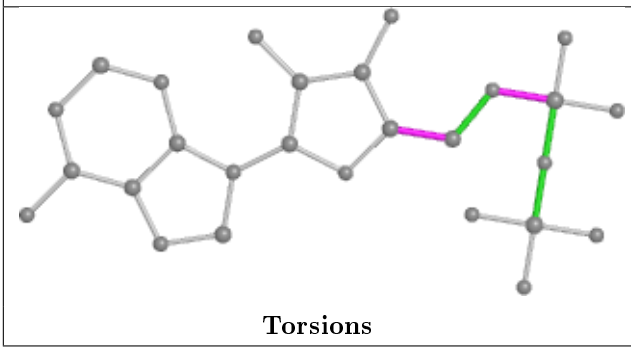
Ligand ADP A 807



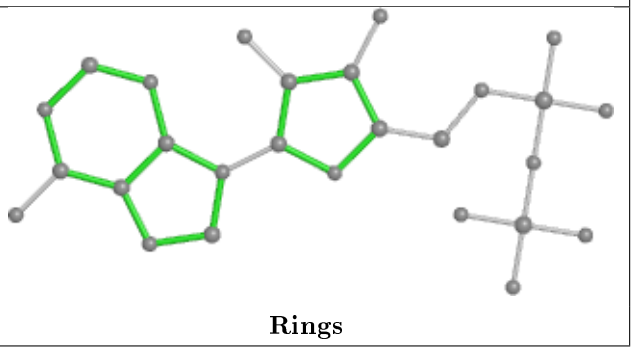
Bond lengths



Bond angles

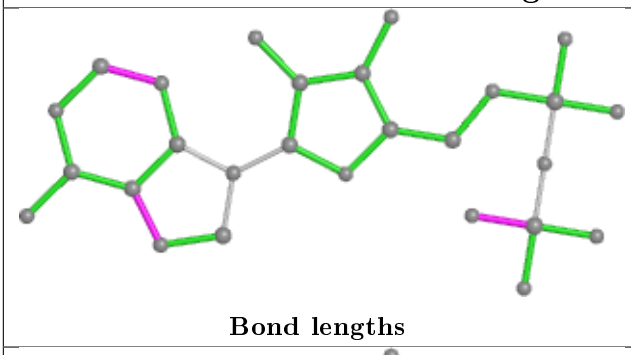


Torsions

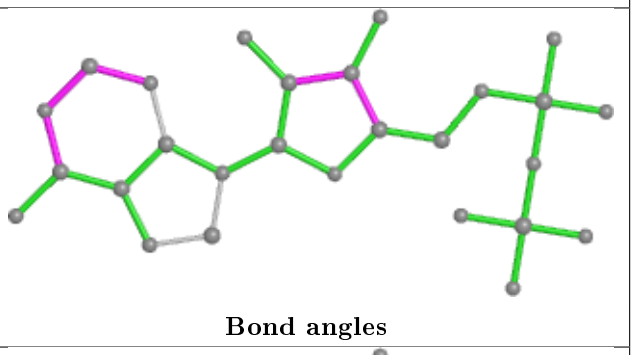


Rings

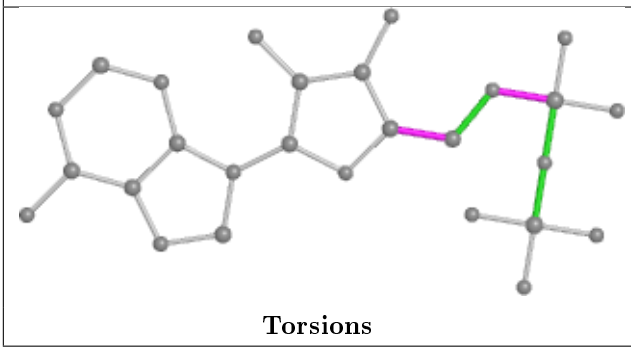
Ligand ADP C 807



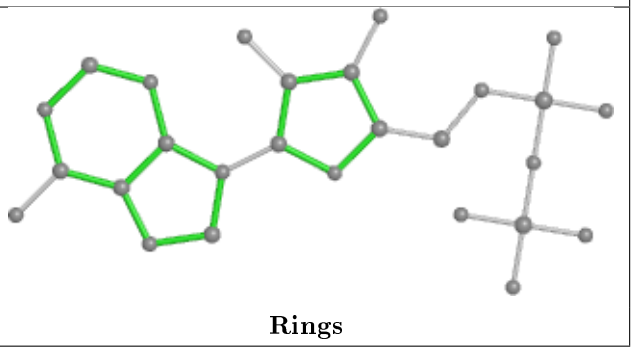
Bond lengths



Bond angles

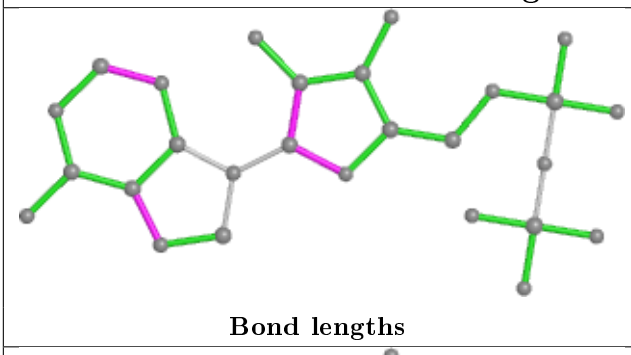


Torsions

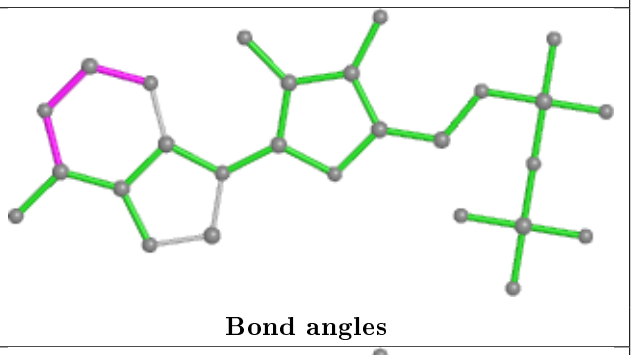


Rings

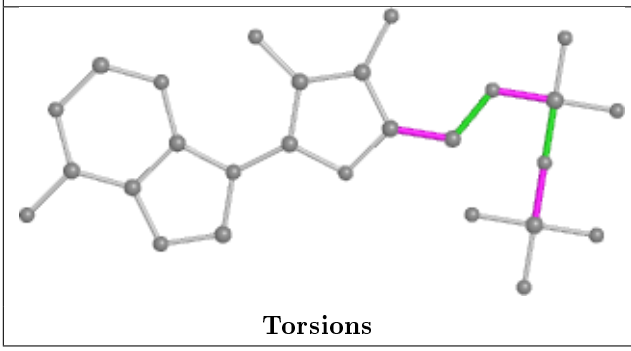
Ligand ADP C 900



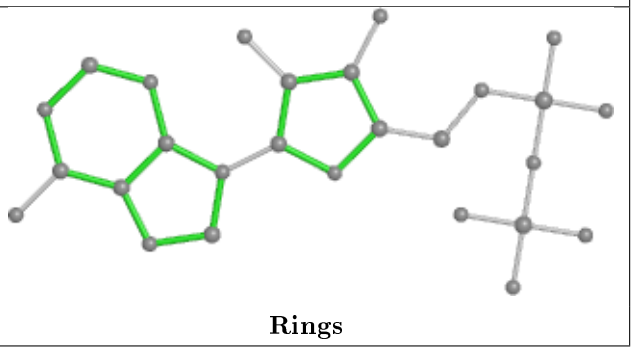
Bond lengths



Bond angles

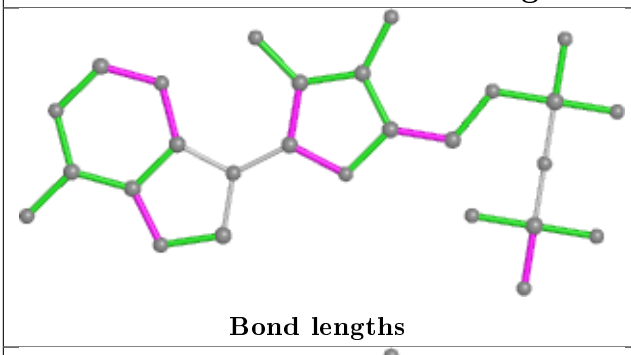


Torsions

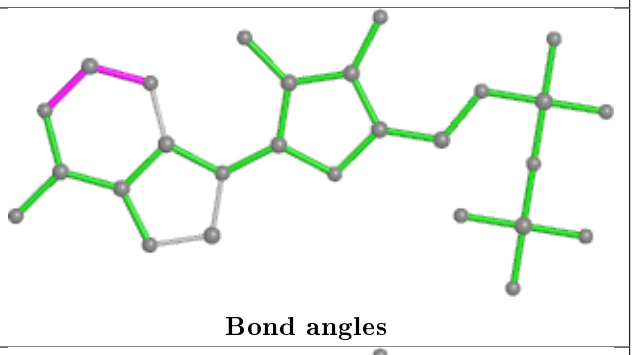


Rings

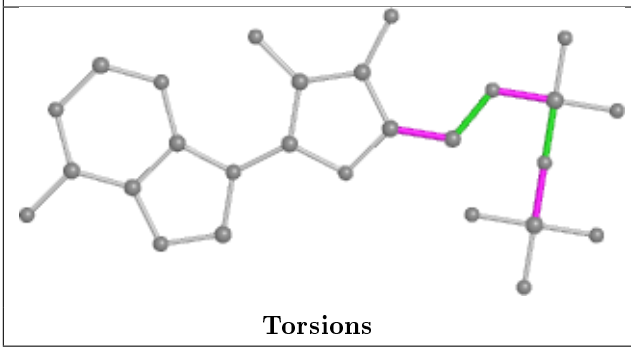
Ligand ADP A 900



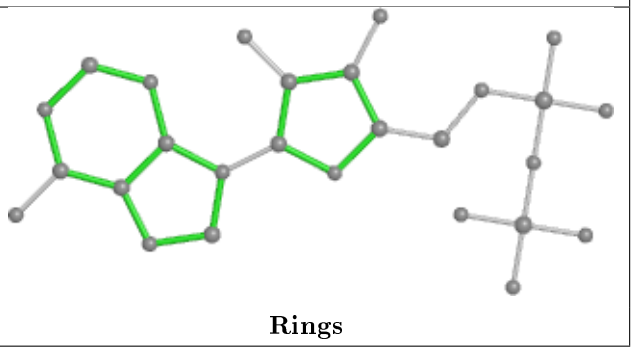
Bond lengths



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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

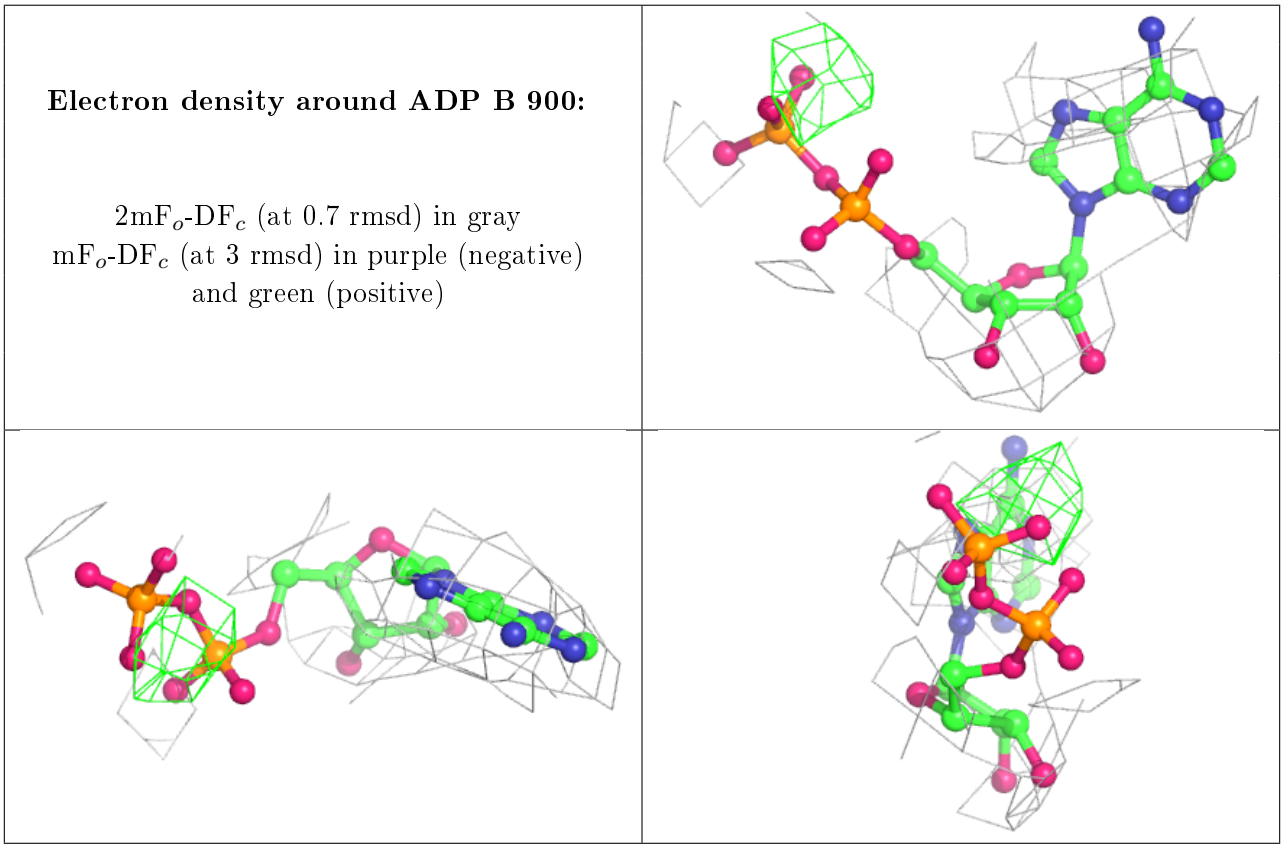
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

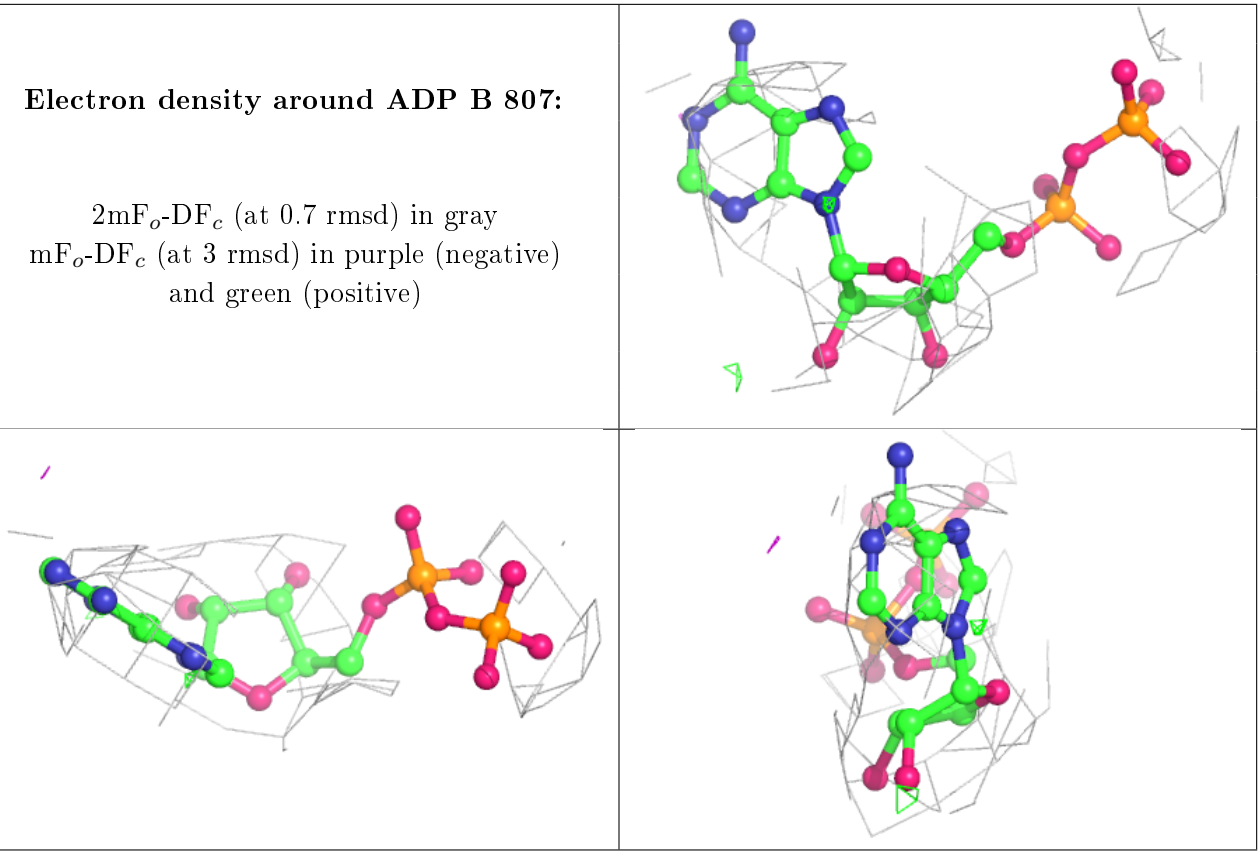
Electron density around ADP B 900:

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



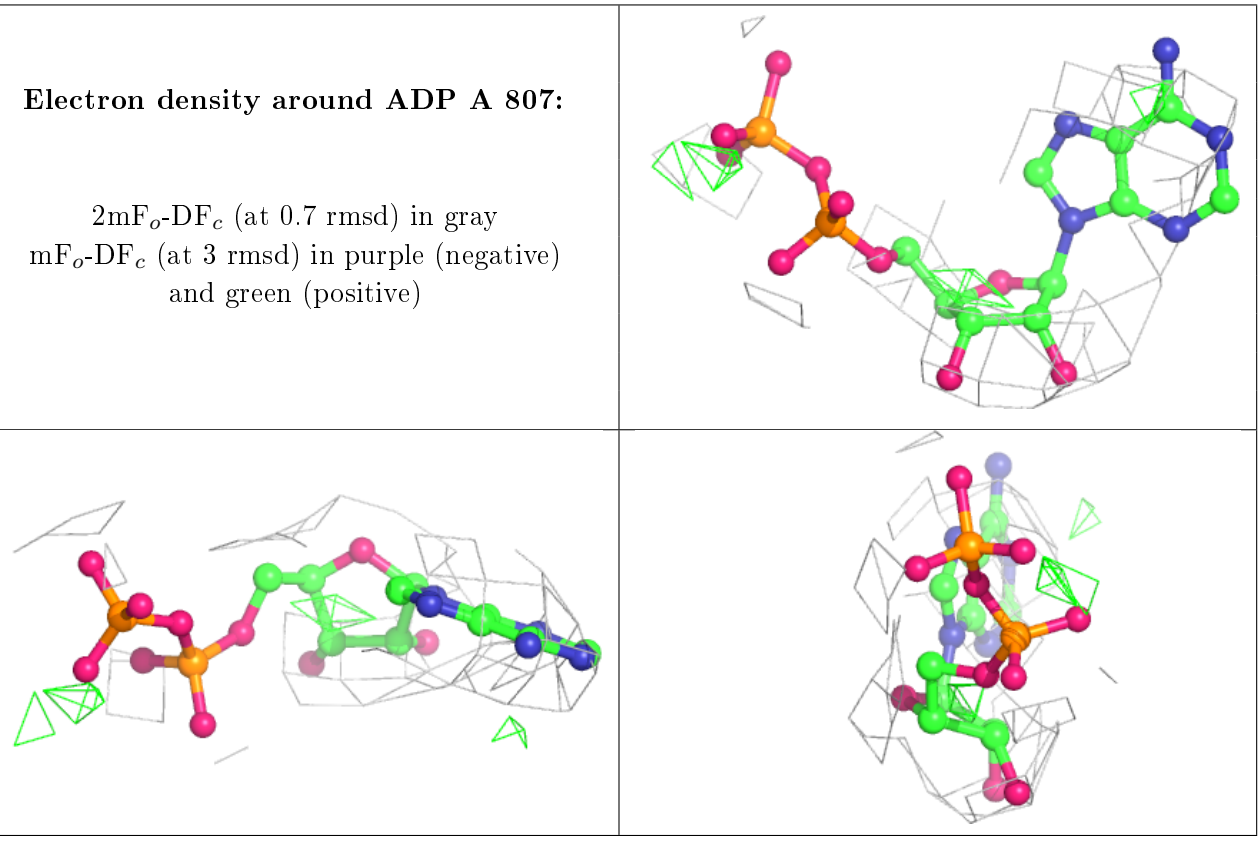
Electron density around ADP B 807:

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



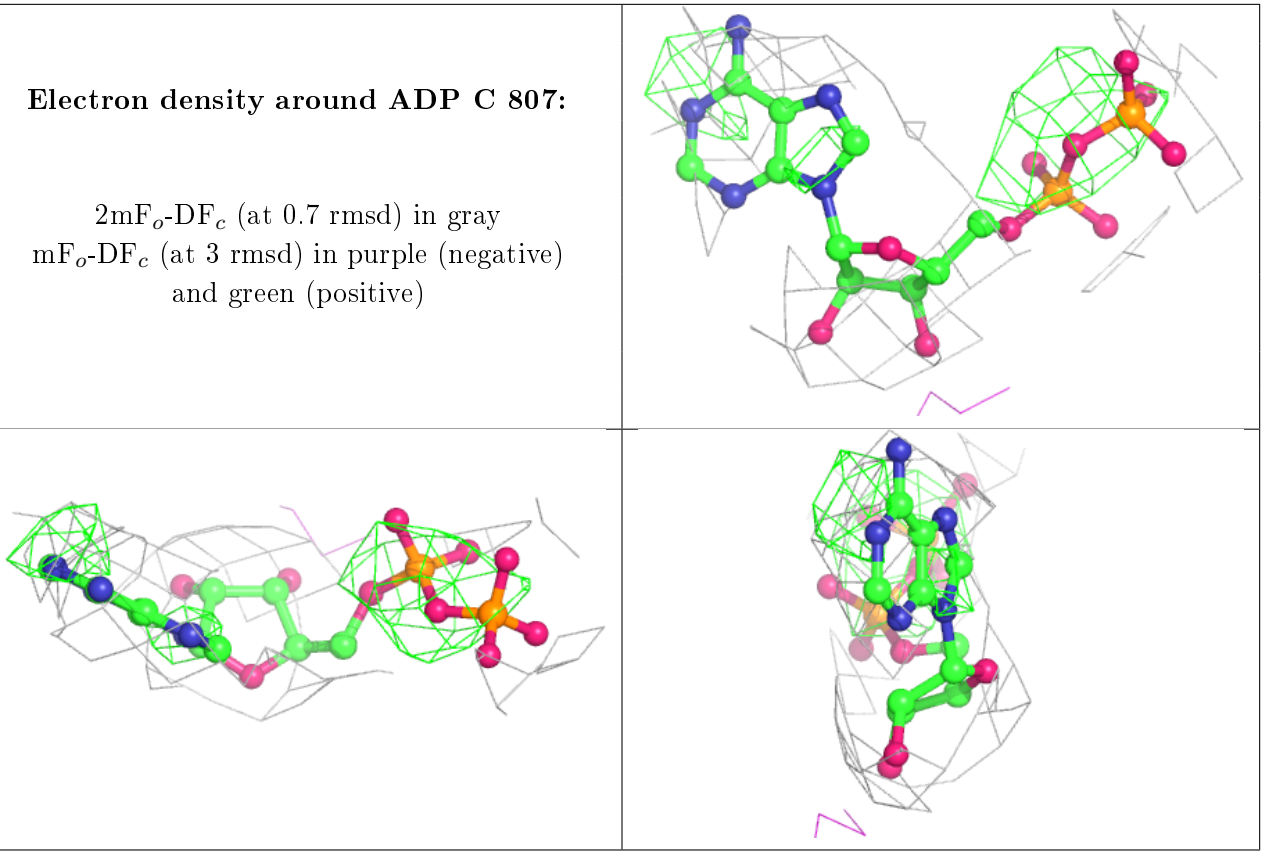
Electron density around ADP A 807:

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



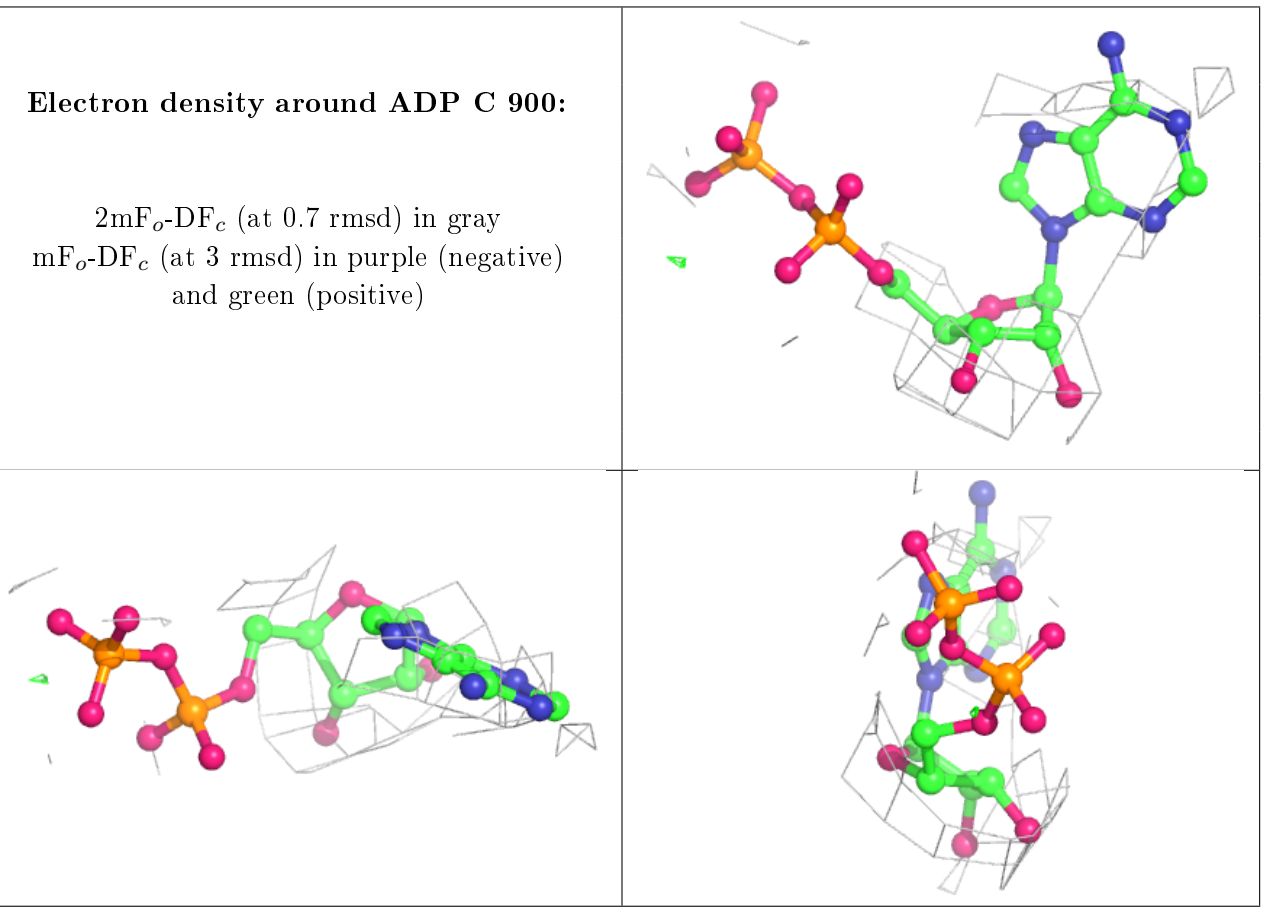
Electron density around ADP C 807:

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



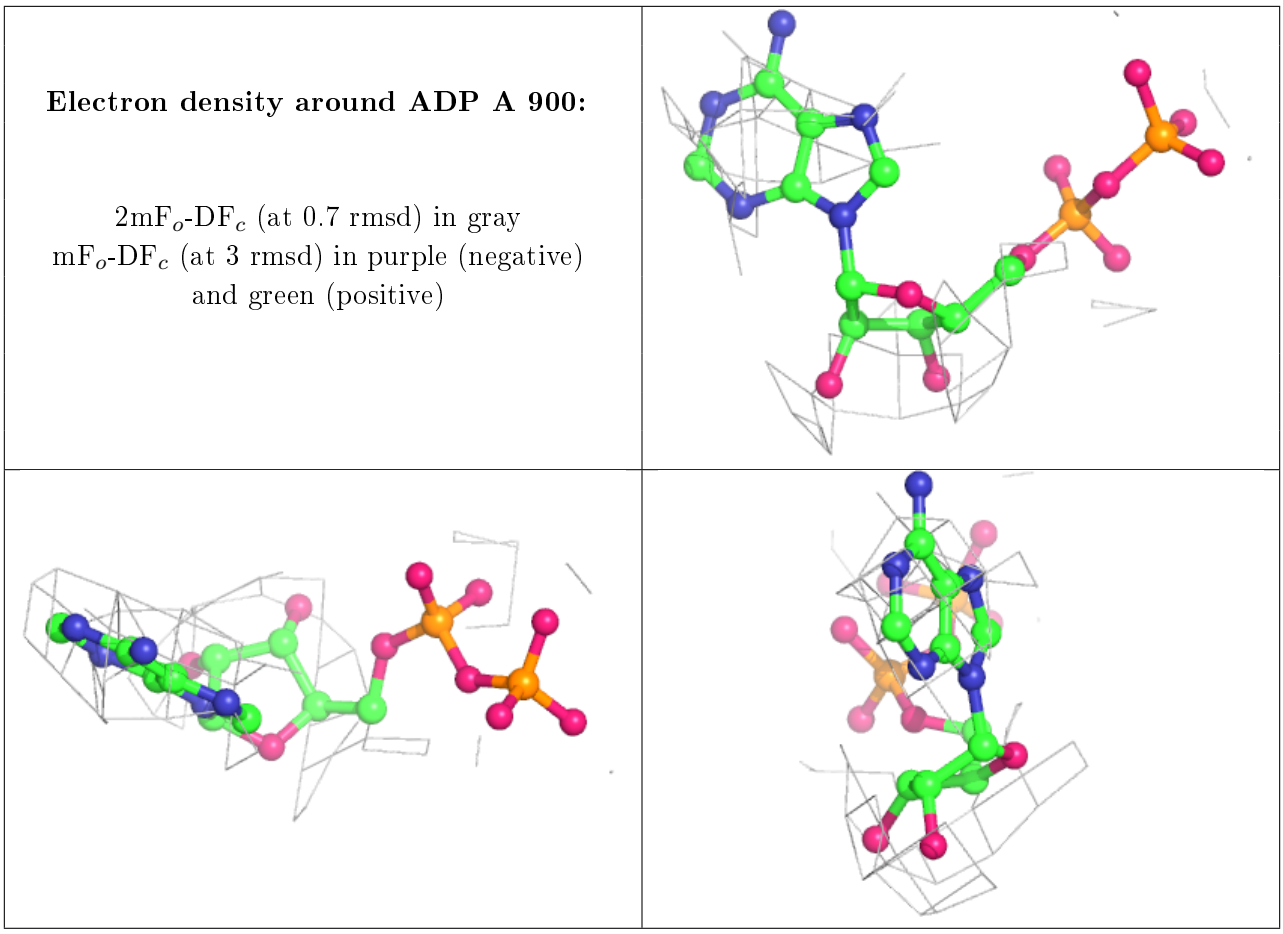
Electron density around ADP C 900:

$2mF_o$-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 900:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.