



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 05:00 PM EDT

PDB ID : 6O8G
Title : Crystal structure of UvrB bound to fully duplex DNA
Authors : Lee, S.-J.; Sung, R.-J.; Verdine, G.L.
Deposited on : 2019-03-10
Resolution : 2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

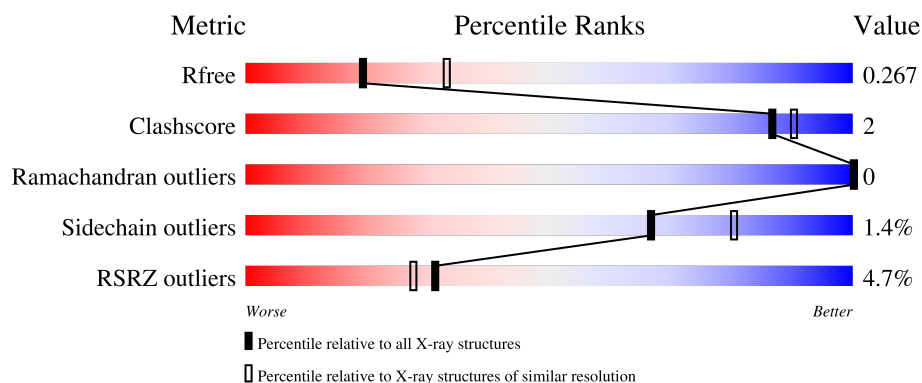
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 $\leq 5\%$. 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	593	<div> <div>8%</div> <div>89% 6% 5%</div> </div>
1	B	593	<div> <div>5%</div> <div>91% 5%</div> </div>
1	C	593	<div> <div>8%</div> <div>87% 7% 6%</div> </div>
2	D	15	<div> <div>73% 27%</div> </div>
2	F	15	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	15	<div> <div></div> <div>7%</div> <div>80%</div> <div>20%</div> </div>
3	E	16	<div> <div></div> <div>6%</div> <div>75%</div> <div>25%</div> </div>
3	G	16	<div> <div></div> <div>6%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
3	I	16	<div> <div></div> <div>75%</div> <div>25%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15645 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 UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4560	2872	816	862	10			
1	B	568	Total	C	N	O	S	0	0	0
			4584	2887	824	863	10			
1	C	560	Total	C	N	O	S	0	0	0
			4518	2847	809	853	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	CYS	SER	conflict	UNP P56981
A	144	SER	CYS	conflict	UNP P56981
A	190	ARG	-	insertion	UNP P56981
A	211	SER	CYS	conflict	UNP P56981
A	233	GLU	LYS	conflict	UNP P56981
A	303	SER	CYS	conflict	UNP P56981
B	91	CYS	SER	conflict	UNP P56981
B	144	SER	CYS	conflict	UNP P56981
B	190	ARG	-	insertion	UNP P56981
B	211	SER	CYS	conflict	UNP P56981
B	233	GLU	LYS	conflict	UNP P56981
B	303	SER	CYS	conflict	UNP P56981
C	91	CYS	SER	conflict	UNP P56981
C	144	SER	CYS	conflict	UNP P56981
C	190	ARG	-	insertion	UNP P56981
C	211	SER	CYS	conflict	UNP P56981
C	233	GLU	LYS	conflict	UNP P56981
C	303	SER	CYS	conflict	UNP P56981

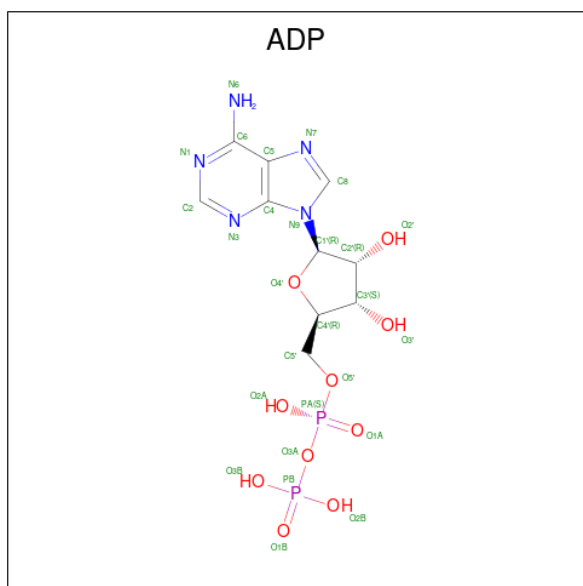
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*TP*CP*CP*AP*TP*CP*GP*CP*GP*CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	15	Total	C	N	O	P	0	0	0
			296	143	49	90	14			
2	F	15	Total	C	N	O	P	0	0	0
			296	143	49	90	14			
2	H	15	Total	C	N	O	P	0	0	0
			296	143	49	90	14			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*GP*TP*AP*GP*CP*GP*CP*GP*AP*TP*GP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	16	Total	C	N	O	P	0	0	0
			335	158	70	92	15			
3	G	15	Total	C	N	O	P	0	0	0
			316	148	65	88	15			
3	I	16	Total	C	N	O	P	0	0	0
			335	158	70	92	15			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

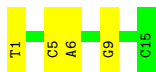
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total	O	0	0
			18	18		
7	B	4	Total	O	0	0
			4	4		
7	C	4	Total	O	0	0
			4	4		

- Molecule 1: UvrABC system protein B





- Molecule 2: DNA (5'-D(*TP*CP*TP*CP*CP*AP*TP*CP*GP*CP*GP*CP*TP*AP*C)-3')



- Molecule 2: DNA (5'-D(*TP*CP*TP*CP*CP*AP*TP*CP*GP*CP*GP*CP*TP*AP*C)-3')

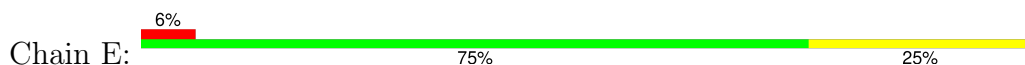


There are no outlier residues recorded for this chain.

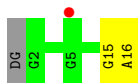
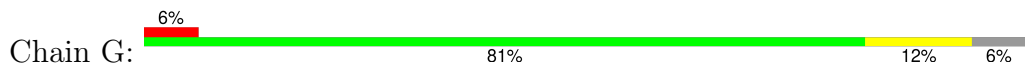
- Molecule 2: DNA (5'-D(*TP*CP*TP*CP*CP*AP*TP*CP*GP*CP*GP*CP*TP*AP*C)-3')



- Molecule 3: DNA (5'-D(*GP*GP*TP*AP*GP*CP*GP*CP*GP*AP*TP*GP*GP*AP*GP*A)-3')

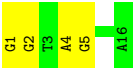


- Molecule 3: DNA (5'-D(*GP*GP*TP*AP*GP*CP*GP*CP*GP*AP*TP*GP*GP*AP*GP*A)-3')



- Molecule 3: DNA (5'-D(*GP*GP*TP*AP*GP*CP*GP*CP*GP*AP*TP*GP*GP*AP*GP*A)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.69Å 201.18Å 62.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.64 48.24 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.24-2.64) 99.2 (48.24-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.220 , 0.274 0.219 , 0.267	Depositor DCC
R_{free} test set	3254 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15645	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, 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	0.34	0/4636	0.57	0/6259
1	B	0.32	0/4659	0.56	0/6290
1	C	0.34	0/4592	0.55	0/6202
2	D	0.33	0/329	0.75	0/504
2	F	0.26	0/329	0.75	0/504
2	H	0.30	0/329	0.75	0/504
3	E	0.33	0/378	0.81	0/584
3	G	0.34	0/356	0.74	0/549
3	I	0.33	0/378	0.71	0/584
All	All	0.33	0/15986	0.59	0/21980

There are no bond length outliers.

There are no bond angle outliers.

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	4560	0	4584	20	0
1	B	4584	0	4631	13	0
1	C	4518	0	4555	24	0
2	D	296	0	171	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	296	0	171	0	0
2	H	296	0	171	4	0
3	E	335	0	180	2	0
3	G	316	0	168	1	0
3	I	335	0	180	2	0
4	A	27	0	12	2	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
5	B	1	0	0	1	0
6	E	1	0	0	0	0
7	A	18	0	0	0	0
7	B	4	0	0	0	0
7	C	4	0	0	0	0
All	All	15645	0	14847	63	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 2.

All (63) 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:C:303:SER:OG	1:C:306:ILE:HB	1.86	0.76
1:C:67:LYS:CG	1:C:90:VAL:HG21	2.28	0.63
1:C:90:VAL:HG22	1:C:91:CYS:N	2.12	0.63
1:C:451:THR:HG22	1:C:529:ARG:HH22	1.65	0.62
1:C:449:LEU:HB3	1:C:505:LEU:HD13	1.80	0.61
1:C:67:LYS:HG2	1:C:90:VAL:HG21	1.82	0.61
3:G:15:DG:H2''	3:G:16:DA:H5'	1.83	0.60
1:C:90:VAL:HG22	1:C:91:CYS:O	2.03	0.58
3:E:4:DA:H4'	3:E:5:DG:OP1	2.03	0.58
1:A:95:TYR:O	1:A:96:TYR:HB2	2.05	0.56
1:B:67:LYS:HD3	1:B:93:TYR:CG	2.42	0.55
1:A:60:THR:HG22	1:A:334:LEU:HB3	1.90	0.54
1:B:475:LEU:HA	1:B:479:ILE:HD12	1.90	0.53
3:I:1:DG:H4'	3:I:2:DG:O5'	2.08	0.53
1:C:162:ARG:HD2	2:D:1:DT:H4'	1.89	0.53
1:C:396:PRO:O	1:C:532:ARG:NH1	2.41	0.52
1:A:503:ASN:HB3	2:D:6:DA:H5'	1.91	0.51
1:A:260:ILE:HG23	1:A:294:LEU:HD22	1.91	0.51
1:B:491:LEU:HD22	1:B:499:LEU:HD22	1.92	0.50
1:A:95:TYR:CD2	1:A:481:THR:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:ILE:HG21	2:H:5:DC:H4'	1.93	0.50
1:B:260:ILE:HG23	1:B:294:LEU:HD22	1.93	0.50
1:A:43:THR:O	4:A:600:ADP:O3B	2.29	0.49
1:C:90:VAL:CG2	1:C:91:CYS:N	2.77	0.48
1:C:88:TYR:CE2	1:C:90:VAL:HG11	2.48	0.48
1:B:156:GLU:OE2	1:B:252:ARG:NH2	2.40	0.48
2:H:11:DG:H2''	2:H:12:DC:C5	2.49	0.48
1:A:87:GLU:HB2	1:A:138:ILE:HG12	1.96	0.48
1:B:341:HIS:CD2	1:B:342:VAL:HG23	2.50	0.47
1:C:411:ILE:HG23	1:C:570:ARG:HG2	1.95	0.47
1:C:289:ARG:NH2	2:H:12:DC:OP1	2.48	0.47
2:H:11:DG:H2''	2:H:12:DC:C6	2.49	0.47
1:B:466:LYS:O	1:B:468:ALA:O	2.33	0.46
1:A:89:PHE:CD2	1:A:325:LEU:HD22	2.50	0.46
1:A:337:VAL:CG2	1:A:389:ILE:HD11	2.46	0.46
1:A:449:LEU:HB3	1:A:505:LEU:HD13	1.98	0.46
1:A:67:LYS:CE	2:D:9:DG:OP2	2.64	0.46
3:I:4:DA:H2''	3:I:5:DG:O5'	2.16	0.46
1:A:491:LEU:HD22	1:A:499:LEU:HD22	1.98	0.45
1:A:543:ARG:NH2	4:A:600:ADP:O1A	2.49	0.45
1:C:475:LEU:HD13	1:C:504:LEU:HD12	1.99	0.45
1:A:62:VAL:HG13	1:A:139:VAL:HA	2.00	0.44
1:A:502:ILE:HG21	2:D:5:DC:H4'	2.00	0.44
1:B:240:HIS:HB2	5:B:602:CL:CL	2.56	0.43
1:B:159:VAL:CG2	1:B:243:ILE:HB	2.49	0.43
1:A:65:HIS:HB3	1:A:343:THR:OG1	2.18	0.43
1:B:130:LEU:HD23	1:B:136:VAL:HG11	2.01	0.43
1:C:92:TYR:HB3	1:C:116:ASN:OD1	2.19	0.42
1:B:92:TYR:HB3	1:B:116:ASN:ND2	2.34	0.42
1:A:58:LYS:O	1:A:60:THR:HG23	2.19	0.42
1:B:64:ALA:HB3	1:B:70:ALA:HB2	2.01	0.41
1:C:65:HIS:HB3	1:C:343:THR:OG1	2.20	0.41
1:C:87:GLU:HB2	1:C:138:ILE:HG12	2.02	0.41
1:A:180:GLN:OE1	1:A:302:PHE:HB3	2.20	0.41
1:A:67:LYS:HA	1:A:70:ALA:HB3	2.01	0.41
1:C:472:VAL:HG12	1:C:473:ALA:N	2.35	0.41
1:B:344:LEU:HB2	1:B:345:PRO:HD3	2.02	0.41
1:C:179:ILE:HA	1:C:250:VAL:HG21	2.02	0.41
1:C:316:ARG:NH2	1:C:321:THR:O	2.51	0.41
3:E:14:DA:H2'	3:E:15:DG:C8	2.56	0.41
1:C:17:GLN:N	1:C:18:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PRO:CB	1:C:258:LEU:HD22	2.51	0.40
1:C:412:ILE:HD12	1:C:412:ILE:N	2.36	0.40

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	560/593 (94%)	538 (96%)	22 (4%)	0	100	100
1	B	564/593 (95%)	540 (96%)	24 (4%)	0	100	100
1	C	554/593 (93%)	533 (96%)	21 (4%)	0	100	100
All	All	1678/1779 (94%)	1611 (96%)	67 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	493/520 (95%)	490 (99%)	3 (1%)	86	93
1	B	497/520 (96%)	491 (99%)	6 (1%)	71	83
1	C	490/520 (94%)	478 (98%)	12 (2%)	49	67
All	All	1480/1560 (95%)	1459 (99%)	21 (1%)	67	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	203	PHE
1	A	333	PHE
1	B	175	ARG
1	B	203	PHE
1	B	208	ASP
1	B	419	ASP
1	B	504	LEU
1	B	505	LEU
1	C	66	ASN
1	C	67	LYS
1	C	69	LEU
1	C	92	TYR
1	C	95	TYR
1	C	121	LYS
1	C	192	THR
1	C	203	PHE
1	C	289	ARG
1	C	350	MET
1	C	467	GLU
1	C	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	B	116	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
4	ADP	B	601	-	24,29,29	0.94	2 (8%)	29,45,45	1.25	2 (6%)
4	ADP	A	600	-	24,29,29	1.06	3 (12%)	29,45,45	1.24	2 (6%)
4	ADP	C	600	-	24,29,29	0.96	2 (8%)	29,45,45	1.34	3 (10%)

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
4	ADP	B	601	-	-	0/12/32/32	0/3/3/3
4	ADP	A	600	-	-	5/12/32/32	0/3/3/3
4	ADP	C	600	-	-	3/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ADP	PA-O3A	2.42	1.62	1.59
4	C	600	ADP	C2-N3	2.39	1.35	1.32
4	A	600	ADP	C2-N3	2.28	1.35	1.32
4	B	601	ADP	O4'-C1'	2.20	1.43	1.40
4	A	600	ADP	O4'-C1'	2.19	1.43	1.40
4	C	600	ADP	O4'-C1'	2.16	1.43	1.40
4	B	601	ADP	C2-N3	2.14	1.35	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	ADP	N3-C2-N1	-4.39	122.72	128.67
4	C	600	ADP	N3-C2-N1	-4.27	122.87	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ADP	N3-C2-N1	-4.27	122.88	128.67
4	C	600	ADP	C4-C5-N7	-2.71	106.47	109.34
4	A	600	ADP	C4-C5-N7	-2.50	106.70	109.34
4	B	601	ADP	C4-C5-N7	-2.42	106.78	109.34
4	C	600	ADP	O4'-C1'-N9	2.16	111.61	108.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

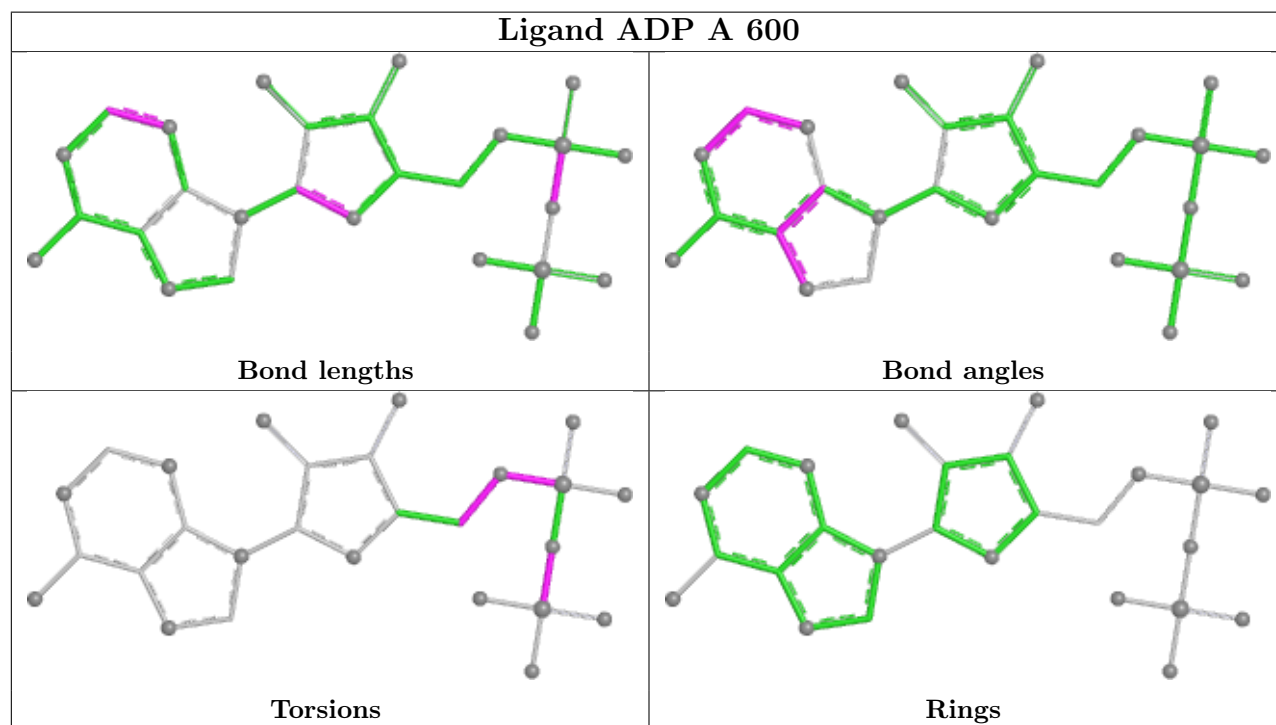
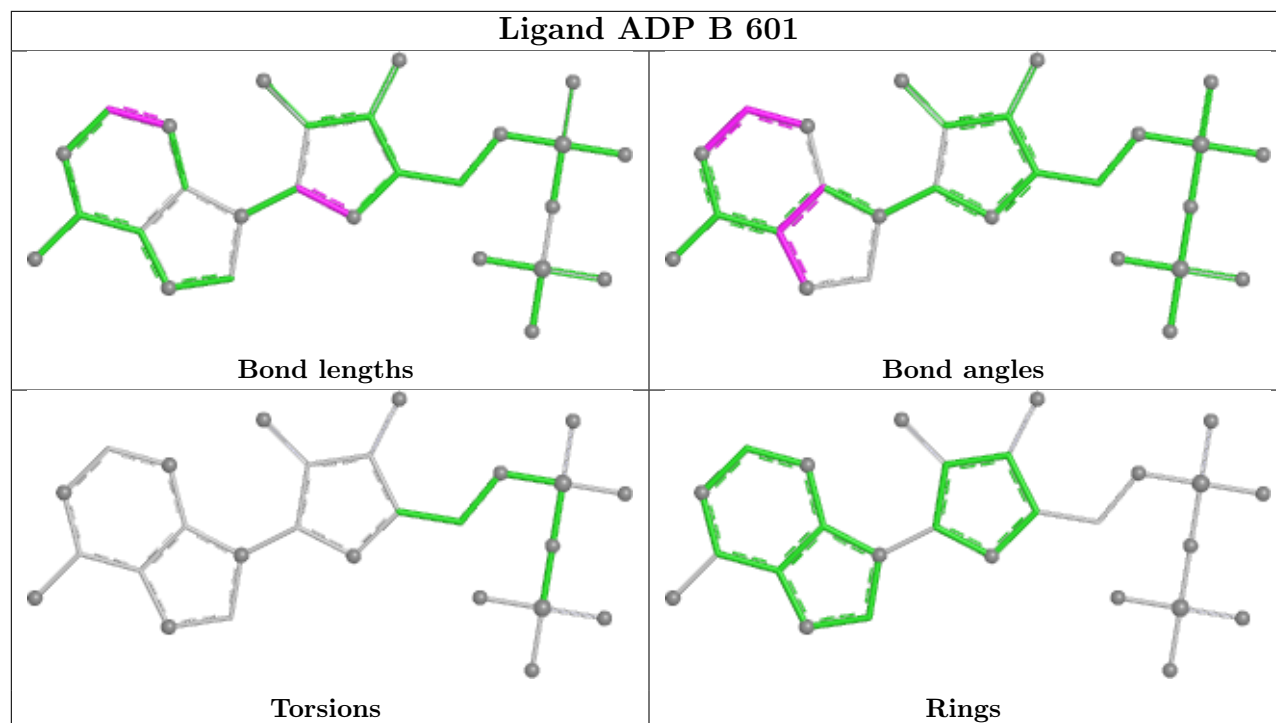
Mol	Chain	Res	Type	Atoms
4	A	600	ADP	C5'-O5'-PA-O1A
4	A	600	ADP	C5'-O5'-PA-O3A
4	C	600	ADP	C5'-O5'-PA-O1A
4	C	600	ADP	C5'-O5'-PA-O2A
4	C	600	ADP	C5'-O5'-PA-O3A
4	A	600	ADP	C5'-O5'-PA-O2A
4	A	600	ADP	C4'-C5'-O5'-PA
4	A	600	ADP	PA-O3A-PB-O3B

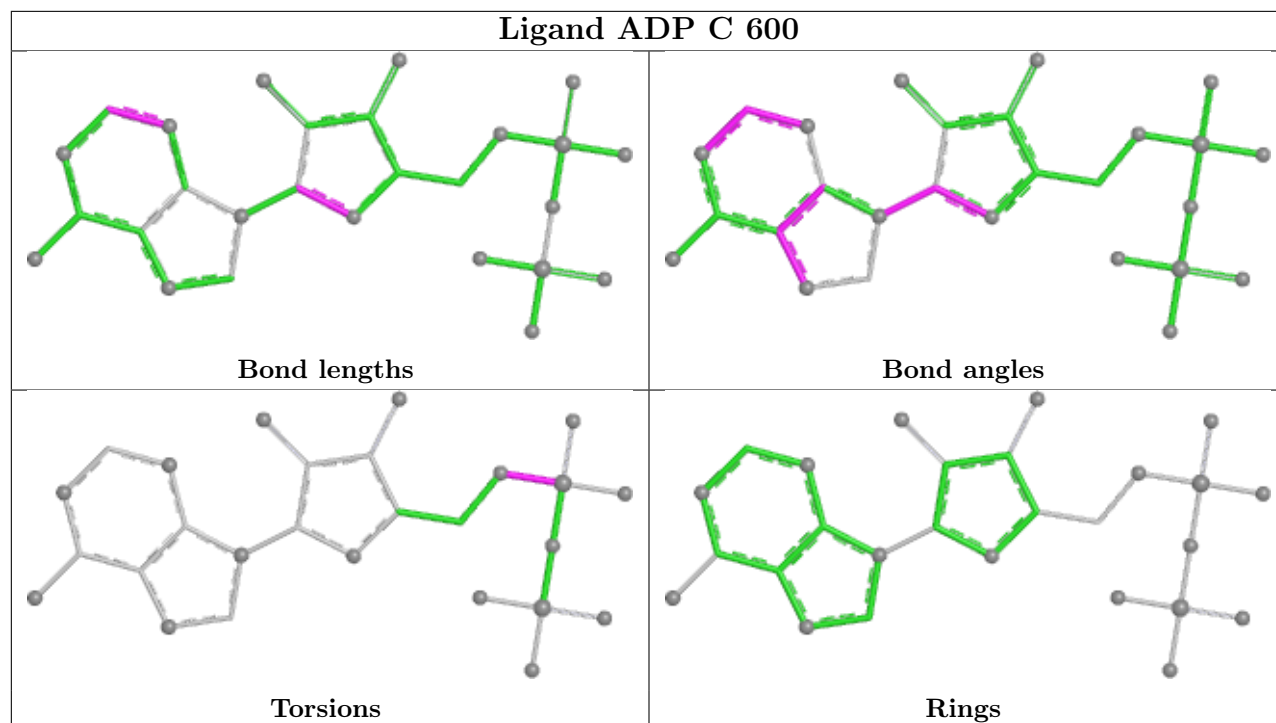
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 ⓘ

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	564/593 (95%)	-0.04	7 (1%) 79 77	37, 57, 86, 129	0
1	B	568/593 (95%)	0.14	28 (4%) 29 25	44, 67, 110, 149	0
1	C	560/593 (94%)	0.32	46 (8%) 11 9	40, 66, 124, 144	0
2	D	15/15 (100%)	-0.55	0 100 100	50, 61, 94, 110	0
2	F	15/15 (100%)	-0.37	0 100 100	57, 78, 119, 125	0
2	H	15/15 (100%)	-0.52	1 (6%) 17 15	57, 70, 97, 128	0
3	E	16/16 (100%)	-0.49	1 (6%) 20 16	52, 68, 98, 108	0
3	G	15/16 (93%)	-0.07	1 (6%) 17 15	53, 70, 125, 136	0
3	I	16/16 (100%)	-0.57	0 100 100	60, 74, 81, 92	0
All	All	1784/1872 (95%)	0.11	84 (4%) 31 27	37, 64, 112, 149	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	LEU	6.0
1	C	219	ASP	5.7
1	B	304	SER	5.6
1	B	282	GLU	4.7
1	C	216	PHE	4.5
1	C	178	ASP	4.4
1	B	277	GLN	4.1
1	C	214	VAL	4.1
1	B	280	LEU	4.0
1	C	95	TYR	3.9
1	C	365	GLY	3.9
1	C	166	GLU	3.9
1	C	232	GLY	3.8
1	B	275	ARG	3.7
1	A	302	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	212	ILE	3.6
1	C	132	GLU	3.6
1	C	224	ILE	3.6
1	C	217	PHE	3.5
1	B	297	MET	3.4
1	B	290	THR	3.4
1	B	489	ARG	3.4
1	C	213	ARG	3.4
1	B	482	LEU	3.3
1	C	585	PRO	3.3
1	C	195	VAL	3.3
1	B	256	MET	3.1
1	B	230	LEU	3.1
1	B	270	ARG	3.0
1	B	209	GLU	3.0
1	C	92	TYR	2.9
1	B	291	ARG	2.9
1	C	167	ILE	2.9
1	C	165	MET	2.9
1	C	173	LEU	2.8
1	C	482	LEU	2.8
1	C	170	ASN	2.8
1	B	363	ASP	2.8
1	B	286	LEU	2.7
1	C	169	ARG	2.7
1	C	220	GLU	2.7
1	C	218	GLY	2.6
1	C	199	VAL	2.6
1	C	209	GLU	2.6
1	B	443	GLU	2.6
1	B	365	GLY	2.5
1	C	210	HIS	2.5
1	C	202	ILE	2.5
1	C	221	ILE	2.5
1	B	305	GLY	2.5
1	B	362	VAL	2.5
3	E	1	DG	2.4
1	C	162	ARG	2.4
1	C	229	ALA	2.4
3	G	5	DG	2.4
1	C	215	GLU	2.3
1	B	233	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	92	TYR	2.2
1	C	223	ARG	2.2
1	C	193	PHE	2.2
1	C	200	VAL	2.2
2	H	1	DT	2.2
1	B	268	GLU	2.2
1	C	235	LEU	2.2
1	A	115	ILE	2.2
1	B	93	TYR	2.1
1	A	507	GLU	2.1
1	B	295	GLU	2.1
1	B	284	GLN	2.1
1	C	287	GLU	2.1
1	C	181	TYR	2.1
1	B	481	THR	2.1
1	C	222	GLU	2.1
1	B	366	PHE	2.1
1	A	239	GLU	2.0
1	B	293	ASP	2.0
1	C	354	ASP	2.0
1	C	284	GLN	2.0
1	A	531	GLU	2.0
1	C	198	ASP	2.0
1	C	172	LEU	2.0
1	C	234	VAL	2.0
1	C	496	TYR	2.0
1	A	235	LEU	2.0

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,

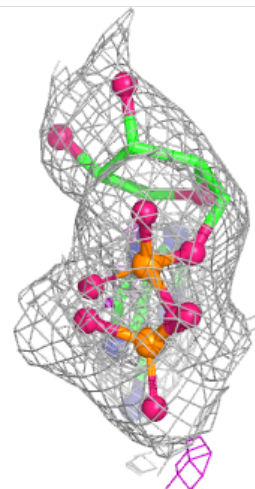
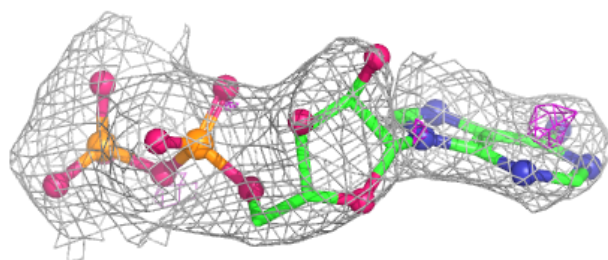
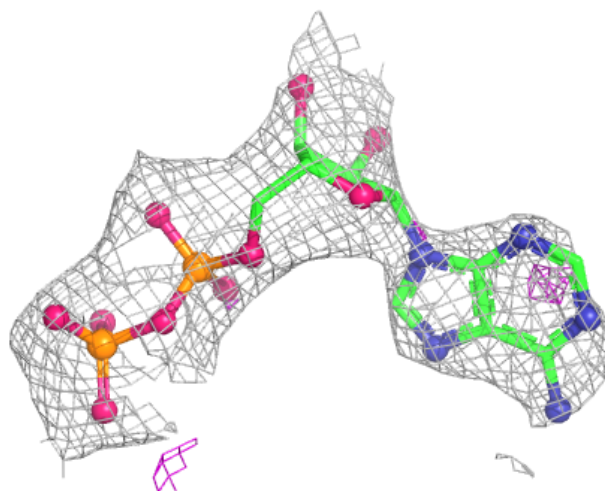
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	E	700	1/1	0.81	0.26	59,59,59,59	0
4	ADP	A	600	27/27	0.87	0.20	78,93,105,109	0
5	CL	B	602	1/1	0.88	0.14	100,100,100,100	0
4	ADP	C	600	27/27	0.89	0.19	73,85,96,98	0
4	ADP	B	601	27/27	0.92	0.15	82,86,91,94	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.

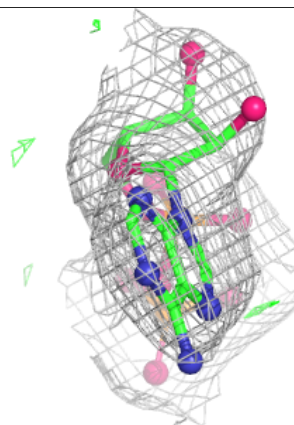
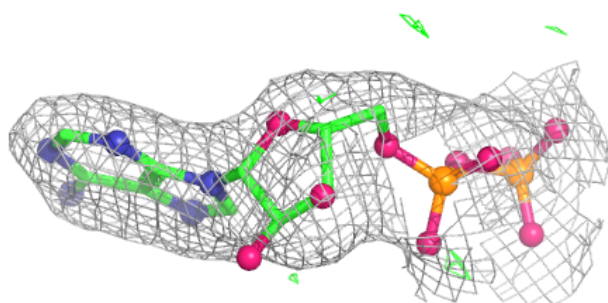
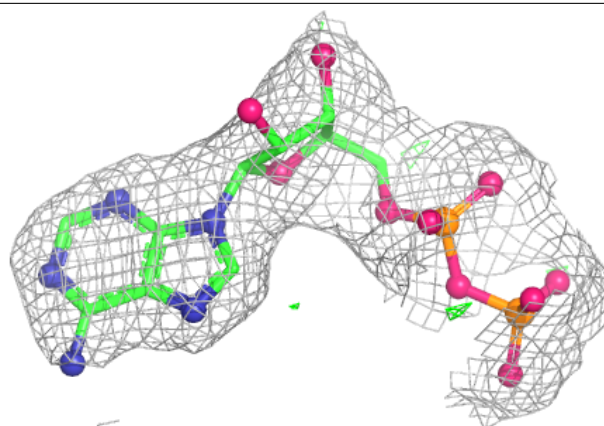
Electron density around ADP A 600:

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

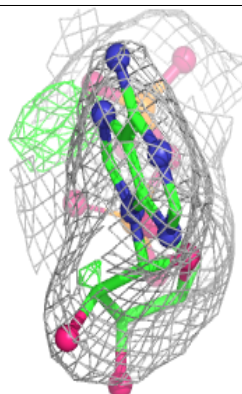
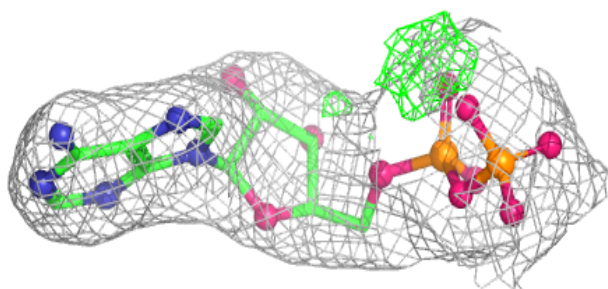
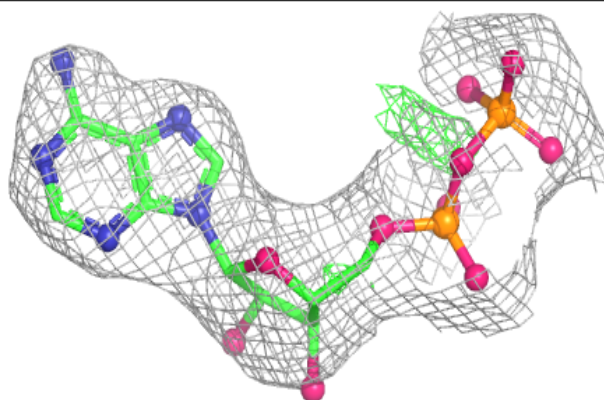


Electron density around ADP C 600:

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

**Electron density around ADP B 601:**

$2mF_o-DF_c$ (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.