



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:50 pm BST

PDB ID : 6D3K
Title : Crystal structure of unphosphorylated human PKR kinase domain in complex with ADP
Authors : Erlandsen, H.; Mayo, C.B.; Robinson, V.L.; Cole, J.L.
Deposited on : 2018-04-16
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) 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

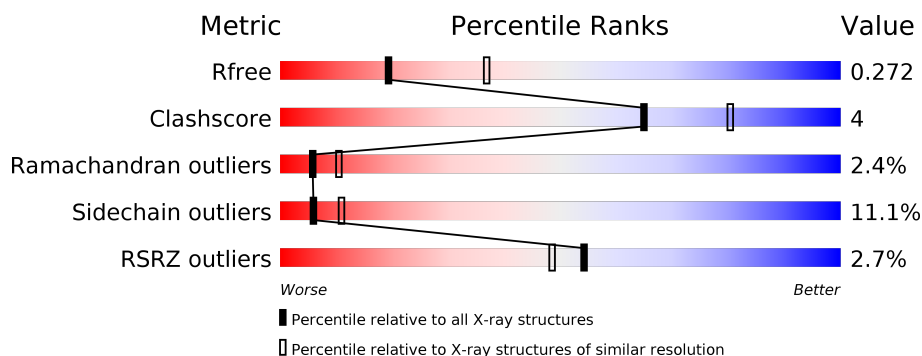
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	323	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 11%, yellow 11%, yellow 66%, green 66%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 66% 11% • 20% </div> </div>
1	B	323	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 12%, yellow 12%, yellow 63%, green 63%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 63% 12% • 21% </div> </div>
1	C	323	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 14%, yellow 14%, yellow 64%, green 64%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 64% 14% • 20% </div> </div>

2 Entry composition [i](#)

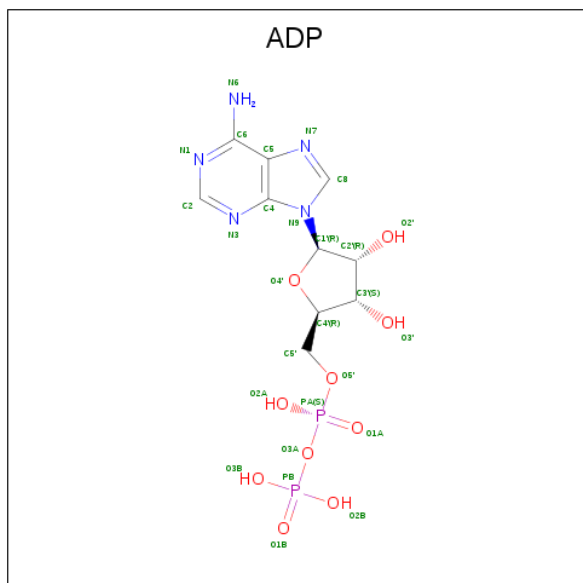
There are 6 unique types of molecules in this entry. The entry contains 6485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	254	Total	C	N	O	S	0	0	0
			2080	1338	352	383	7			
1	A	258	Total	C	N	O	S	0	0	0
			2107	1355	356	389	7			
1	C	258	Total	C	N	O	S	0	0	0
			2107	1353	358	389	7			

- 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	B	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		

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

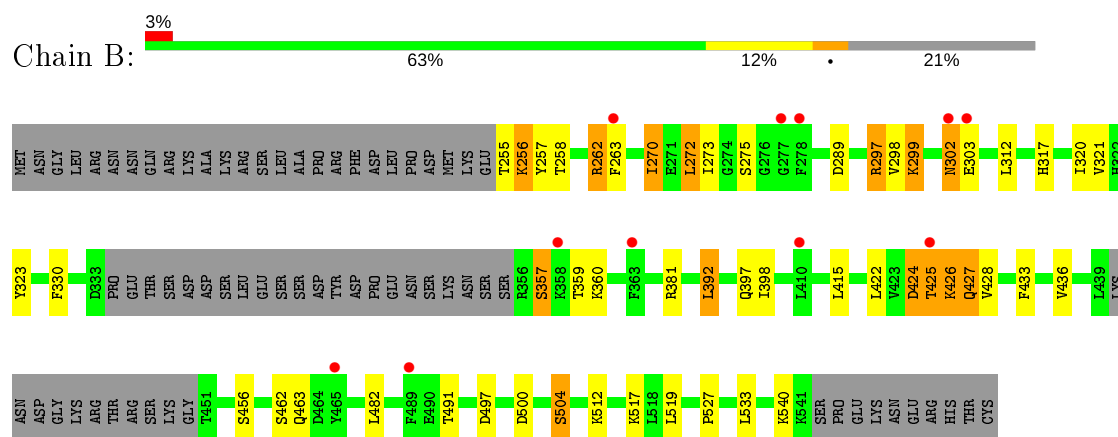
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	15	Total	O	0	0
			15	15		
6	A	21	Total	O	0	0
			21	21		
6	C	16	Total	O	0	0
			16	16		

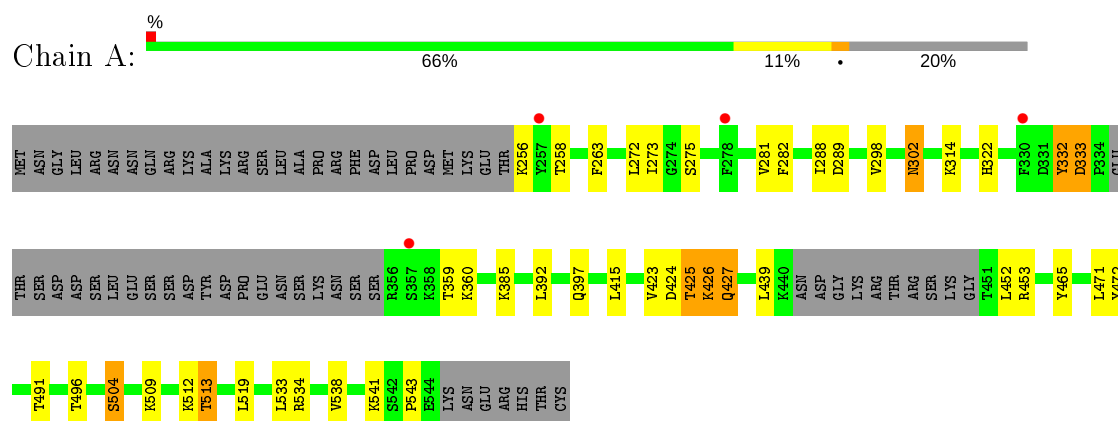
3 Residue-property plots [i](#)

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 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.

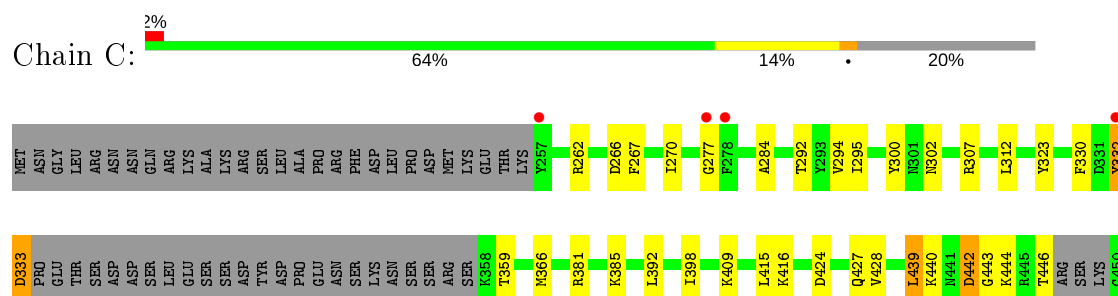
- Molecule 1: Interferon-induced, double-stranded RNA-activated protein kinase



- Molecule 1: Interferon-induced, double-stranded RNA-activated protein kinase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.48 Å 159.60 Å 172.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	172.99 – 2.60 88.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (172.99-2.60) 97.2 (88.58-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.62 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.209 , 0.266 0.216 , 0.272	Depositor DCC
R_{free} test set	2245 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6485	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: MG, PO4, ADP, SO4

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	0.67	0/2145	0.87	1/2875 (0.0%)
1	B	0.62	0/2116	0.85	1/2834 (0.0%)
1	C	0.69	0/2143	0.89	0/2869
All	All	0.66	0/6404	0.87	2/8578 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	297	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	332	TYR	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	ASP	Peptide
1	B	357	SER	Peptide

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	2107	0	2149	12	0
1	B	2080	0	2129	18	0
1	C	2107	0	2153	24	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
5	C	15	0	0	0	0
6	A	21	0	0	1	0
6	B	15	0	0	0	0
6	C	16	0	0	0	0
All	All	6485	0	6467	53	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 4.

All (53) 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:307:ARG:CZ	1:C:442:ASP:OD1	1.66	1.41
1:C:307:ARG:NE	1:C:442:ASP:OD1	1.92	1.02
1:C:439:LEU:HD12	1:C:439:LEU:H	1.36	0.89
1:C:307:ARG:NH2	1:C:442:ASP:OD1	2.15	0.80
1:B:397:GLN:HE22	1:B:427:GLN:HA	1.49	0.77
1:C:439:LEU:HD12	1:C:439:LEU:N	2.07	0.70
1:B:302:ASN:HD22	1:B:302:ASN:C	2.00	0.65
1:A:322:HIS:HB3	6:A:705:HOH:O	2.01	0.60
1:A:273:ILE:HG22	1:A:281:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:LYS:O	1:C:439:LEU:HD11	2.01	0.59
1:C:307:ARG:NH1	1:C:442:ASP:OD1	2.31	0.59
1:A:424:ASP:O	1:A:426:LYS:N	2.36	0.59
1:B:398:ILE:HG13	1:B:428:VAL:HG21	1.86	0.57
1:A:397:GLN:HE22	1:A:427:GLN:HA	1.69	0.56
1:B:392:LEU:HD13	1:B:482:LEU:HD21	1.89	0.54
1:B:517:LYS:HB3	1:B:527:PRO:HD3	1.88	0.54
1:B:381:ARG:HG2	1:B:381:ARG:O	2.08	0.53
2:C:601:ADP:O1A	2:C:601:ADP:O2B	2.26	0.53
1:C:409:LYS:C	1:C:439:LEU:HD11	2.30	0.52
1:C:504:SER:OG	1:C:506:ILE:HG22	2.10	0.51
1:B:258:THR:HG22	1:B:297:ARG:NH1	2.25	0.51
1:A:509:LYS:O	1:A:513:THR:HG22	2.10	0.51
1:B:392:LEU:CD1	1:B:482:LEU:HD21	2.42	0.49
1:B:312:LEU:HB3	1:B:323:TYR:HB2	1.95	0.48
1:C:440:LYS:HB2	1:C:440:LYS:HE3	1.57	0.47
1:B:359:THR:HG22	1:B:360:LYS:N	2.29	0.47
1:C:442:ASP:HB3	1:C:443:GLY:H	1.66	0.46
1:C:468:GLU:HA	1:C:471:LEU:HD22	1.98	0.46
1:A:534:ARG:O	1:A:538:VAL:HG23	2.16	0.46
1:C:398:ILE:HG13	1:C:428:VAL:HG21	1.98	0.46
1:B:456:SER:HA	1:A:472:TYR:CD2	2.50	0.45
1:C:295:ILE:HD12	1:C:295:ILE:N	2.31	0.45
1:C:332:TYR:O	1:C:333:ASP:HB2	2.17	0.45
1:B:299:LYS:HE3	1:B:359:THR:HG21	1.98	0.45
1:C:509:LYS:O	1:C:513:THR:HG23	2.16	0.44
1:A:424:ASP:C	1:A:426:LYS:N	2.71	0.44
1:A:359:THR:HG22	1:A:360:LYS:N	2.33	0.43
1:B:263:PHE:CE1	1:B:270:ILE:HD13	2.53	0.43
1:B:424:ASP:O	1:B:426:LYS:N	2.52	0.43
1:B:262:ARG:NH2	1:C:266:ASP:OD2	2.52	0.42
1:C:294:VAL:C	1:C:295:ILE:HD12	2.39	0.42
1:B:317:HIS:HB3	1:B:320:ILE:HD12	2.02	0.42
1:C:312:LEU:HB3	1:C:323:TYR:HB2	2.02	0.42
1:A:272:LEU:HD12	1:A:282:PHE:CE1	2.55	0.41
1:A:423:VAL:HG22	1:A:427:GLN:HB3	2.01	0.41
1:B:433:PHE:O	1:B:436:VAL:HG12	2.21	0.41
1:C:366:MET:HE2	2:C:601:ADP:HN61	1.86	0.41
1:C:267:PHE:HB3	1:C:284:ALA:HB1	2.03	0.41
1:C:455:MET:O	1:C:499:ARG:NH2	2.50	0.41
1:C:453:ARG:HG2	1:C:495:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ALA:O	1:C:292:THR:HA	2.22	0.40
1:B:255:THR:HB	1:B:256:LYS:HG3	2.03	0.40
1:A:302:ASN:C	1:A:302:ASN:HD22	2.23	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	252/323 (78%)	227 (90%)	18 (7%)	7 (3%)	5	7
1	B	248/323 (77%)	222 (90%)	18 (7%)	8 (3%)	4	6
1	C	252/323 (78%)	231 (92%)	18 (7%)	3 (1%)	13	27
All	All	752/969 (78%)	680 (90%)	54 (7%)	18 (2%)	6	10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	ILE
1	B	303	GLU
1	B	425	THR
1	B	426	LYS
1	A	333	ASP
1	A	425	THR
1	A	426	LYS
1	A	439	LEU
1	B	462	SER
1	B	504	SER
1	C	444	LYS
1	B	272	LEU
1	B	540	LYS
1	A	543	PRO

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Mol	Chain	Res	Type
1	C	277	GLY
1	A	332	TYR
1	A	504	SER
1	C	270	ILE

5.3.2 Protein sidechains ⓘ

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	233/294 (79%)	207 (89%)	26 (11%)	6	10
1	B	230/294 (78%)	203 (88%)	27 (12%)	5	10
1	C	232/294 (79%)	208 (90%)	24 (10%)	7	13
All	All	695/882 (79%)	618 (89%)	77 (11%)	6	11

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	256	LYS
1	B	257	TYR
1	B	262	ARG
1	B	270	ILE
1	B	272	LEU
1	B	275	SER
1	B	289	ASP
1	B	298	VAL
1	B	299	LYS
1	B	302	ASN
1	B	321	VAL
1	B	330	PHE
1	B	357	SER
1	B	392	LEU
1	B	415	LEU
1	B	422	LEU
1	B	424	ASP
1	B	425	THR

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Mol	Chain	Res	Type
1	B	427	GLN
1	B	463	GLN
1	B	491	THR
1	B	497	ASP
1	B	500	ASP
1	B	504	SER
1	B	512	LYS
1	B	519	LEU
1	B	533	LEU
1	A	256	LYS
1	A	258	THR
1	A	263	PHE
1	A	275	SER
1	A	288	ILE
1	A	289	ASP
1	A	298	VAL
1	A	302	ASN
1	A	314	LYS
1	A	385	LYS
1	A	392	LEU
1	A	415	LEU
1	A	425	THR
1	A	427	GLN
1	A	452	LEU
1	A	453	ARG
1	A	465	TYR
1	A	471	LEU
1	A	491	THR
1	A	496	THR
1	A	504	SER
1	A	512	LYS
1	A	513	THR
1	A	519	LEU
1	A	533	LEU
1	A	541	LYS
1	C	262	ARG
1	C	300	TYR
1	C	302	ASN
1	C	330	PHE
1	C	332	TYR
1	C	333	ASP
1	C	359	THR

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Mol	Chain	Res	Type
1	C	381	ARG
1	C	385	LYS
1	C	392	LEU
1	C	415	LEU
1	C	416	LYS
1	C	424	ASP
1	C	427	GLN
1	C	439	LEU
1	C	442	ASP
1	C	446	THR
1	C	452	LEU
1	C	457	PRO
1	C	471	LEU
1	C	500	ASP
1	C	512	LYS
1	C	519	LEU
1	C	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	302	ASN
1	B	319	ASN
1	B	397	GLN
1	B	427	GLN
1	B	483	HIS
1	B	516	GLN
1	A	302	ASN
1	A	319	ASN
1	A	376	GLN
1	A	397	GLN
1	A	412	HIS
1	A	516	GLN
1	C	302	ASN
1	C	376	GLN
1	C	412	HIS
1	C	516	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\# Z > 2$
5	SO4	A	606	-	4,4,4	0.47	0	6,6,6	0.34	0
5	SO4	C	604	-	4,4,4	0.47	0	6,6,6	0.63	0
2	ADP	B	601	4	24,29,29	0.90	2 (8%)	29,45,45	1.85	11 (37%)
3	PO4	C	607	-	4,4,4	0.91	0	6,6,6	1.44	1 (16%)
5	SO4	B	604	-	4,4,4	0.40	0	6,6,6	0.32	0
5	SO4	A	604	-	4,4,4	0.34	0	6,6,6	1.15	0
3	PO4	A	602	-	4,4,4	0.77	0	6,6,6	1.04	0
2	ADP	C	601	4	24,29,29	1.07	2 (8%)	29,45,45	1.68	8 (27%)
3	PO4	C	602	-	4,4,4	1.36	0	6,6,6	1.04	0
2	ADP	A	601	4	24,29,29	0.91	1 (4%)	29,45,45	1.62	7 (24%)
5	SO4	C	605	-	4,4,4	0.51	0	6,6,6	0.50	0
5	SO4	C	606	-	4,4,4	0.37	0	6,6,6	0.40	0
5	SO4	A	605	-	4,4,4	0.39	0	6,6,6	0.32	0
3	PO4	B	602	-	4,4,4	0.65	0	6,6,6	0.79	0

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	C	601	4	-	2/12/32/32	0/3/3/3
2	ADP	A	601	4	-	3/12/32/32	0/3/3/3
2	ADP	B	601	4	-	8/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ADP	C5-C4	2.46	1.47	1.40
2	B	601	ADP	C5-C4	2.20	1.46	1.40
2	C	601	ADP	C5-C4	2.20	1.46	1.40
2	C	601	ADP	C2-N3	2.19	1.35	1.32
2	B	601	ADP	C5-N7	-2.00	1.32	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ADP	N3-C2-N1	-3.55	123.13	128.68
2	A	601	ADP	O2B-PB-O1B	3.52	124.48	110.68
2	C	601	ADP	PA-O3A-PB	-3.45	120.97	132.83
2	B	601	ADP	C3'-C2'-C1'	3.30	105.95	100.98
2	B	601	ADP	N3-C2-N1	-3.28	123.56	128.68
2	B	601	ADP	O2B-PB-O3A	-3.18	93.98	104.64
2	A	601	ADP	N3-C2-N1	-3.11	123.81	128.68
2	C	601	ADP	C3'-C2'-C1'	3.04	105.56	100.98
2	C	601	ADP	C1'-N9-C4	-2.91	121.54	126.64
2	C	601	ADP	O2A-PA-O1A	2.64	125.27	112.24
2	B	601	ADP	O2B-PB-O1B	2.63	120.97	110.68
2	B	601	ADP	O4'-C4'-C3'	2.63	110.31	105.11
2	B	601	ADP	N6-C6-N1	2.48	123.72	118.57
2	B	601	ADP	O5'-C5'-C4'	2.46	117.47	108.99
2	B	601	ADP	O3B-PB-O3A	2.45	112.84	104.64
2	C	601	ADP	O3B-PB-O2B	2.37	116.70	107.64
2	A	601	ADP	O2B-PB-O3A	-2.37	96.69	104.64
2	B	601	ADP	C2-N1-C6	2.36	122.78	118.75
2	B	601	ADP	PA-O5'-C5'	-2.32	108.05	121.68
3	C	607	PO4	O3-P-O2	2.31	115.38	107.97
2	A	601	ADP	C1'-N9-C4	-2.30	122.59	126.64
2	A	601	ADP	C2-N1-C6	2.27	122.64	118.75
2	B	601	ADP	O3B-PB-O2B	2.27	116.31	107.64
2	A	601	ADP	O3A-PB-O1B	-2.15	99.25	111.19
2	C	601	ADP	C4-C5-N7	-2.14	107.17	109.40
2	A	601	ADP	N6-C6-N1	2.14	123.02	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	ADP	O5'-PA-O1A	-2.09	100.90	109.07

There are no chirality outliers.

All (13) torsion outliers are listed below:

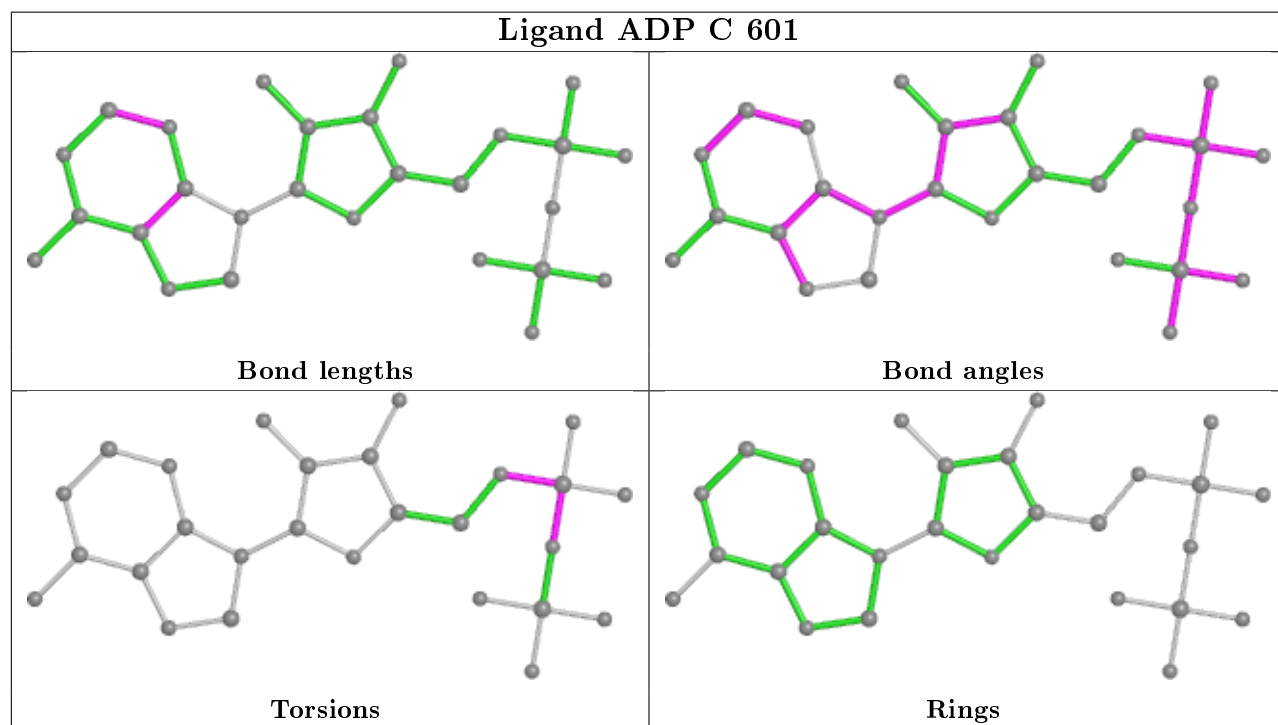
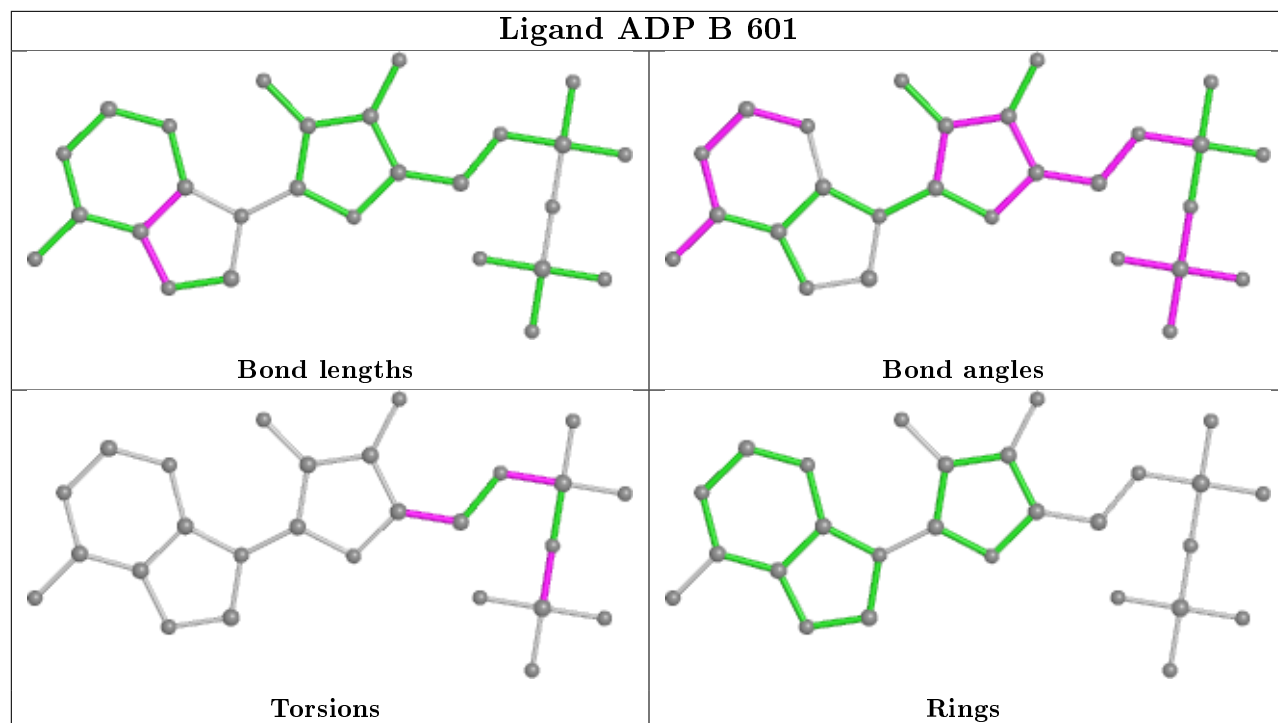
Mol	Chain	Res	Type	Atoms
2	B	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	C5'-O5'-PA-O1A
2	B	601	ADP	C5'-O5'-PA-O2A
2	B	601	ADP	O4'-C4'-C5'-O5'
2	A	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	PA-O3A-PB-O1B
2	B	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	C5'-O5'-PA-O3A
2	C	601	ADP	PB-O3A-PA-O2A
2	C	601	ADP	C5'-O5'-PA-O1A
2	A	601	ADP	PA-O3A-PB-O1B

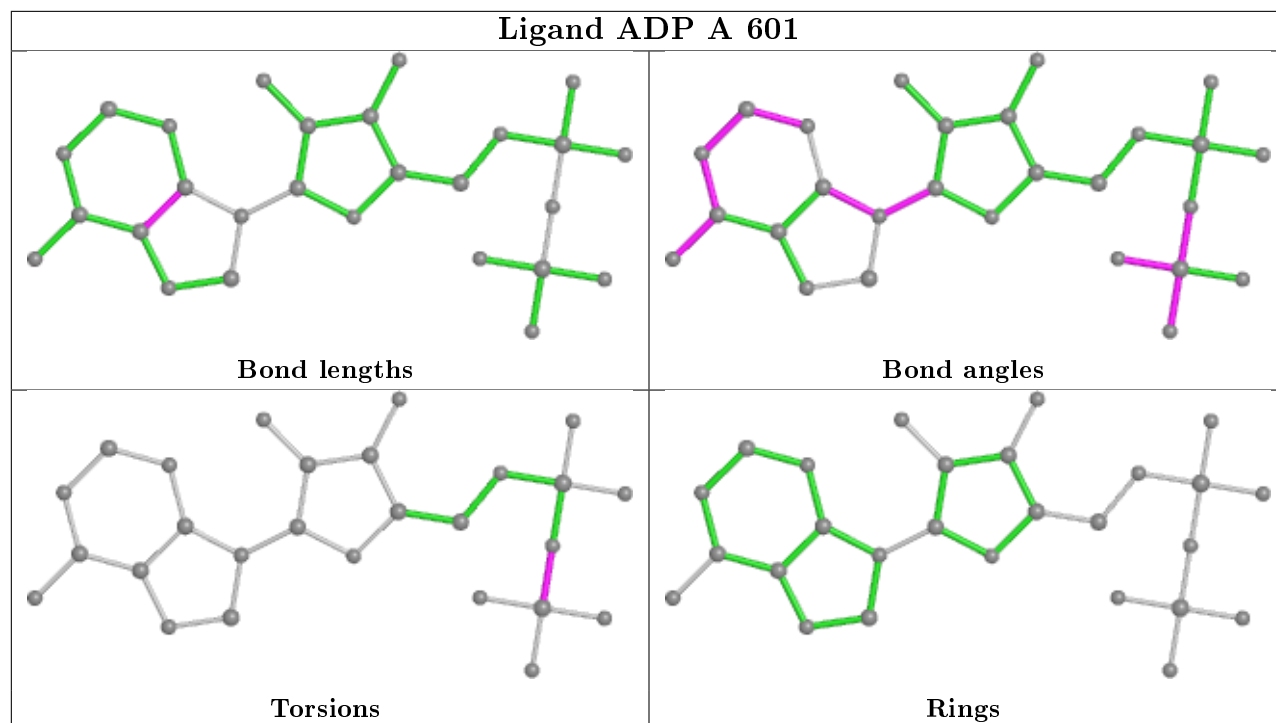
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	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	258/323 (79%)	0.32	4 (1%) 72 68	48, 76, 130, 152	0
1	B	254/323 (78%)	0.41	11 (4%) 35 28	59, 88, 138, 171	0
1	C	258/323 (79%)	0.37	6 (2%) 60 54	54, 79, 129, 162	0
All	All	770/969 (79%)	0.37	21 (2%) 54 48	48, 82, 130, 171	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	LYS	4.2
1	A	278	PHE	3.4
1	A	357	SER	3.2
1	C	257	TYR	3.1
1	B	303	GLU	3.1
1	C	332	TYR	3.1
1	B	278	PHE	3.0
1	C	278	PHE	2.9
1	A	330	PHE	2.7
1	B	263	PHE	2.6
1	A	257	TYR	2.5
1	C	489	PHE	2.5
1	B	363	PHE	2.4
1	B	410	LEU	2.2
1	B	277	GLY	2.2
1	B	465	TYR	2.1
1	C	277	GLY	2.1
1	B	302	ASN	2.1
1	C	452	LEU	2.1
1	B	489	PHE	2.1
1	B	425	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

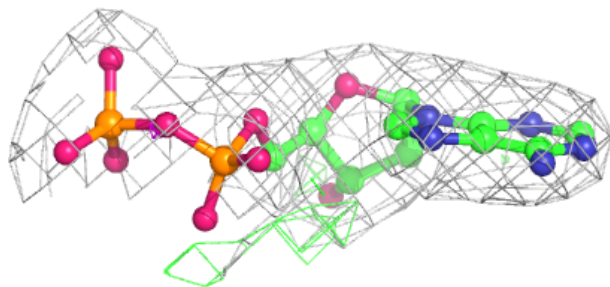
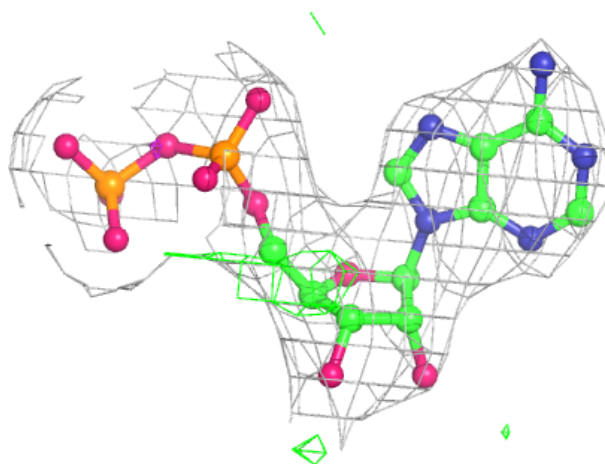
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	C	606	5/5	0.87	0.17	114,129,145,164	0
3	PO4	A	602	5/5	0.88	0.12	104,118,123,131	0
5	SO4	A	605	5/5	0.91	0.14	108,117,144,144	0
3	PO4	B	602	5/5	0.91	0.13	97,124,136,148	0
5	SO4	B	604	5/5	0.92	0.12	120,125,135,146	0
3	PO4	C	602	5/5	0.94	0.20	66,88,105,108	0
4	MG	B	603	1/1	0.94	0.17	66,66,66,66	0
5	SO4	A	606	5/5	0.94	0.12	112,112,127,135	0
3	PO4	C	607	5/5	0.95	0.22	89,105,110,112	0
5	SO4	C	605	5/5	0.95	0.11	117,118,126,132	0
2	ADP	B	601	27/27	0.96	0.17	63,81,92,105	0
5	SO4	C	604	5/5	0.97	0.14	74,79,83,87	0
5	SO4	A	604	5/5	0.97	0.14	65,84,85,91	0
2	ADP	A	601	27/27	0.97	0.19	59,70,83,92	0
2	ADP	C	601	27/27	0.98	0.18	63,73,83,90	0
4	MG	C	603	1/1	0.98	0.13	65,65,65,65	0
4	MG	A	603	1/1	0.99	0.10	72,72,72,72	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.

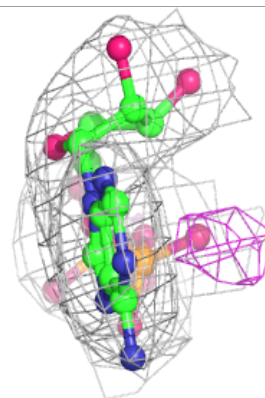
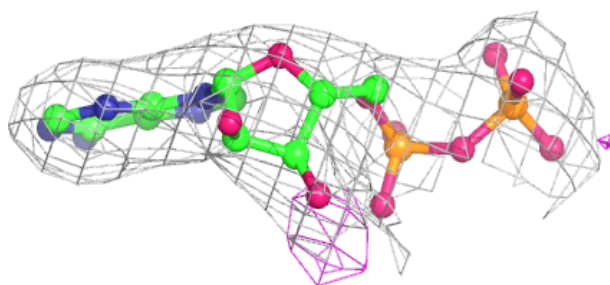
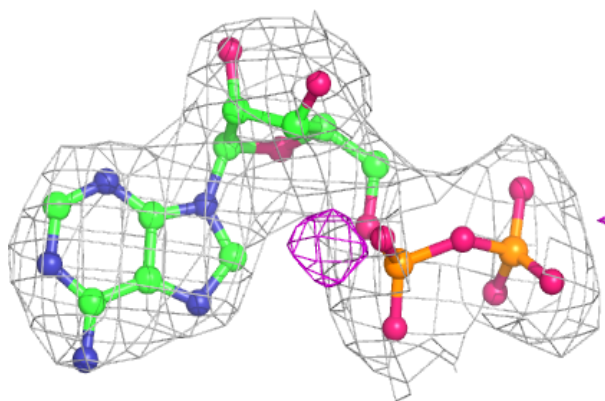
Electron density around ADP B 601:

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

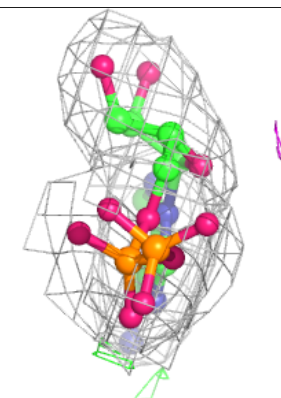
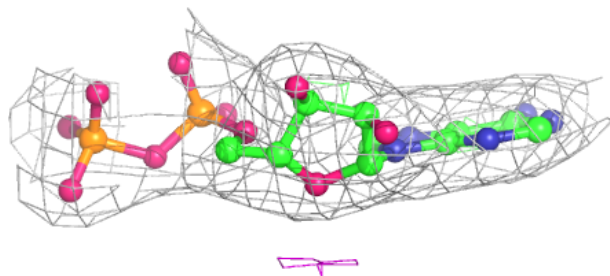
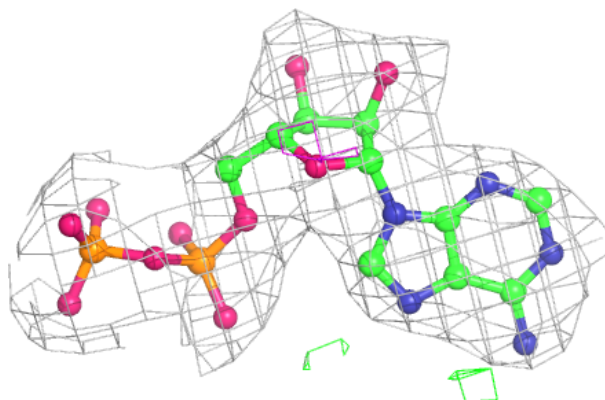


Electron density around ADP A 601:

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

**Electron density around ADP C 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.