



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 12:24 PM EST

PDB ID : 4P69
Title : Acek (D477A) ICDH complex
Authors : Jimin, Z.; Nan, W.; Shu, W.; Zongchao, J.
Deposited on : 2014-03-22
Resolution : 3.30 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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

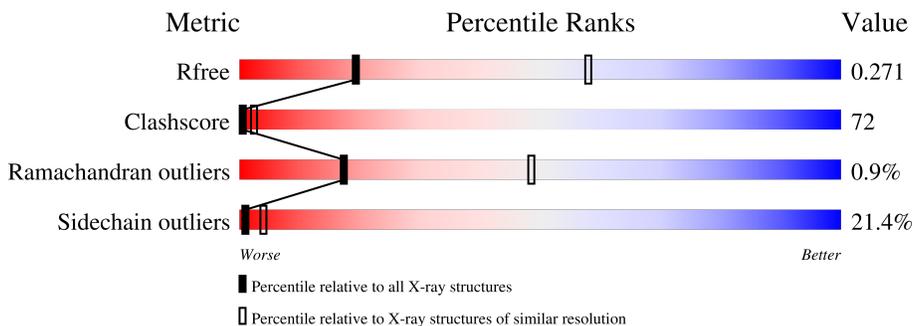
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	568	
1	B	568	
2	C	415	
2	D	415	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15755 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	Total	C	N	O	S	0	0	0
			4575	2946	799	809	21			
1	B	561	Total	C	N	O	S	0	0	0
			4649	2992	815	821	21			

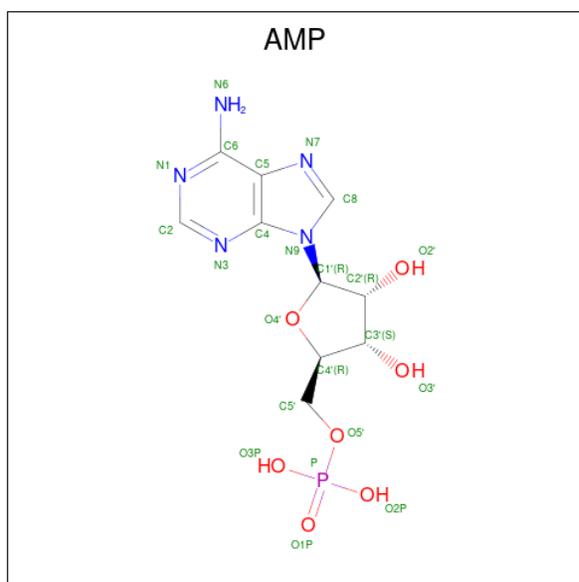
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ALA	ASP	engineered mutation	UNP Q8X607
B	477	ALA	ASP	engineered mutation	UNP Q8X607

- Molecule 2 is a protein called Isocitrate dehydrogenase [NADP].

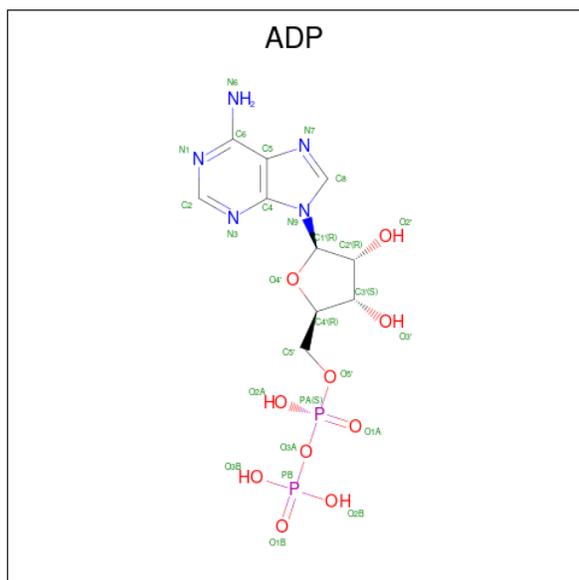
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			
2	D	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

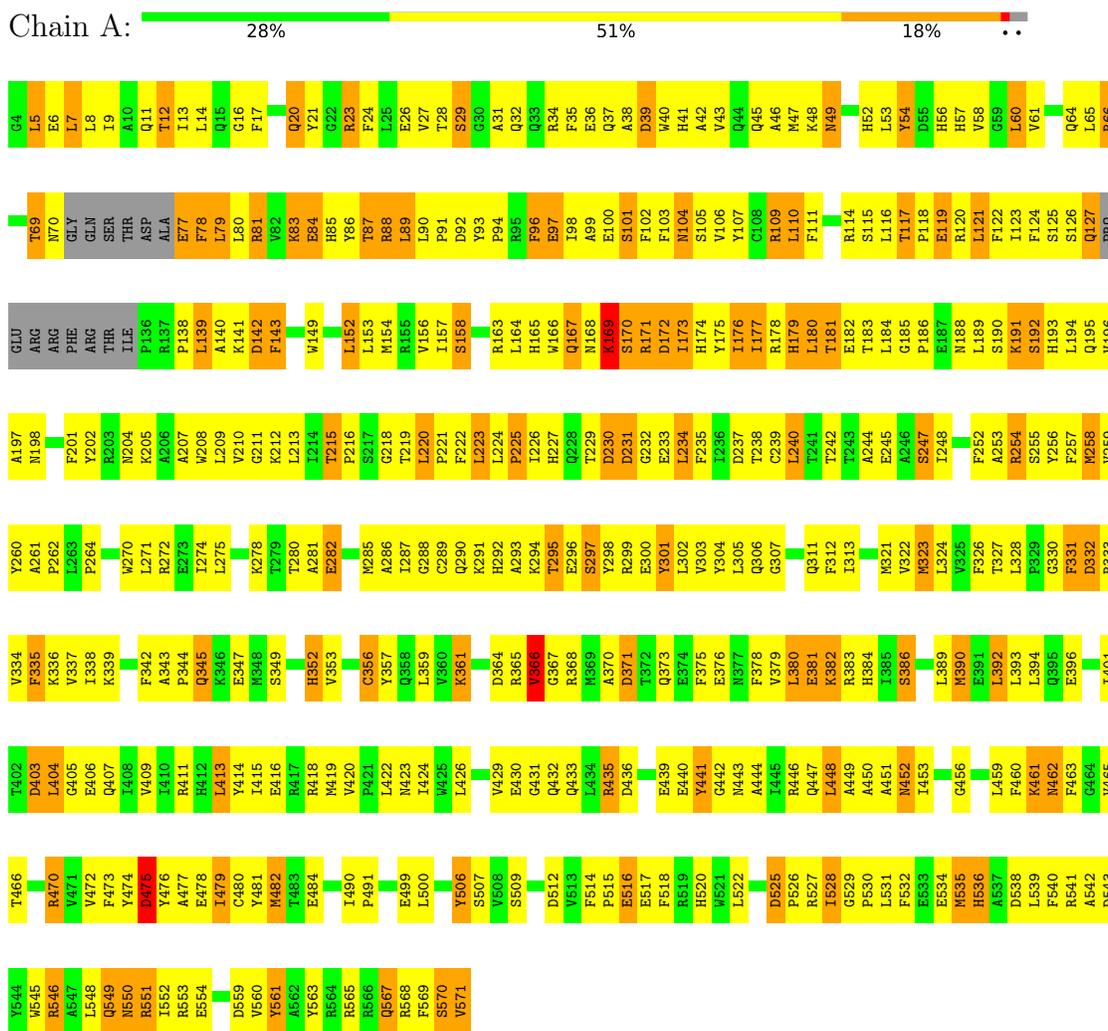
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	4	Total 4	O 4	0	0
5	C	7	Total 7	O 7	0	0
5	D	7	Total 7	O 7	0	0

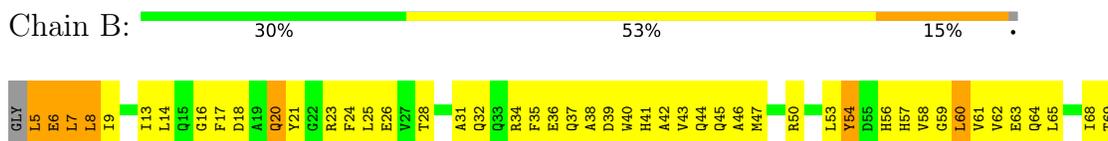
3 Residue-property plots

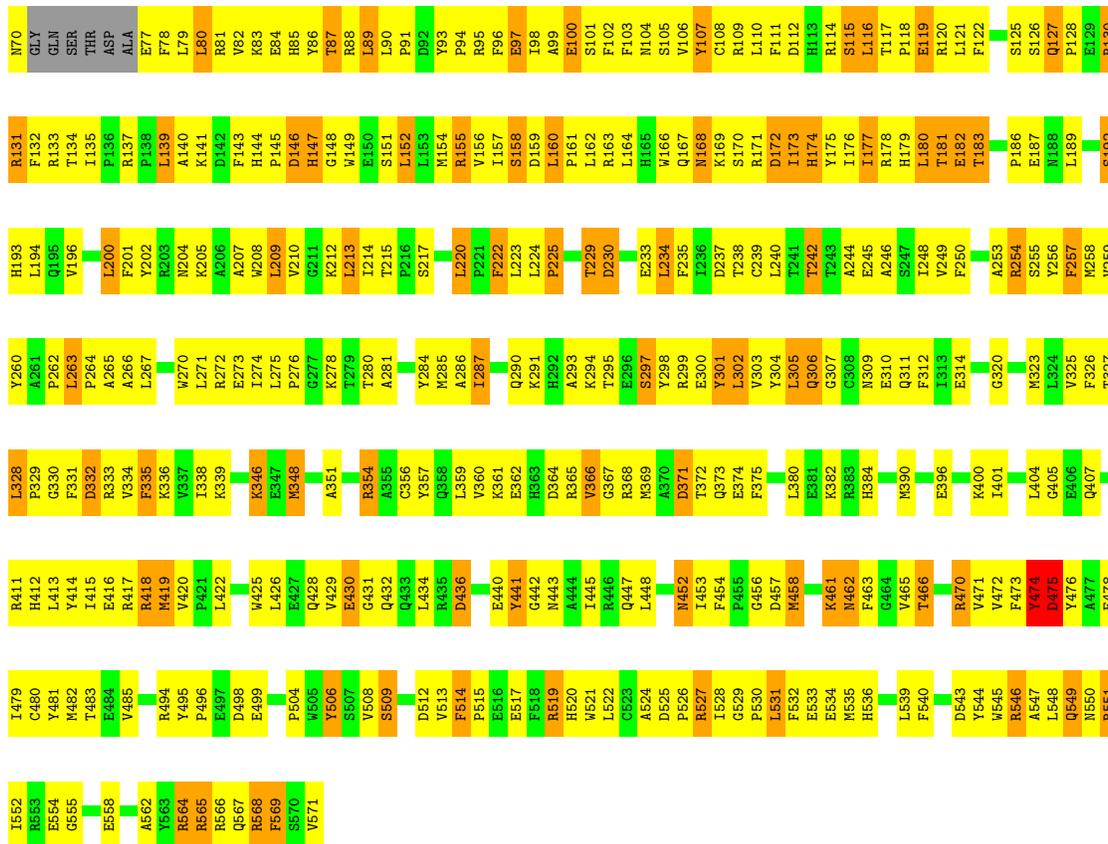
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Isocitrate dehydrogenase kinase/phosphatase

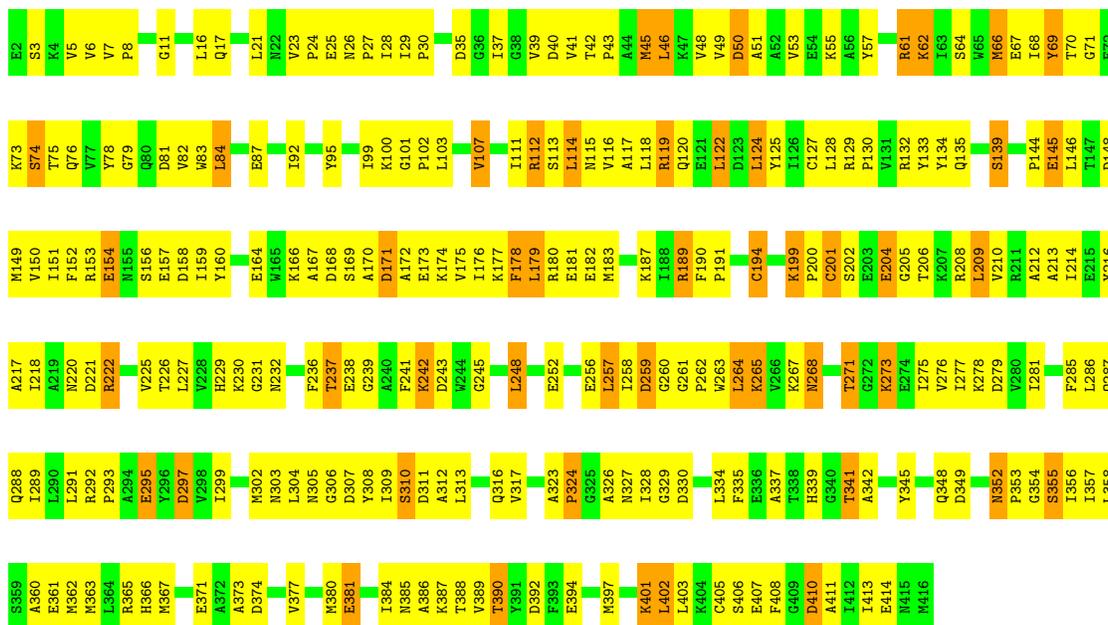


- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase

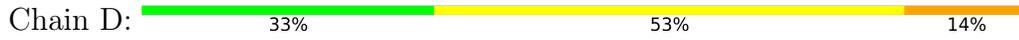




● Molecule 2: Isocitrate dehydrogenase [NADP]



● Molecule 2: Isocitrate dehydrogenase [NADP]



E2	S3	K4	V5	V6	V7	Q10	G11	K12	K13	I14	T15	L16	Q17	M18	G19	K20	L21	N22	V23	P24	E25	N26	P27	L28	L29	P30	Y31	E33	G36	I37	G38	V39	D40	V41	T42	P43	A44	M45	L46	K47	V48	V49	V53	Y57	K58	G59	E60	R61	M66	S67	L68	Y69	T70			
G71	S74	T75	Y78	G79	Q80	D81	W82	W83	L84	P85	T88	L89	D90	L91	I92	R93	E94	Y95	R96	Y97	A98	I99	K100	G101	P102	L103	T104	L105	P106	I111	R112	S113	L114	M115	M116	A117	L118	R119	L122	D123	L124	Y125	I126	C127	L128	R129	P130	E60	V131	R132	Y133	Y134	Q135	G136	T137	
P138	V141	P144	D148	M149	V150	I151	F152	R153	E154	E157	D158	L159	Y160	A161	G162	I163	E164	W165	K166	A167	D168	S169	D171	A170	D171	A172	S173	K174	V175	L176	K177	F178	L179	R180	E181	E182	M183	G184	V185	R189	F190	P191	E192	H193	C194	G195	I196	G197	I198	K199	P200	C201	S202	E203	E204	
G205	T206	K207	R208	L209	V210	R211	A212	A213	L214	E215	Y216	A217	L218	A219	N220	D221	R222	Q223	S224	T225	L226	L227	H228	K230	G231	N232	L233	M234	K235	T236	T237	E238	G239	A240	F241	K242	D243	W244	G245	Y246	Q247	L248	A249	R250	L257	G260	G261	P262	W263	L264	K265	V266	K267	N268	P269	N270
T271	G272	K273	E274	L275	V276	L277	K278	D279	V280	L281	A282	D283	A284	P285	L286	Q287	Q288	L289	L290	L291	R292	P293	A294	E295	Y296	D297	V298	L299	A300	C301	K302	N303	L304	D307	S310	D311	A312	L313	Q316	T322	A323	P324	G325	A326	N327	L328	G329	D330	E331	C332	F335	E336	A337	T338		
H339	G340	T341	A342	Y345	Q346	V351	N352	P353	G354	S355	L356	L357	L358	S359	A360	E361	K362	K363	K367	G368	K369	T370	E371	A372	L375	L376	V377	E381	G382	A383	L384	N385	A386	K387	T388	V389	T390	Y391	D392	F393	E394	R395	L396	K397	D398	G399	A400	K401	L402	L403	K404	C405	S406			
E407	F408	G409	D410	A411	L412	L413	E414	N415	N416																																															

4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	198.16Å 198.16Å 156.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 3.30 29.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.97-3.30) 99.4 (29.95-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.31Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.177 , 0.247 0.221 , 0.271	Depositor DCC
R_{free} test set	2657 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	99.5	Xtrriage
Anisotropy	0.211	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15755	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.91	0/4699	0.74	2/6367 (0.0%)
1	B	0.92	0/4776	0.73	3/6473 (0.0%)
2	C	1.00	0/3266	0.77	2/4417 (0.0%)
2	D	0.93	0/3266	0.79	3/4417 (0.1%)
All	All	0.93	0/16007	0.75	10/21674 (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
2	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	352	ASN	C-N-CD	-15.54	86.42	120.60
1	B	514	PHE	C-N-CD	-9.84	98.96	120.60
1	A	169	LYS	N-CA-C	-7.42	90.97	111.00
2	C	261	GLY	N-CA-C	-5.92	98.31	113.10
2	D	261	GLY	N-CA-C	-5.88	98.40	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	GLU	Peptide
2	C	70	THR	Peptide

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	4575	0	4464	753	3
1	B	4649	0	4550	688	0
2	C	3205	0	3213	418	2
2	D	3205	0	3211	437	3
3	A	23	0	12	2	0
3	B	23	0	12	6	0
4	A	27	0	12	7	0
4	B	27	0	12	6	0
5	A	3	0	0	0	0
5	B	4	0	0	1	0
5	C	7	0	0	2	0
5	D	7	0	0	2	0
All	All	15755	0	15486	2256	5

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 72.

The worst 5 of 2256 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)
2:D:261:GLY:HA3	2:D:263:TRP:CZ3	1.26	1.69
1:A:7:LEU:CD1	1:A:85:HIS:CD2	1.76	1.66
1:B:40:TRP:CZ3	1:B:205:LYS:HE2	1.36	1.59
1:A:525:ASP:CB	1:A:528:ILE:HD12	1.31	1.54
2:D:154:GLU:C	2:D:303:ASN:HD21	1.04	1.52

All (5) 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:A:499:GLU:OE1	2:D:345:TYR:OH[3_555]	1.57	0.63
1:A:507:SER:OG	2:C:279:ASP:OD1[3_555]	1.61	0.59
2:D:295:GLU:OE2	2:D:398:ASP:OD1[2_455]	1.84	0.36
1:A:520:HIS:NE2	2:D:104:THR:OG1[3_555]	2.09	0.11
2:C:135:GLN:NE2	2:C:401:LYS:N[3_445]	2.18	0.02

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	548/568 (96%)	528 (96%)	15 (3%)	5 (1%)	17	48
1	B	557/568 (98%)	548 (98%)	7 (1%)	2 (0%)	34	66
2	C	413/415 (100%)	398 (96%)	13 (3%)	2 (0%)	29	61
2	D	413/415 (100%)	391 (95%)	14 (3%)	8 (2%)	8	34
All	All	1931/1966 (98%)	1865 (97%)	49 (2%)	17 (1%)	17	48

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	200	PRO
2	D	200	PRO
1	A	69	THR
1	A	570	SER
2	D	231	GLY

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	485/498 (97%)	370 (76%)	115 (24%)	1	2
1	B	494/498 (99%)	390 (79%)	104 (21%)	1	4
2	C	337/337 (100%)	271 (80%)	66 (20%)	1	5
2	D	337/337 (100%)	269 (80%)	68 (20%)	1	5
All	All	1653/1670 (99%)	1300 (79%)	353 (21%)	1	4

5 of 353 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	84	LEU
2	D	13	LYS
2	C	124	LEU
2	C	248	LEU
2	D	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	HIS
1	B	462	ASN
2	D	18	ASN
1	B	373	GLN
1	B	549	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

4 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
3	AMP	A	601	-	22,25,25	0.92	1 (4%)	25,38,38	1.41	2 (8%)
4	ADP	A	602	-	24,29,29	1.13	2 (8%)	29,45,45	1.56	6 (20%)
4	ADP	B	601	-	24,29,29	1.34	4 (16%)	29,45,45	2.12	12 (41%)
3	AMP	B	602	-	22,25,25	0.97	2 (9%)	25,38,38	1.38	5 (20%)

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
3	AMP	A	601	-	-	0/6/26/26	0/3/3/3
4	ADP	A	602	-	-	6/12/32/32	0/3/3/3
4	ADP	B	601	-	-	8/12/32/32	0/3/3/3
3	AMP	B	602	-	-	4/6/26/26	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	ADP	C2-N3	2.88	1.36	1.32
4	A	602	ADP	O4'-C1'	2.64	1.44	1.41
4	B	601	ADP	C5-C4	2.61	1.47	1.40
4	B	601	ADP	O4'-C1'	2.47	1.44	1.41
3	A	601	AMP	O4'-C1'	2.24	1.44	1.41

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	ADP	O3B-PB-O3A	-5.50	86.18	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	AMP	N3-C2-N1	-3.91	122.57	128.68
4	B	601	ADP	O3B-PB-O1B	3.51	124.42	110.68
4	A	602	ADP	O3B-PB-O1B	3.40	124.00	110.68
4	B	601	ADP	C4-C5-N7	-3.11	106.15	109.40

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

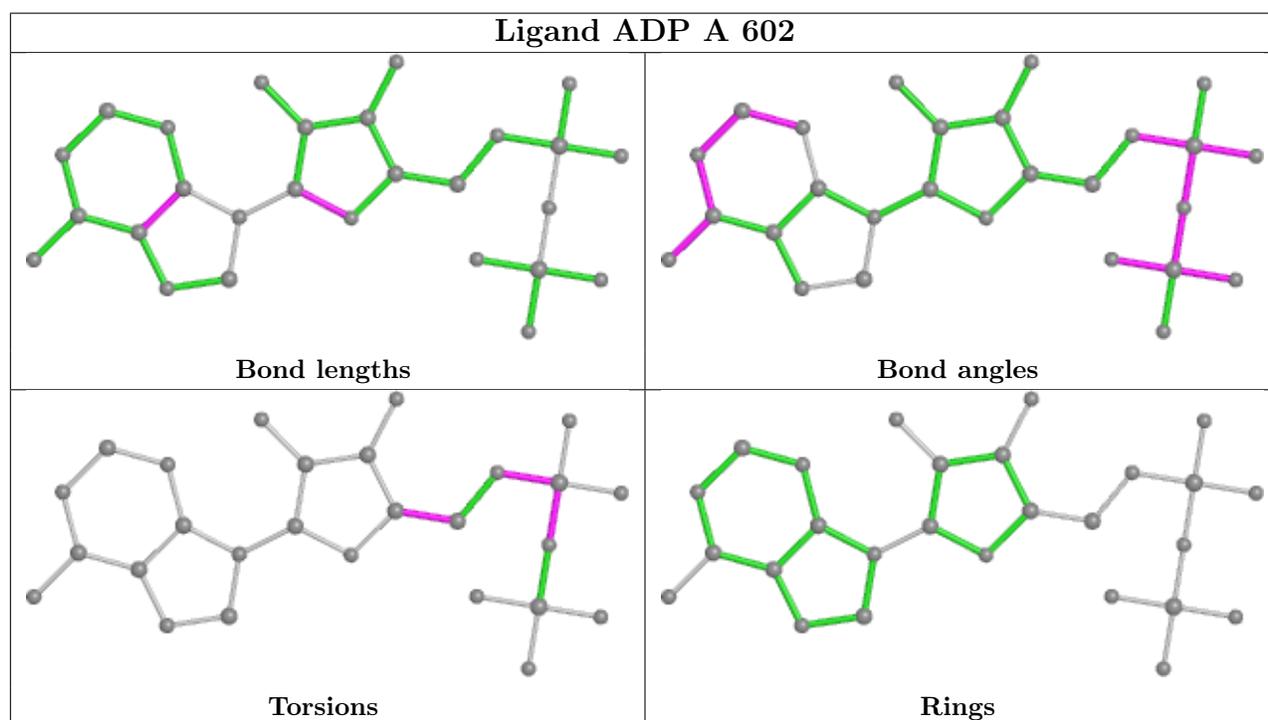
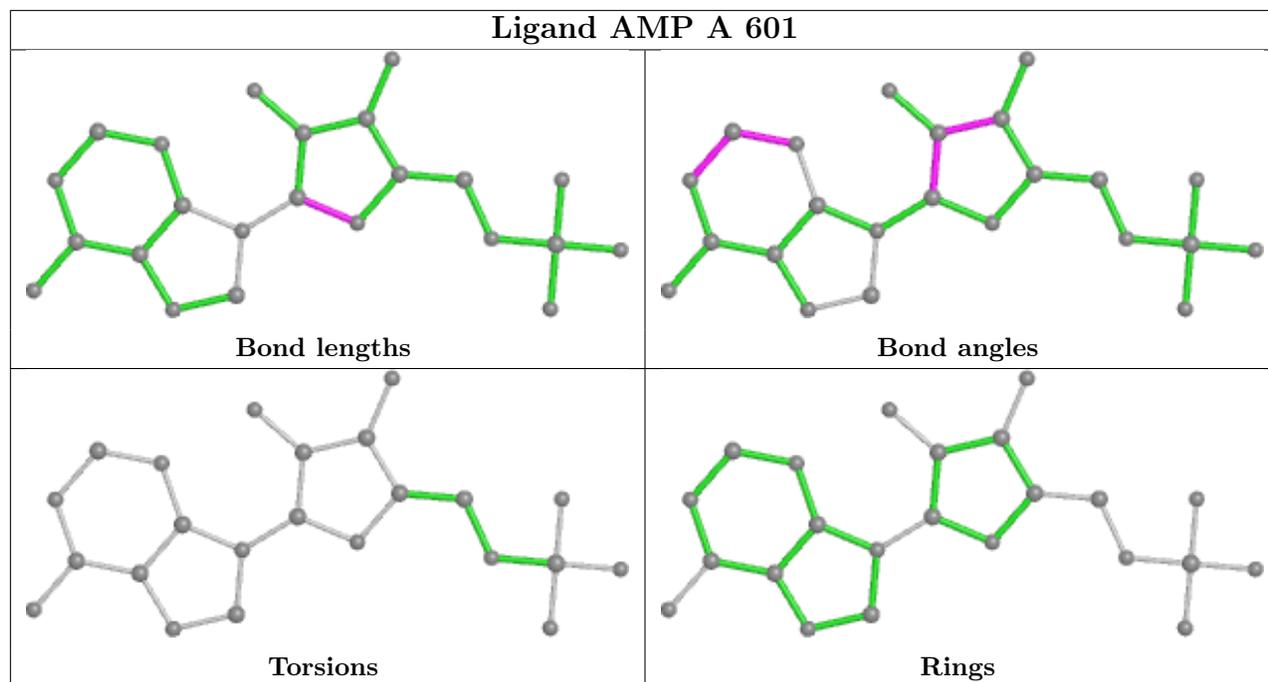
Mol	Chain	Res	Type	Atoms
3	B	602	AMP	C5'-O5'-P-O2P
3	B	602	AMP	C5'-O5'-P-O3P
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	O4'-C4'-C5'-O5'

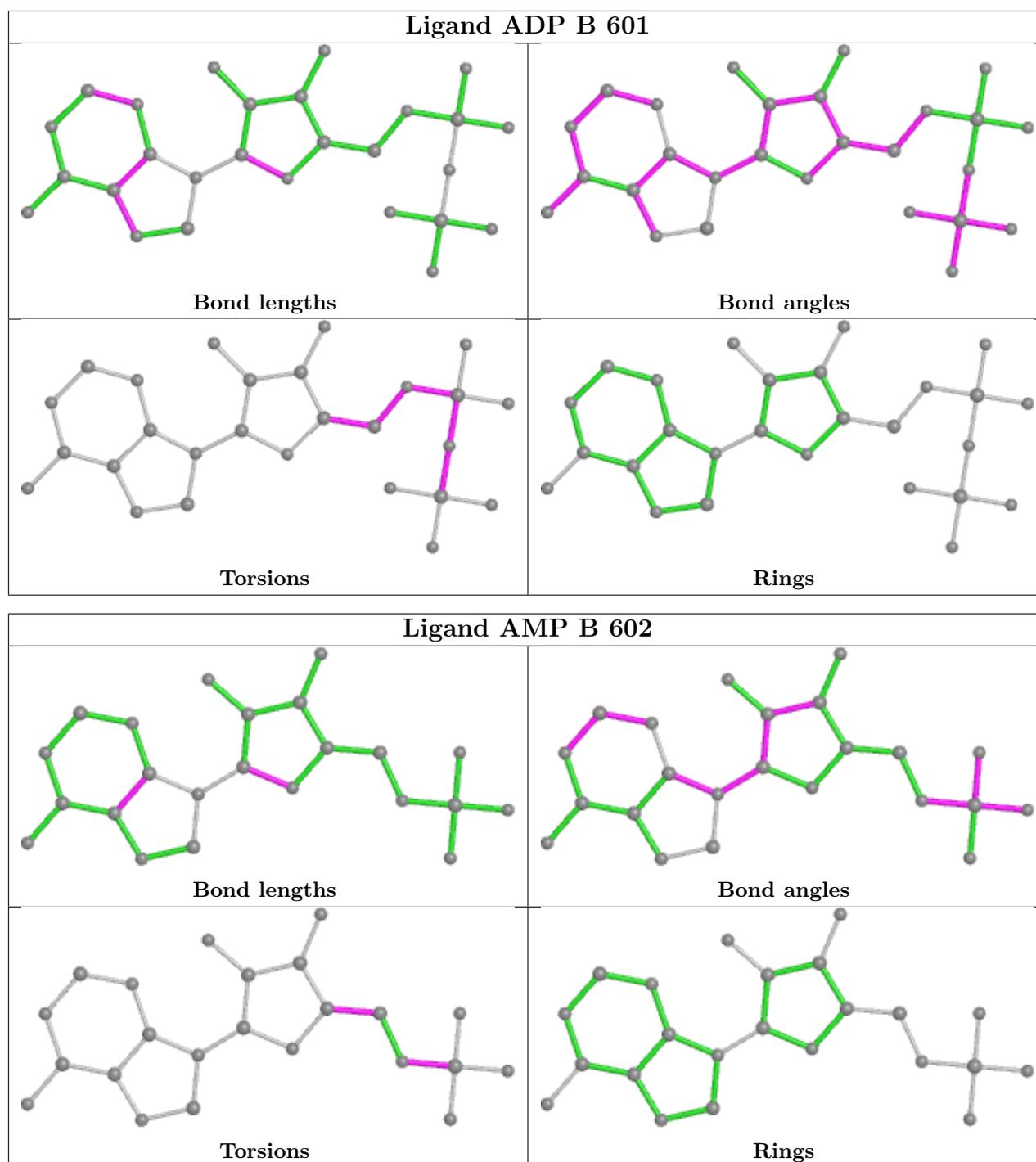
There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	AMP	2	0
4	A	602	ADP	7	0
4	B	601	ADP	6	0
3	B	602	AMP	6	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

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.

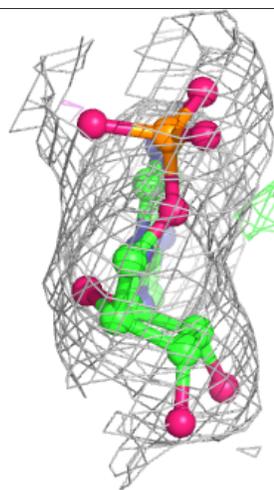
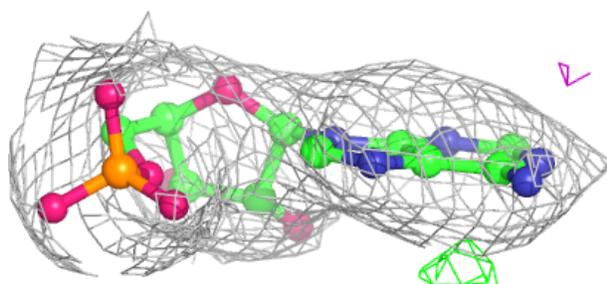
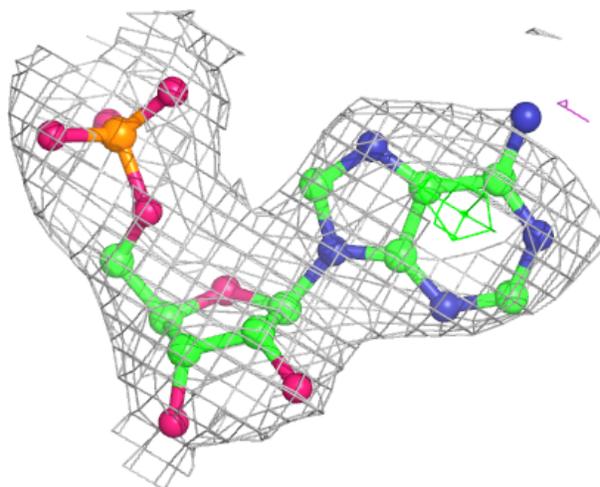
6.4 Ligands

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.

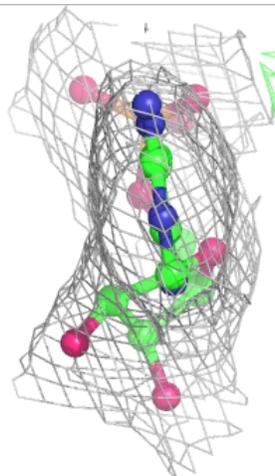
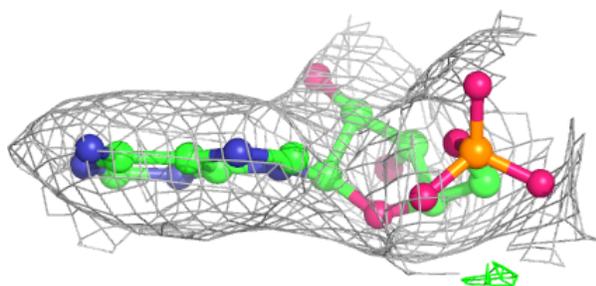
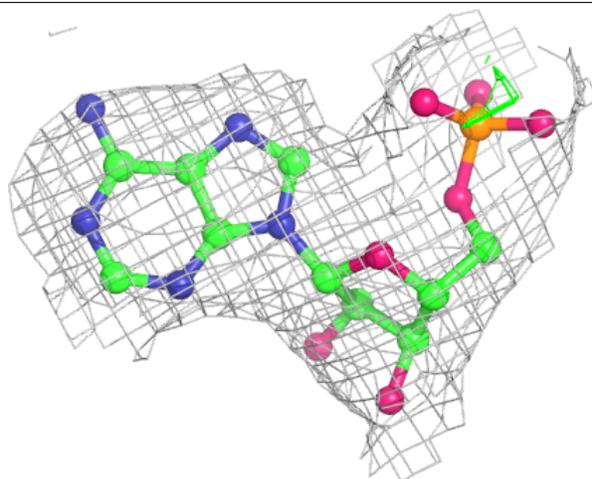
Electron density around AMP A 601:

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



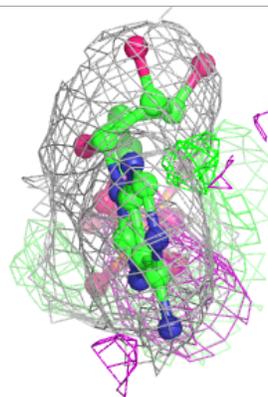
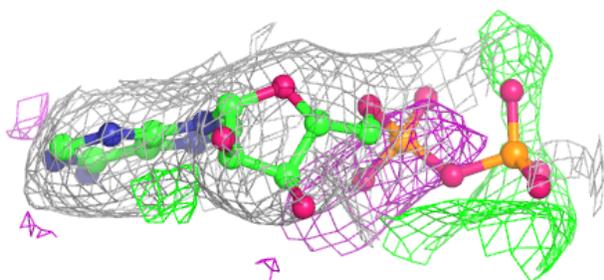
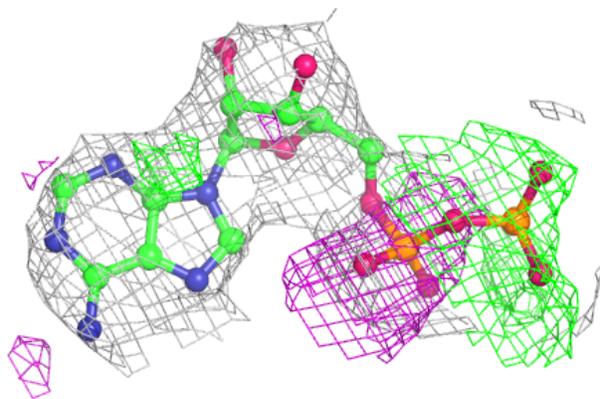
Electron density around AMP B 602:

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

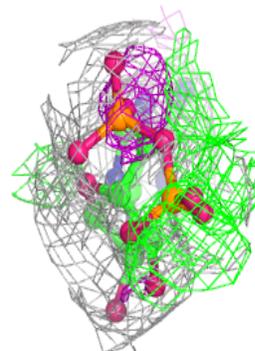
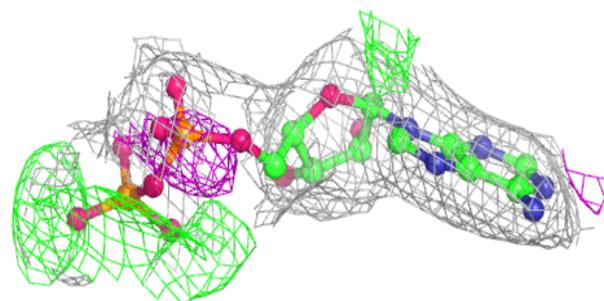
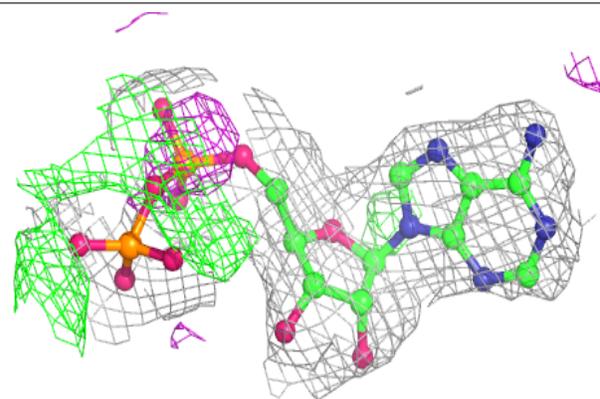


Electron density around ADP A 602:

$2mF_o-DF_c$ (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

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