



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 01:28 AM EDT

PDB ID : 2XAL
Title : Lead derivative of Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *A. thaliana* in complex with ADP and IP6.
Authors : Gonzalez, B.; Banos-Sanz, J.I.; Villate, M.; Brearley, C.A.; Sanz-Aparicio, J.
Deposited on : 2010-03-31
Resolution : 3.20 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 : 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

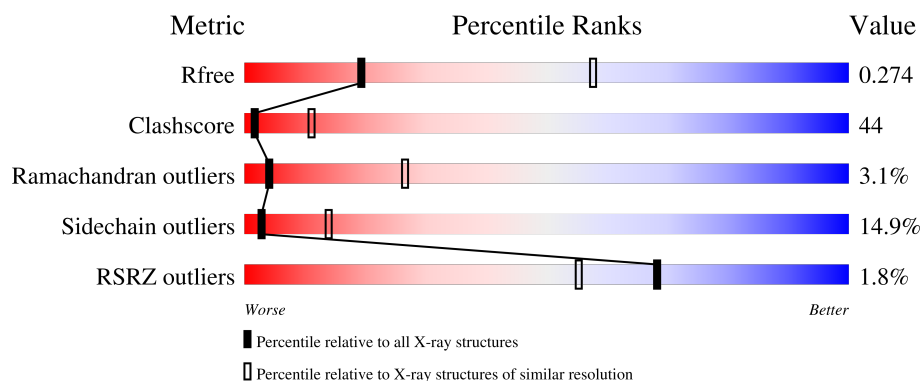
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	451	 2% 42% 40% 10% 7%
1	B	451	 2% 39% 45% 10% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6851 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.

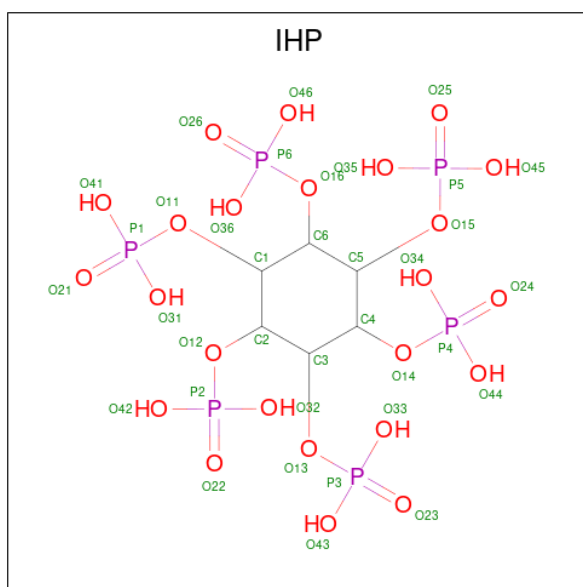
- Molecule 1 is a protein called INOSITOL-PENTAKISPHOSPHATE 2-KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3338	2120	565	640	13			
1	B	425	Total	C	N	O	S	0	0	0
			3381	2148	574	645	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	SER	ALA	conflict	UNP Q93YN9
A	90	GLN	LYS	conflict	UNP Q93YN9
A	157	THR	SER	conflict	UNP Q93YN9
A	204	ILE	ASN	conflict	UNP Q93YN9
A	224	ARG	SER	conflict	UNP Q93YN9
A	321	CYS	SER	conflict	UNP Q93YN9
A	325	ILE	LEU	conflict	UNP Q93YN9
A	337	ARG	LYS	conflict	UNP Q93YN9
B	54	SER	ALA	conflict	UNP Q93YN9
B	90	GLN	LYS	conflict	UNP Q93YN9
B	157	THR	SER	conflict	UNP Q93YN9
B	204	ILE	ASN	conflict	UNP Q93YN9
B	224	ARG	SER	conflict	UNP Q93YN9
B	321	CYS	SER	conflict	UNP Q93YN9
B	325	ILE	LEU	conflict	UNP Q93YN9
B	337	ARG	LYS	conflict	UNP Q93YN9

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			36	6	24	6		
2	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 3 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Pb	0	0
			2	2		
3	B	2	Total	Pb	0	0
			2	2		

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



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

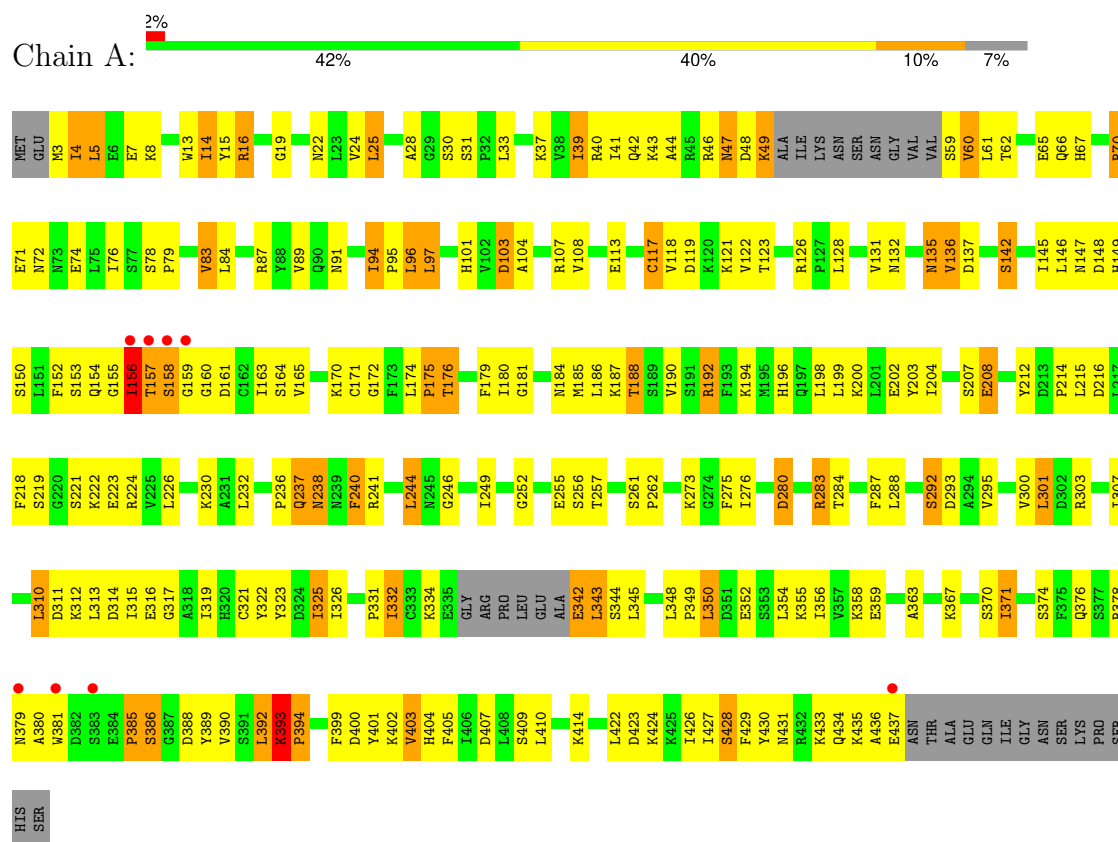
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0

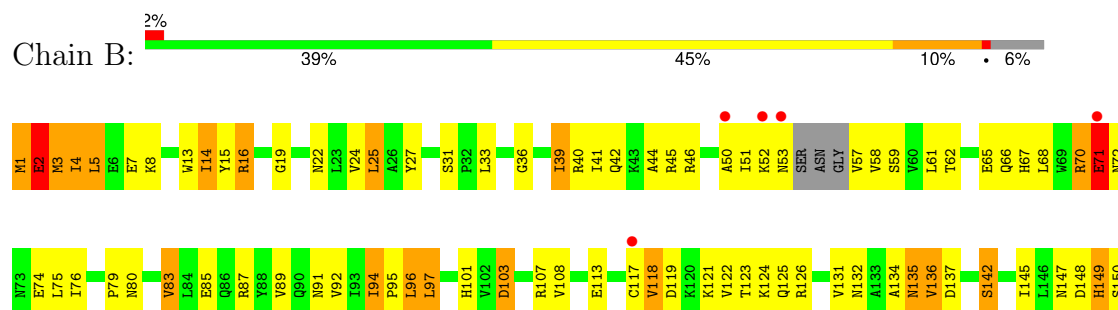
3 Residue-property plots

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 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: INOSITOL-PENTAKISPHOSPHATE 2-KINASE



• Molecule 1: INOSITOL-PENTAKISPHOSPHATE 2-KINASE



ASN	Q376	L310	F218	L151
SER	S377	L311	S219	F152
LYS	R378	K312	G220	SER
PRO	M379	L313	S221	GLN
SER	A380	D314	K222	GLY
HIS	TRP	I315	E223	ILE
SER	ASP	E316	R224	THR
	S383	G317	V225	SER
	E394	A318	L226	GLY
		I319	L232	D161
	D388	H320	P236	V165
	Y389	C321	Q237	
	V390	Y322	N238	K168
	S391	Y323	N239	P169
	L392	D324	F240	K170
	K393	I325	R241	C171
	P394	I326	L244	G172
	T395		E269	F173
	N396	C330	I249	L174
	Q397	P331	G252	P175
	T398	I332	E255	T176
	F399	C333	S256	
	D400	K334	T257	
	Y401	E335		
	K402	G336	K273	F179
	V403	R337	G274	I180
	H404	P338	F275	G181
	F405	L339	I276	K182
	I406	E340	Q277	E183
	D407	A341	S278	N184
	I408	E342	E279	M185
	S409	L343	D280	L186
		S344	G281	K187
	P412	L345	H282	T188
	L413	H346	R283	S189
	K414	A347	T284	V190
	R415	L348	E285	S191
		P349	C286	R192
		L350	F287	F193
	L422	D351	L288	K194
	D423	E352	S282	M195
	K424	S353	V295	H196
	K425	L354	Y296	Q197
	I426	K355		L198
	I427	I356		L199
	S428	V357		K200
	F429	K358		L201
	Y430	E359		E202
		I362		Y203
	K433	A363		I204
	Q434	K367		
	K435			S207
	A436			E208
	E437			
	N438			Y212
	THR	I371		D213
	ALA	K372		P214
	GLU	I373		L215
	GLN	S374		D216
	ILE	F375		L217
	GLY			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.06Å 110.97Å 138.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.71 – 3.20 86.65 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.71-3.20) 99.9 (86.65-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.210 , 0.268 0.214 , 0.274	Depositor DCC
R_{free} test set	768 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6851	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.27% 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: ZN, IHP, ADP, PB

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	0.56	0/3400	0.66	0/4584
1	B	0.56	0/3441	0.65	0/4637
All	All	0.56	0/6841	0.66	0/9221

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	3338	0	3344	263	3
1	B	3381	0	3406	358	4
2	A	36	0	6	1	0
2	B	36	0	6	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	27	0	12	4	0
4	B	27	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	6851	0	6786	604	4

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 44.

The worst 5 of 604 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:46:ARG:HH12	1:B:182:LYS:CG	1.14	1.58
1:B:52:LYS:HA	1:B:57:VAL:O	1.20	1.38
1:B:280:ASP:HB2	1:B:282:HIS:CD2	1.56	1.38
1:A:46:ARG:NH1	1:B:182:LYS:CG	1.86	1.37
1:A:46:ARG:NH1	1:B:182:LYS:HG3	1.36	1.37

All (4) 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:312:LYS:NZ	1:B:202:GLU:CG[1_455]	1.84	0.36
1:B:124:LYS:NZ	1:B:273:LYS:O[4_556]	1.87	0.33
1:A:312:LYS:NZ	1:B:202:GLU:CD[1_455]	2.04	0.16
1:A:381:TRP:CE3	1:B:223:GLU:OE1[3_655]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	414/451 (92%)	366 (88%)	34 (8%)	14 (3%)	3	24
1	B	417/451 (92%)	374 (90%)	31 (7%)	12 (3%)	4	28
All	All	831/902 (92%)	740 (89%)	65 (8%)	26 (3%)	4	26

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ILE

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Mol	Chain	Res	Type
1	A	161	ASP
1	A	343	LEU
1	A	386	SER
1	A	393	LYS

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	374/399 (94%)	322 (86%)	52 (14%)	3	16
1	B	379/399 (95%)	319 (84%)	60 (16%)	2	12
All	All	753/798 (94%)	641 (85%)	112 (15%)	3	14

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LYS
1	B	437	GLU
1	B	97	LEU
1	B	428	SER
1	B	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	ASN
1	B	282	HIS
1	B	397	GLN
1	B	376	GLN
1	B	196	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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$
2	IHP	A	500	3	36,36,36	0.73	0	60,60,60	1.36	10 (16%)
4	ADP	B	600	3	24,29,29	1.03	1 (4%)	29,45,45	1.64	6 (20%)
4	ADP	A	600	3	24,29,29	1.22	2 (8%)	29,45,45	1.43	4 (13%)
2	IHP	B	500	3	36,36,36	0.84	0	60,60,60	1.50	16 (26%)

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	IHP	A	500	3	-	7/30/54/54	0/1/1/1
4	ADP	B	600	3	-	4/12/32/32	0/3/3/3
4	ADP	A	600	3	-	0/12/32/32	0/3/3/3
2	IHP	B	500	3	-	10/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ADP	PA-O3A	4.09	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	ADP	PA-O3A	2.90	1.62	1.59
4	A	600	ADP	C1'-N9	-2.01	1.45	1.49

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ADP	O4'-C1'-N9	-4.30	103.05	108.75
4	A	600	ADP	N3-C2-N1	-3.94	123.33	128.67
4	B	600	ADP	N3-C2-N1	-3.47	123.97	128.67
2	B	500	IHP	P2-O12-C2	-3.26	114.73	123.43
4	A	600	ADP	C1'-N9-C4	-2.97	121.43	126.64

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	IHP	C5-O15-P5-O25
2	A	500	IHP	C3-O13-P3-O23
2	B	500	IHP	C3-O13-P3-O23
4	B	600	ADP	C5'-O5'-PA-O1A
4	B	600	ADP	C5'-O5'-PA-O2A

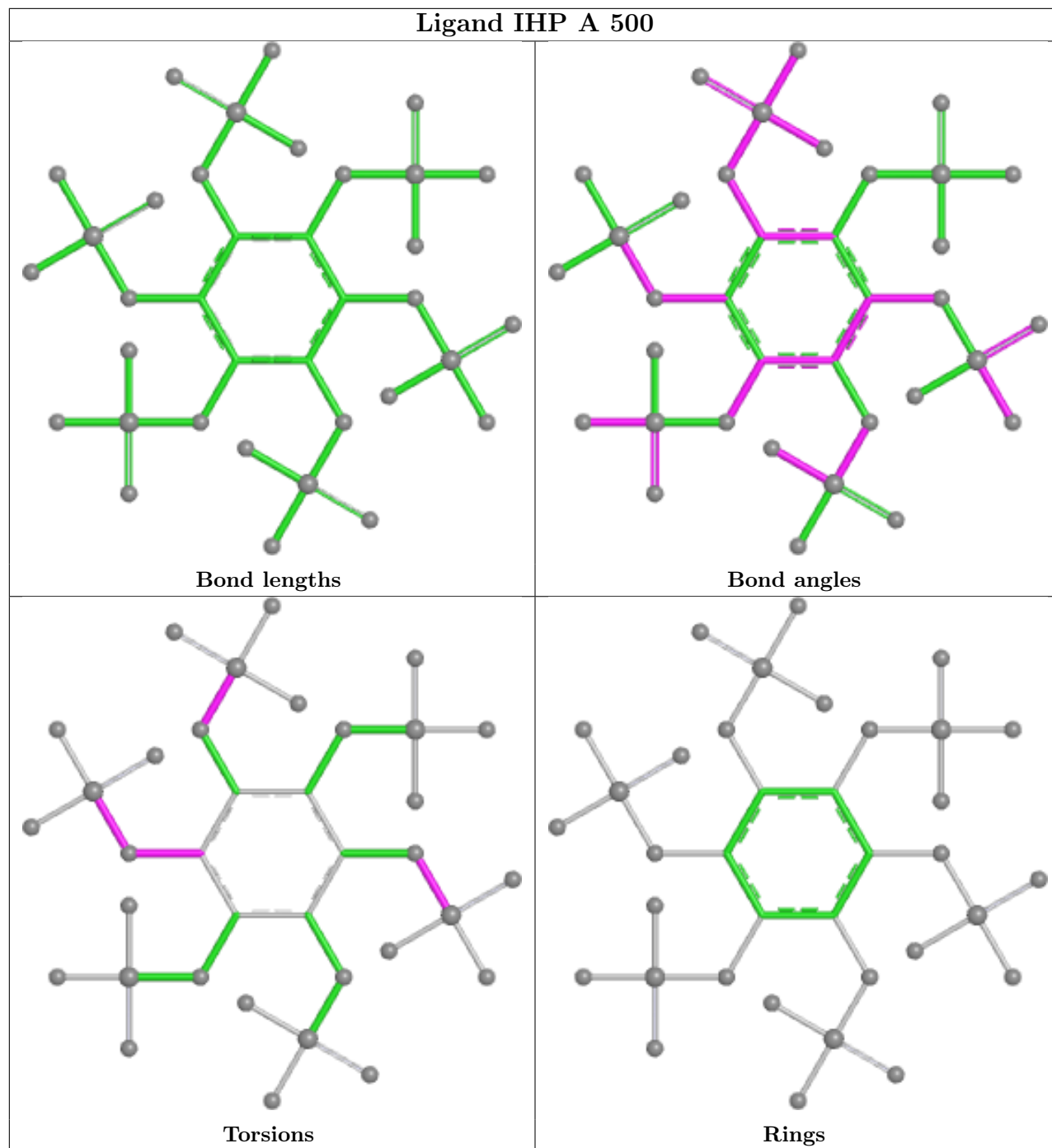
There are no ring outliers.

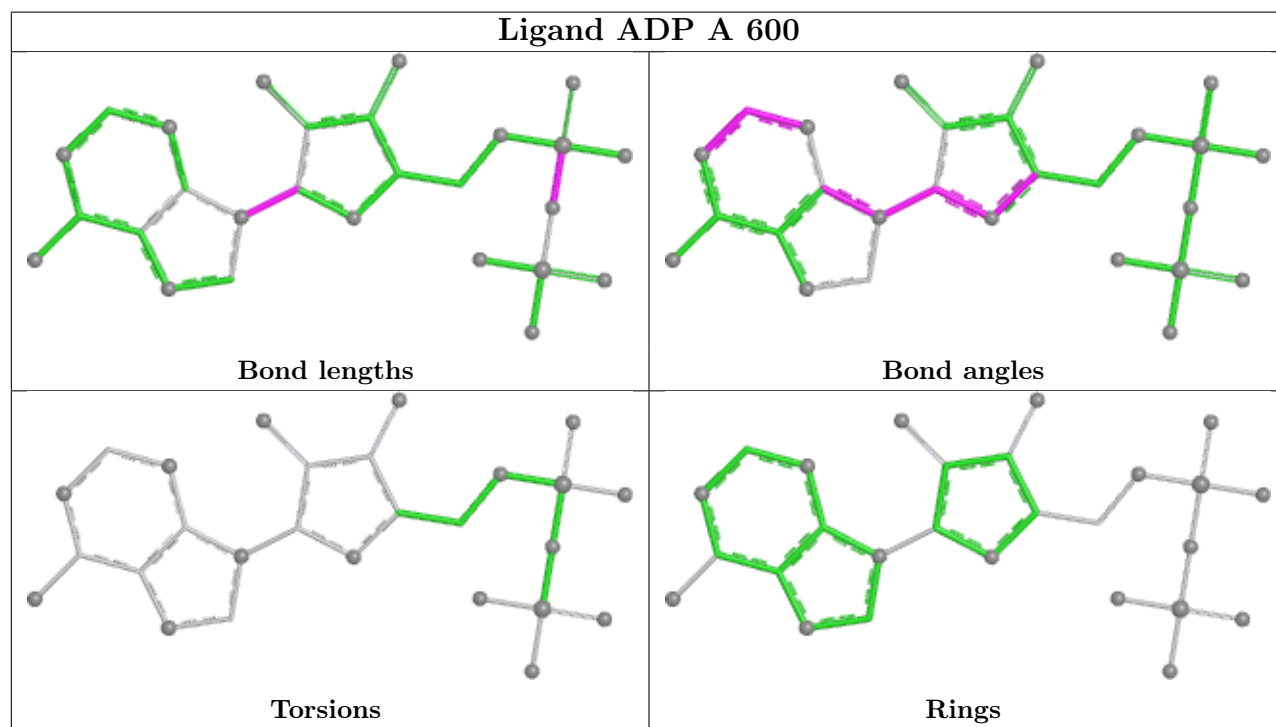
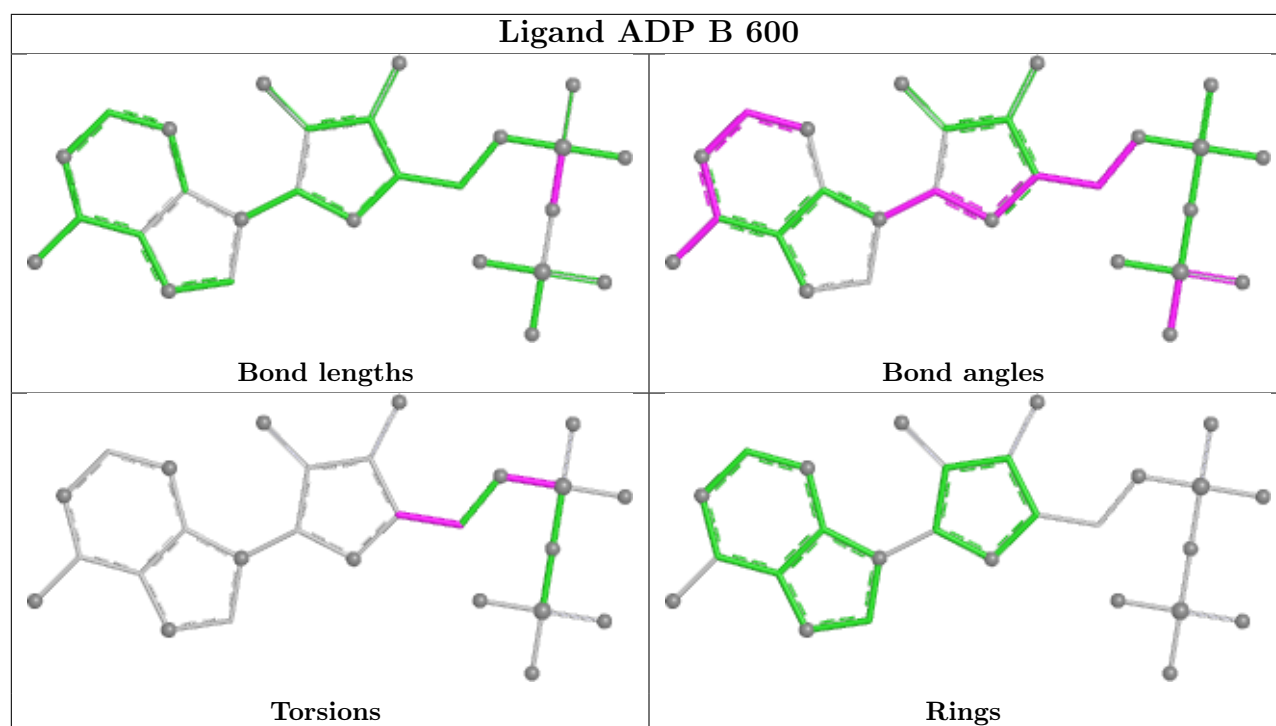
4 monomers are involved in 14 short contacts:

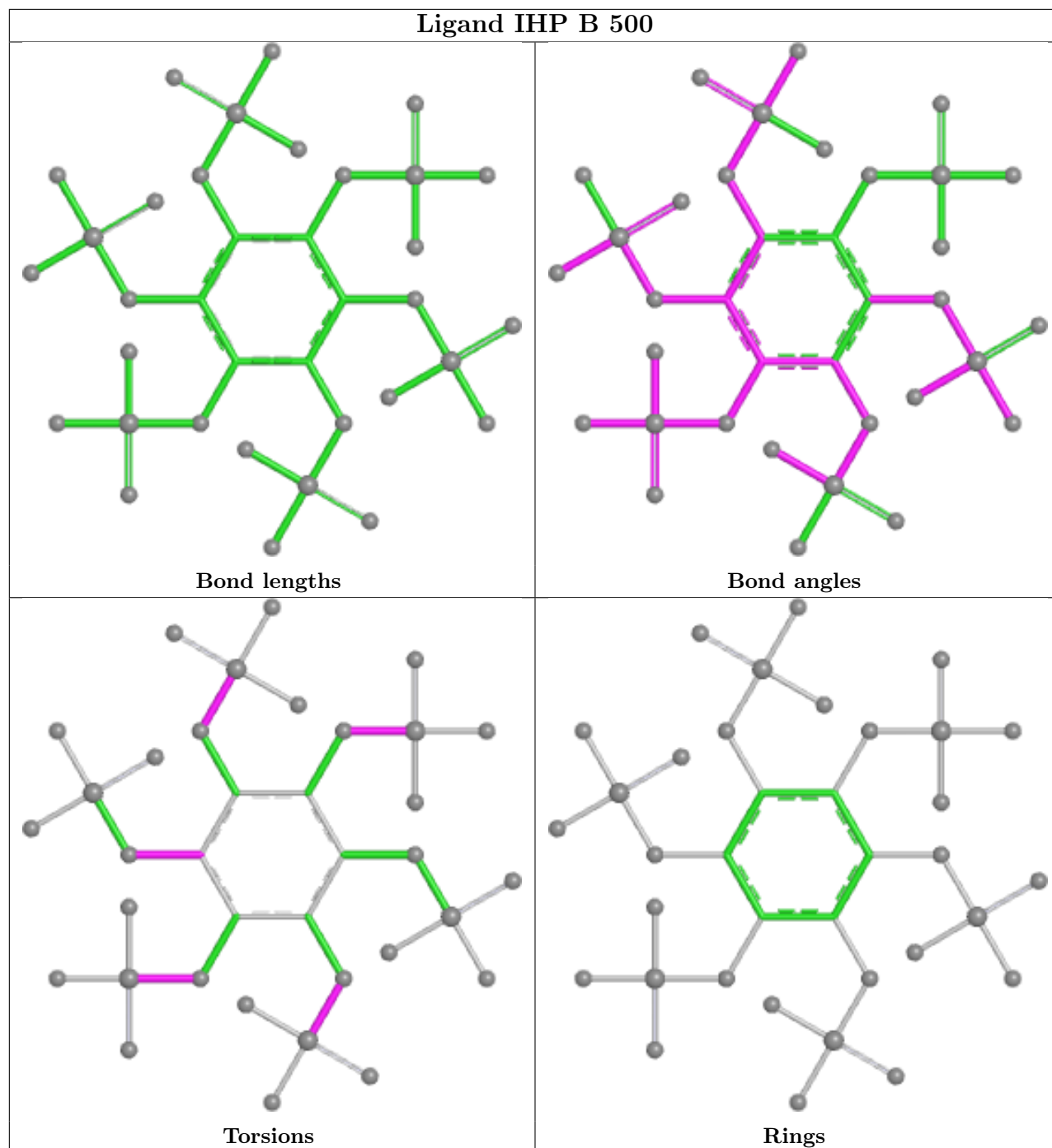
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IHP	1	0
4	B	600	ADP	4	0
4	A	600	ADP	4	0
2	B	500	IHP	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	420/451 (93%)	-0.13	8 (1%) 66 53	9, 21, 41, 54	0
1	B	425/451 (94%)	0.02	7 (1%) 72 59	9, 20, 41, 62	0
All	All	845/902 (93%)	-0.05	15 (1%) 68 55	9, 21, 41, 62	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	GLY	3.1
1	A	383	SER	3.0
1	A	437	GLU	2.9
1	A	379	ASN	2.8
1	B	396	ASN	2.5

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](#)

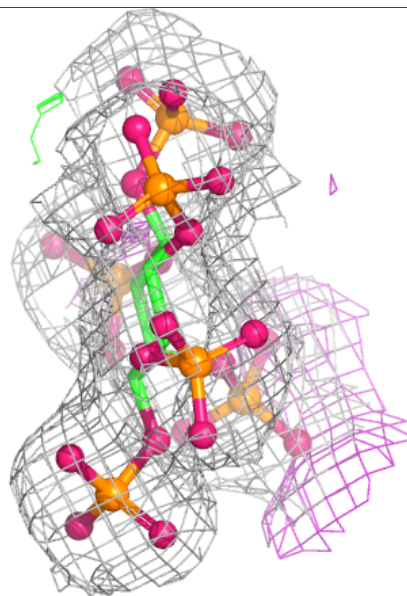
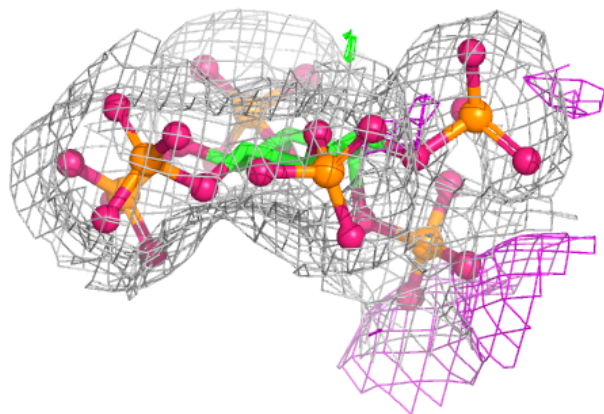
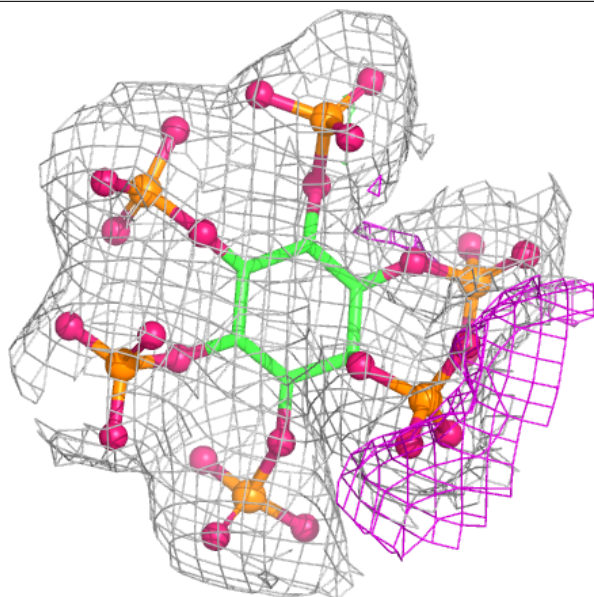
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IHP	B	500	36/36	0.97	0.11	11,14,18,18	0
4	ADP	B	600	27/27	0.97	0.14	4,8,11,11	0
4	ADP	A	600	27/27	0.98	0.13	9,12,23,24	0
2	IHP	A	500	36/36	0.98	0.11	9,12,22,24	0
5	ZN	A	700	1/1	0.98	0.06	33,33,33,33	0
5	ZN	B	700	1/1	0.98	0.06	56,56,56,56	0
3	PB	A	502	1/1	0.99	0.02	20,20,20,20	0
3	PB	B	503	1/1	0.99	0.03	30,30,30,30	0
3	PB	A	501	1/1	0.99	0.04	27,27,27,27	0
3	PB	B	504	1/1	1.00	0.01	22,22,22,22	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.

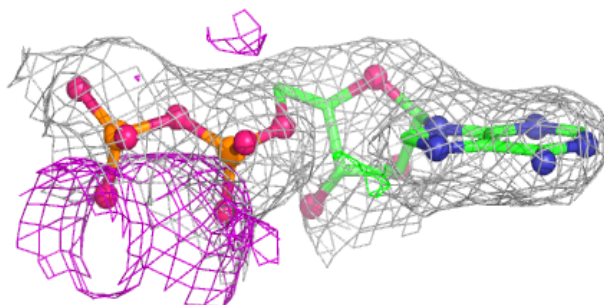
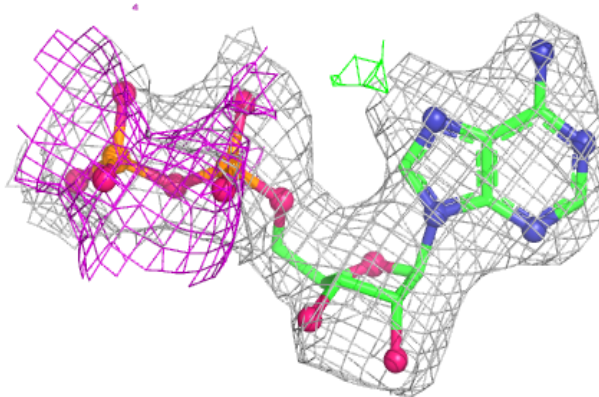
Electron density around IHP B 500:

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

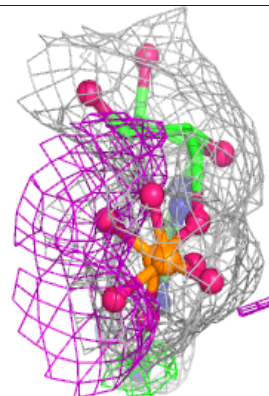
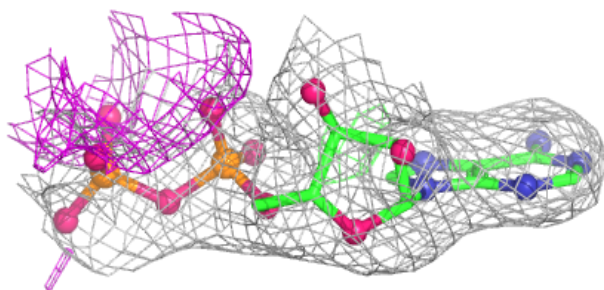
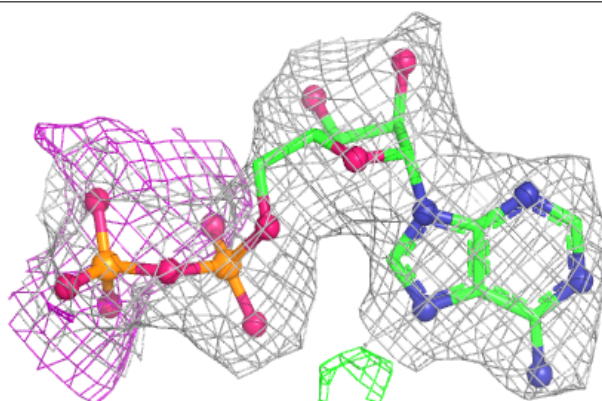


Electron density around ADP B 600:

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

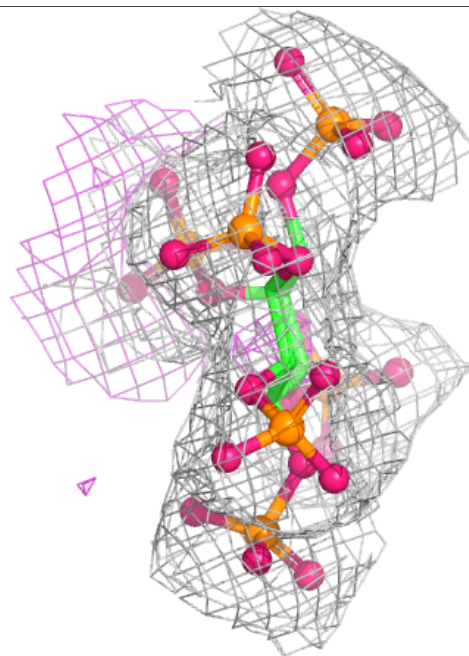
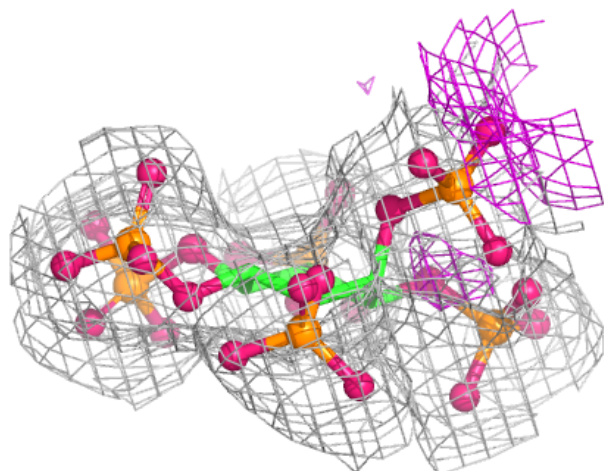
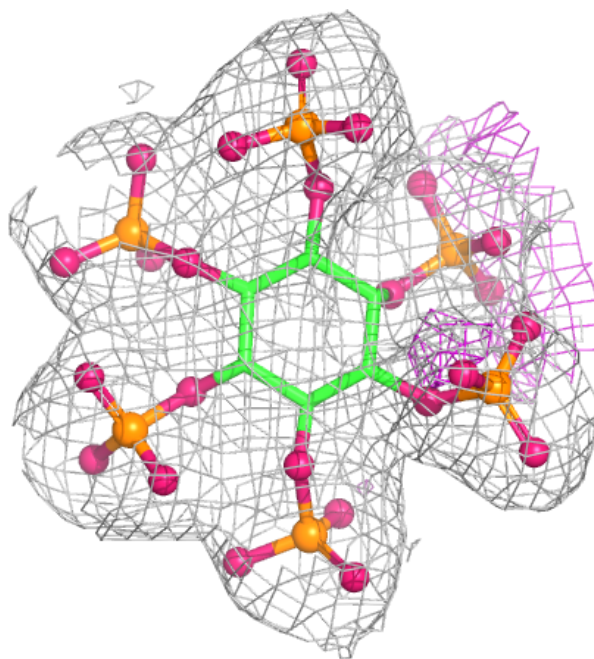
**Electron density around ADP A 600:**

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



Electron density around IHP A 500:

$2mF_o-DF_c$ (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.