



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:49 pm BST

PDB ID : 6GFG
Title : Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from *A. thaliana* in complex with D-chiro-IP6 and ADP
Authors : Whitfield, H.L.; Brearley, C.A.; Hemmings, A.M.
Deposited on : 2018-04-30
Resolution : 3.00 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 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

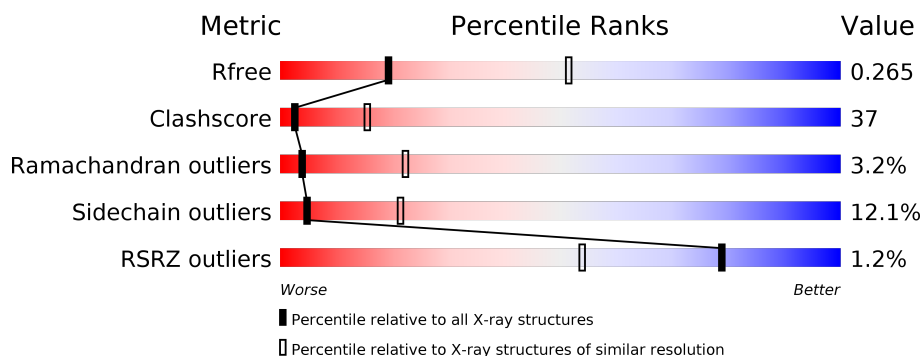
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	470	<div> <div>%</div> <div> <div></div> <div>33%</div> <div>50%</div> <div>7%</div> <div>11%</div> </div> </div>
1	B	470	<div> <div>%</div> <div> <div></div> <div>35%</div> <div>46%</div> <div>7%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6874 atoms, of which 36 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	B	420	Total	C	N	O	S	0	0	0
			3353	2134	564	641	14			
1	A	420	Total	C	N	O	S	0	0	0
			3353	2134	564	641	14			

There are 40 discrepancies between the modelled and reference sequences:

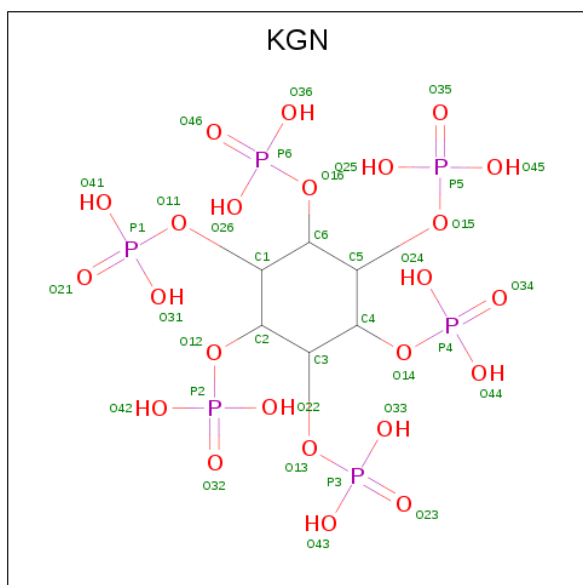
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP A0A178UAB5
B	-17	ALA	-	expression tag	UNP A0A178UAB5
B	-16	HIS	-	expression tag	UNP A0A178UAB5
B	-15	HIS	-	expression tag	UNP A0A178UAB5
B	-14	HIS	-	expression tag	UNP A0A178UAB5
B	-13	HIS	-	expression tag	UNP A0A178UAB5
B	-12	HIS	-	expression tag	UNP A0A178UAB5
B	-11	HIS	-	expression tag	UNP A0A178UAB5
B	-10	SER	-	expression tag	UNP A0A178UAB5
B	-9	SER	-	expression tag	UNP A0A178UAB5
B	-8	GLY	-	expression tag	UNP A0A178UAB5
B	-7	LEU	-	expression tag	UNP A0A178UAB5
B	-6	GLU	-	expression tag	UNP A0A178UAB5
B	-5	VAL	-	expression tag	UNP A0A178UAB5
B	-4	LEU	-	expression tag	UNP A0A178UAB5
B	-3	PHE	-	expression tag	UNP A0A178UAB5
B	-2	GLN	-	expression tag	UNP A0A178UAB5
B	-1	GLY	-	expression tag	UNP A0A178UAB5
B	0	PRO	-	expression tag	UNP A0A178UAB5
B	185	MET	ILE	conflict	UNP A0A178UAB5
A	-18	MET	-	initiating methionine	UNP A0A178UAB5
A	-17	ALA	-	expression tag	UNP A0A178UAB5
A	-16	HIS	-	expression tag	UNP A0A178UAB5
A	-15	HIS	-	expression tag	UNP A0A178UAB5
A	-14	HIS	-	expression tag	UNP A0A178UAB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP A0A178UAB5
A	-12	HIS	-	expression tag	UNP A0A178UAB5
A	-11	HIS	-	expression tag	UNP A0A178UAB5
A	-10	SER	-	expression tag	UNP A0A178UAB5
A	-9	SER	-	expression tag	UNP A0A178UAB5
A	-8	GLY	-	expression tag	UNP A0A178UAB5
A	-7	LEU	-	expression tag	UNP A0A178UAB5
A	-6	GLU	-	expression tag	UNP A0A178UAB5
A	-5	VAL	-	expression tag	UNP A0A178UAB5
A	-4	LEU	-	expression tag	UNP A0A178UAB5
A	-3	PHE	-	expression tag	UNP A0A178UAB5
A	-2	GLN	-	expression tag	UNP A0A178UAB5
A	-1	GLY	-	expression tag	UNP A0A178UAB5
A	0	PRO	-	expression tag	UNP A0A178UAB5
A	185	MET	ILE	conflict	UNP A0A178UAB5

- Molecule 2 is D-chiro inositol hexakisphosphate (three-letter code: KGN) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	O	P	0	0
			42	6	6	24	6		
2	A	1	Total	C	H	O	P	0	0
			42	6	6	24	6		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0
4	A	2	Total Mg 2 2	0	0

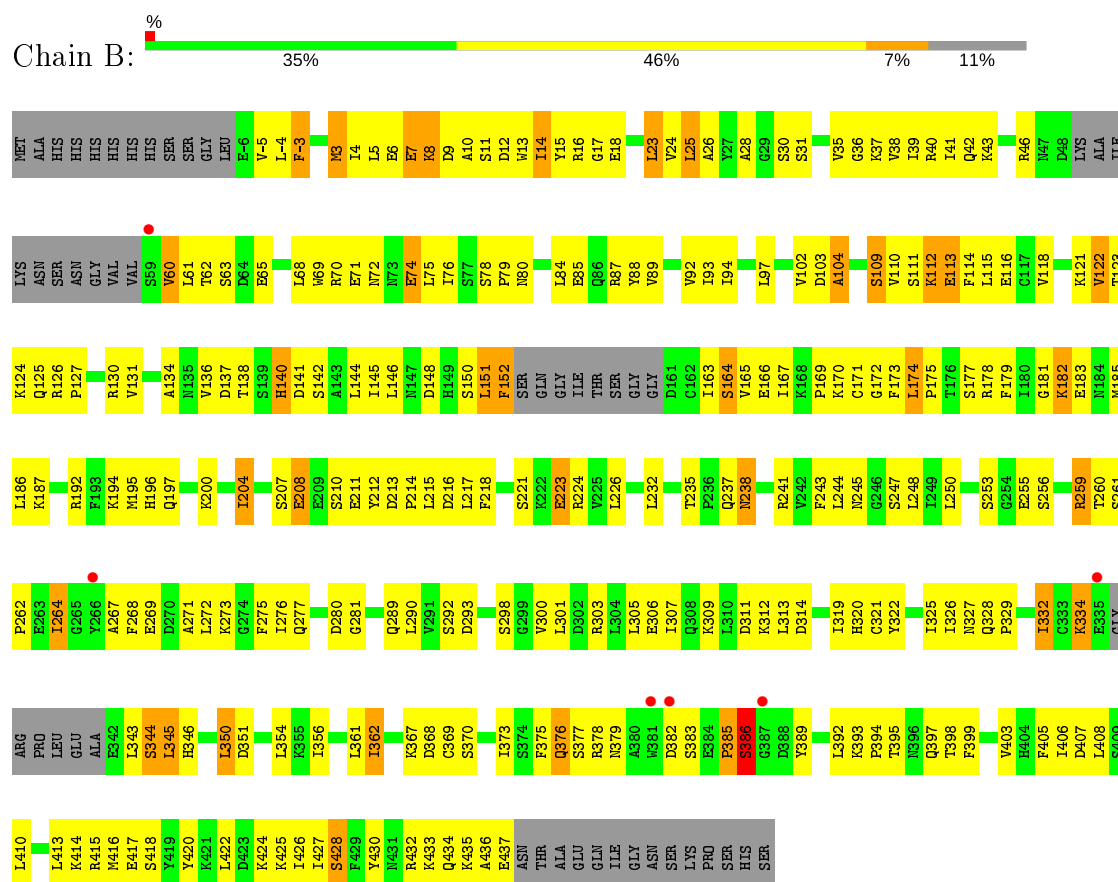
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

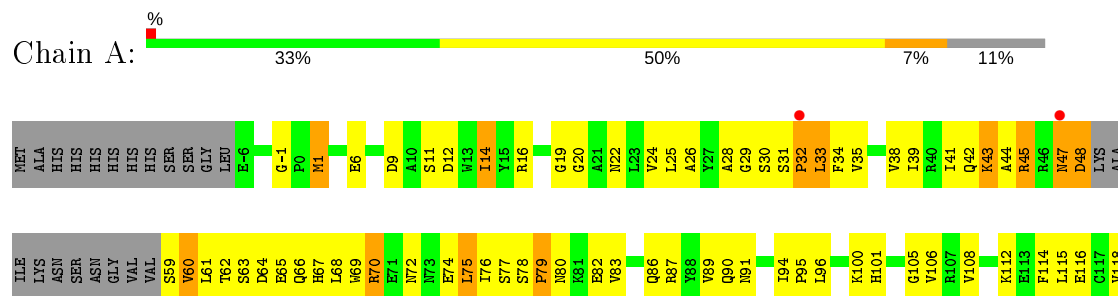
3 Residue-property plots

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: Inositol-pentakisphosphate 2-kinase



• Molecule 1: Inositol-pentakisphosphate 2-kinase



I396	I397	T398	F399	D400	Y401	K402	V403		L410	K411	P412	L413	K414	R415	R416	E417		Y420	K421	L422	D423		I426	I427	S428	F429	Y430	N431	R432	K433	Q434	K435	A436	E437	ASN	THR	ALA	GLU	GLN	ILE	GLY	ASN	SER	LYS	PRO	SER	HIS	SER														
I324	I325	I326	I327	I328	I329	I330	I331	I332	I333	I334	I335	GLY	ARG	PRO	LEU	GLU	ALA	E342	I343	S344	I345	I346		S353	I354		V357	K358		I361	I362	A363		A366	K367		S370	I371	I372	I373	S374	F375	Q376	S377	R378	I379		D382	S383	F384			V389	V390	S391	I392	K393	P394	T395			
C252	S253	G254	E255	S256	T257	G258	R259	T260	S261	F262	E263	I264	G265	Y266	A267	F268	E269	D270	A271	L272	K273	G274	F275	I276	Q277	S278	E279		R283	T284	E285	C286	F287	L288	Q289	L290	V291	S292		V295	Y296		V300	L301	D302	R303	L304	L305	F306	I307		L313		E316		H320	G321	Y322	Y323			
G181	K182	E183			L186	K187		S191		M195	H196		K200	L201	E202	Y203	I204	E205	I206	S207	E208	E209	S210	E211	Y212	D213	P214	L215	D216	L217	F218	S219	G220	SER	GLN	GLY	ILE	THR	SER	GLY	D161	C162	I163	S164	V165	E166	I167	K168	P169	K170	C171	G172	F173	F243	L174	L244		S247	L248	L249	L250	G251
D119	K120	K121	V122	T123	K124	Q125	R126	P127	L128	W129	R130		A133	A134	N135	V136	D137	T138		D141	S142	A143	L144	I145	L146	H147	H149	S150	L151	F152		GLN	GLY	ILE	THR	SER	GLY	D161	C162	I163	S164	V165	E166	I167	K168	P169	K170	C171	G172	F173	F243	L174	L244		S247	L248	L249	L250	G251			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.57Å 60.82Å 82.44Å 89.50° 88.34° 62.54°	Depositor
Resolution (Å)	29.02 – 3.00 29.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.02-3.00) 96.8 (29.02-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.197 , 0.265 0.197 , 0.265	Depositor DCC
R_{free} test set	1065 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.000 for k,h,-l 0.009 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6874	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, MG, ADP, KGN

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	0.48	0/3416	0.61	0/4606
1	B	0.48	0/3416	0.62	1/4606 (0.0%)
All	All	0.48	0/6832	0.61	1/9212 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3353	0	3356	265	0
1	B	3353	0	3356	238	0
2	A	36	6	0	3	0
2	B	36	6	0	2	0
3	A	27	12	12	4	0
3	B	27	12	12	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	6838	36	6736	496	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 37.

The worst 5 of 496 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:378:ARG:HG3	1:A:398:THR:HG23	1.25	1.14
1:B:260:THR:HG23	1:B:264:ILE:HG22	1.45	0.94
1:A:183:GLU:OE1	1:A:183:GLU:N	2.01	0.94
1:B:23:LEU:HD23	1:B:25:LEU:HD21	1.54	0.90
1:B:39:ILE:HG13	1:B:145:ILE:HD13	1.52	0.89

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	412/470 (88%)	344 (84%)	54 (13%)	14 (3%)	3	20
1	B	412/470 (88%)	356 (86%)	44 (11%)	12 (3%)	4	24
All	All	824/940 (88%)	700 (85%)	98 (12%)	26 (3%)	4	22

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	ALA
1	B	385	PRO

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Mol	Chain	Res	Type
1	A	202	GLU
1	A	208	GLU
1	A	327	ASN

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	376/415 (91%)	334 (89%)	42 (11%)	6	24
1	B	376/415 (91%)	327 (87%)	49 (13%)	4	19
All	All	752/830 (91%)	661 (88%)	91 (12%)	5	21

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	376	GLN
1	A	12	ASP
1	A	391	SER
1	B	382	ASP
1	B	418	SER

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

Mol	Chain	Res	Type
1	B	80	ASN
1	A	376	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
3	ADP	B	502	4	24,29,29	0.82	0	29,45,45	1.59	5 (17%)
3	ADP	A	502	4	24,29,29	0.89	1 (4%)	29,45,45	1.50	3 (10%)
2	KGN	A	501	-	36,36,36	0.97	4 (11%)	54,60,60	1.51	6 (11%)
2	KGN	B	501	-	36,36,36	0.94	2 (5%)	54,60,60	1.44	8 (14%)

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	ADP	B	502	4	-	8/12/32/32	0/3/3/3
3	ADP	A	502	4	-	5/12/32/32	0/3/3/3
2	KGN	A	501	-	-	5/30/54/54	0/1/1/1
2	KGN	B	501	-	-	8/30/54/54	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	KGN	P4-O14	2.91	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ADP	C5-C4	2.30	1.47	1.40
2	B	501	KGN	P6-O16	2.16	1.63	1.59
2	A	501	KGN	P3-O13	2.08	1.63	1.59
2	A	501	KGN	P6-O16	2.07	1.63	1.59

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	KGN	C3-C2-C1	5.39	122.20	110.41
3	B	502	ADP	N3-C2-N1	-4.02	122.39	128.68
3	A	502	ADP	PA-O3A-PB	-3.97	119.20	132.83
2	B	501	KGN	O16-C6-C5	3.74	117.50	108.69
2	A	501	KGN	O16-C6-C5	3.64	117.28	108.69

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	ADP	O4'-C4'-C5'-O5'
3	B	502	ADP	PA-O3A-PB-O2B
3	B	502	ADP	C5'-O5'-PA-O2A
2	B	501	KGN	C3-O13-P3-O23
2	B	501	KGN	C2-C3-O13-P3

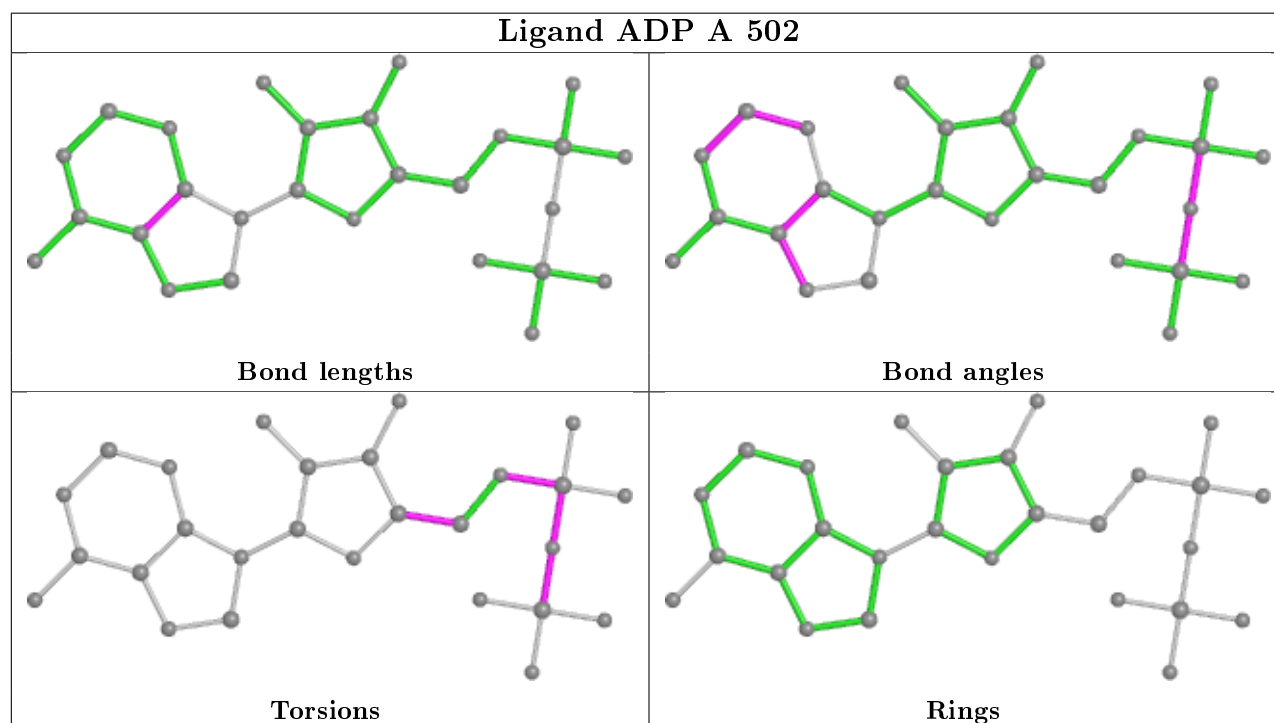
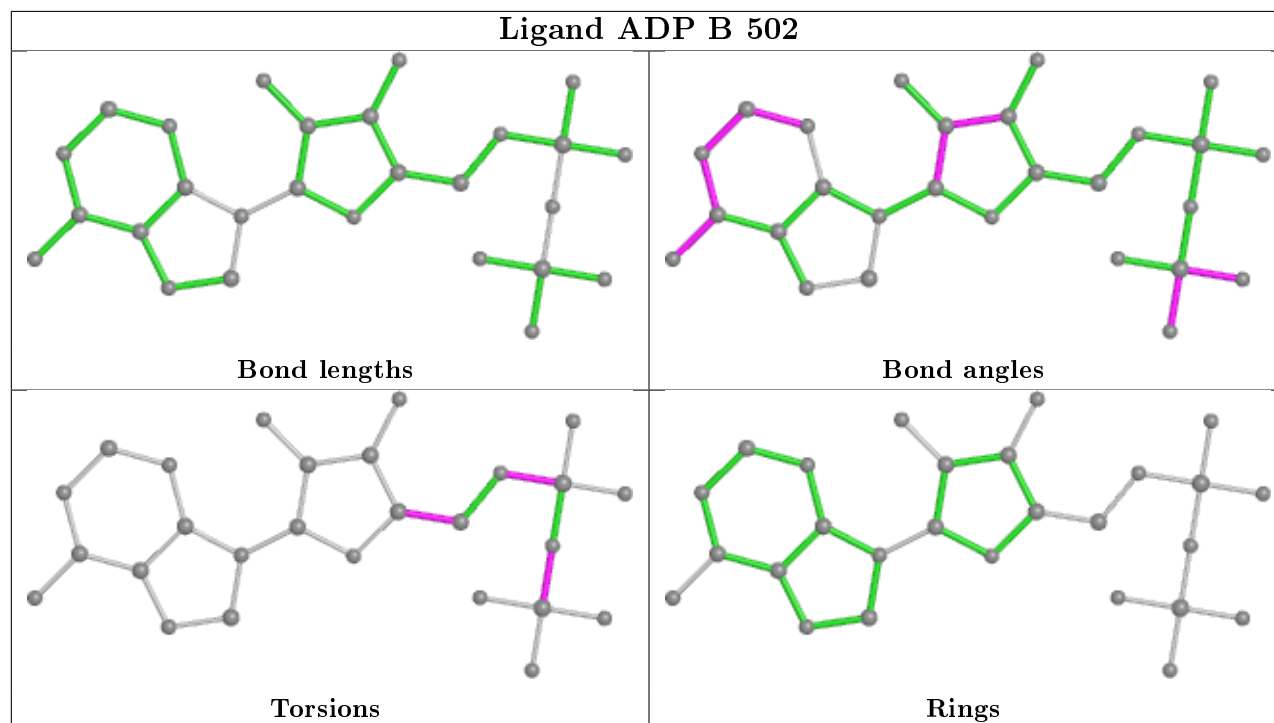
There are no ring outliers.

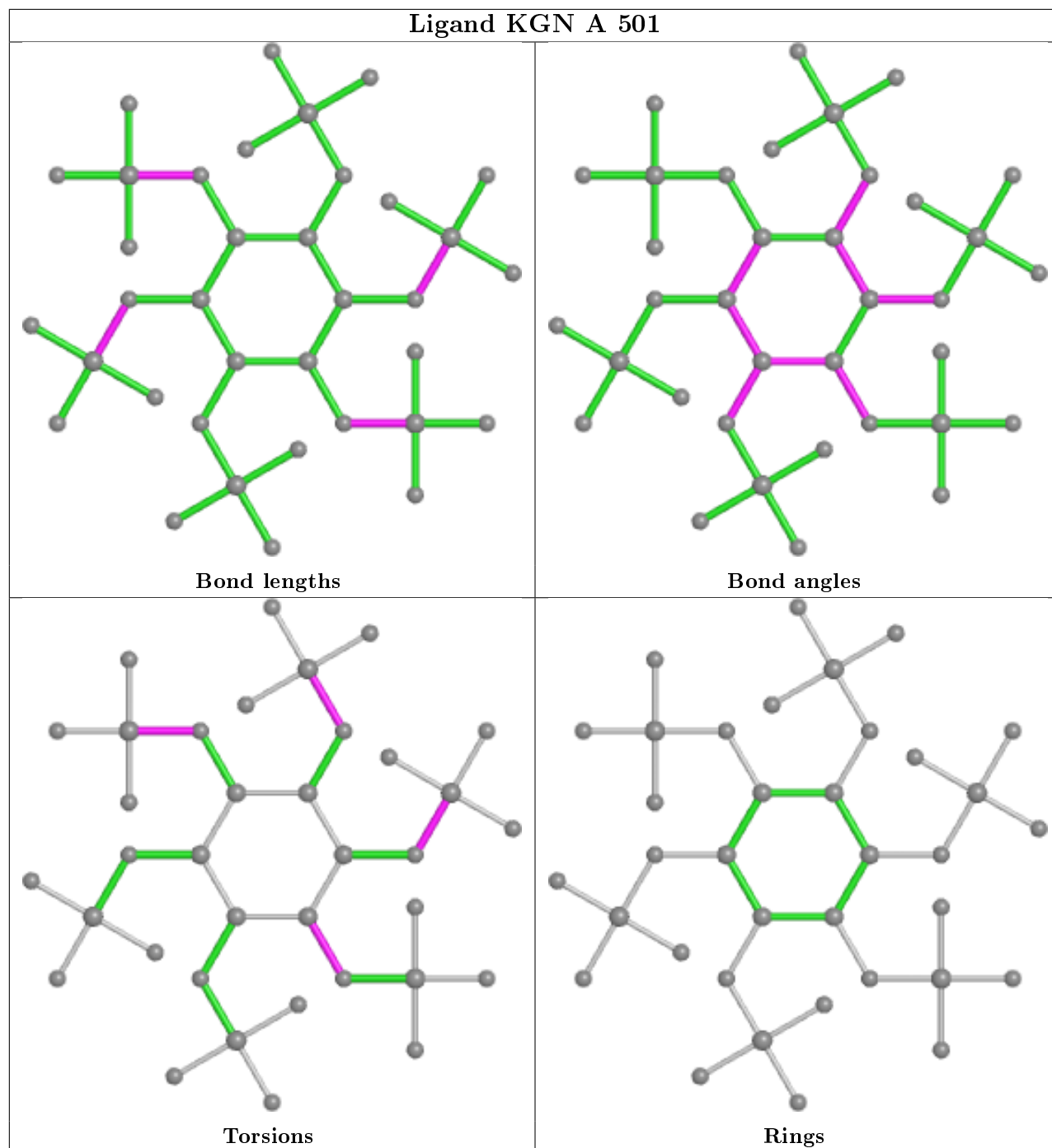
4 monomers are involved in 12 short contacts:

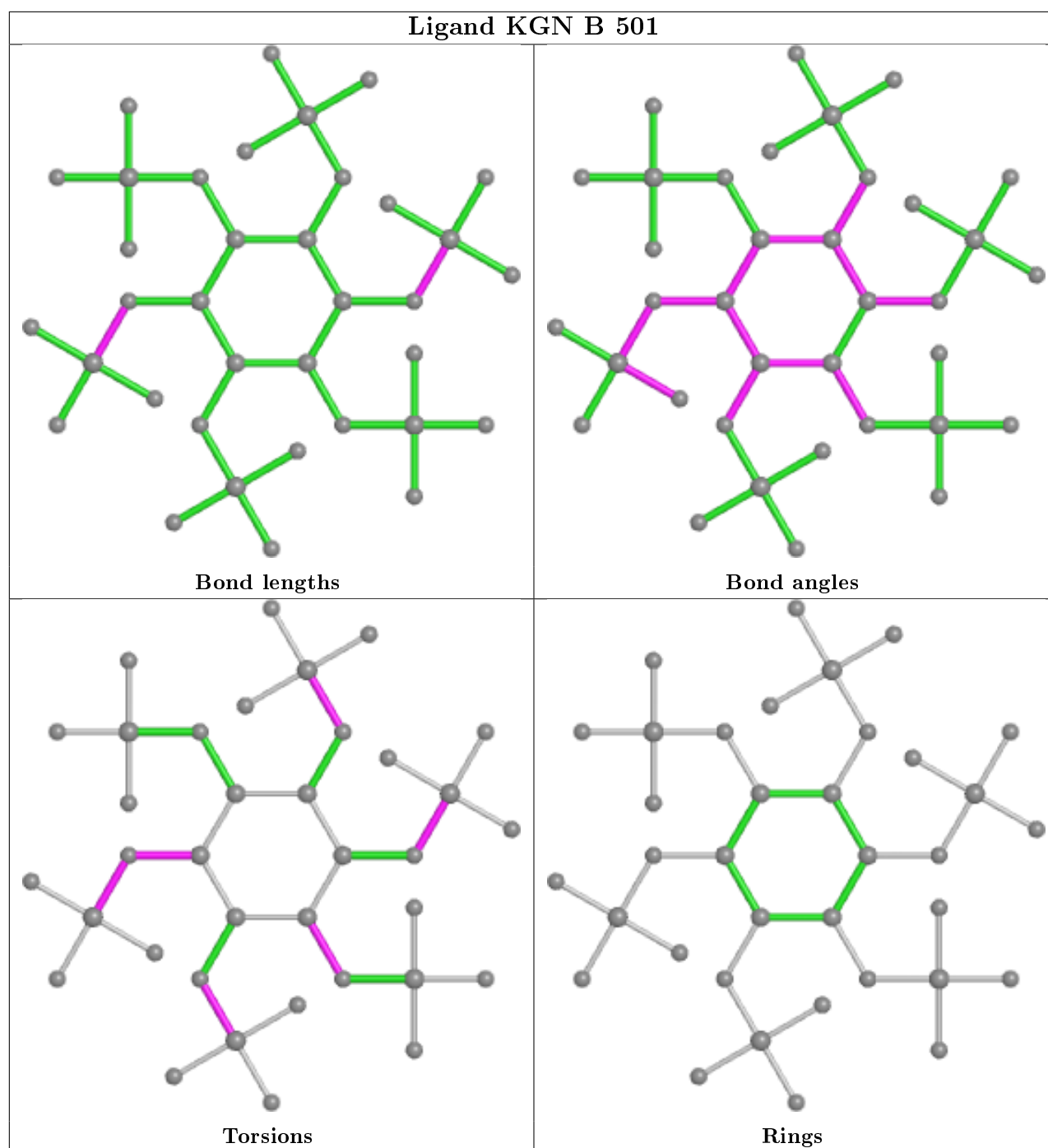
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ADP	3	0
3	A	502	ADP	4	0
2	A	501	KGN	3	0
2	B	501	KGN	2	0

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 [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	420/470 (89%)	-0.26	4 (0%)	82 59	27, 53, 84, 147	0
1	B	420/470 (89%)	-0.30	6 (1%)	75 49	25, 47, 78, 113	0
All	All	840/940 (89%)	-0.28	10 (1%)	79 54	25, 50, 81, 147	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	SER	3.4
1	A	47	ASN	3.1
1	B	382	ASP	2.8
1	A	382	ASP	2.7
1	B	381	TRP	2.7

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](#)

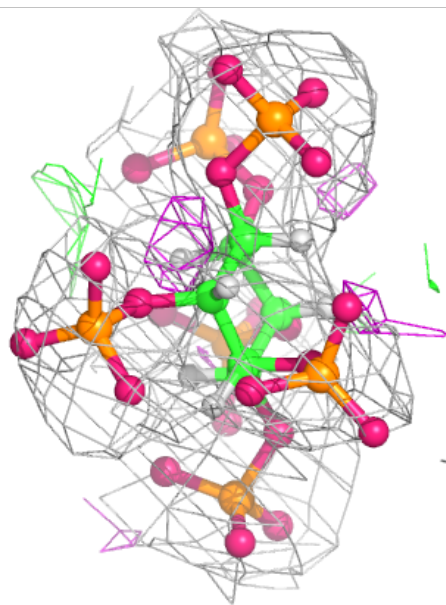
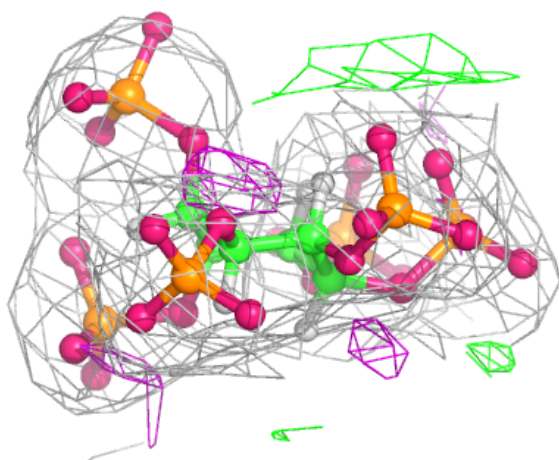
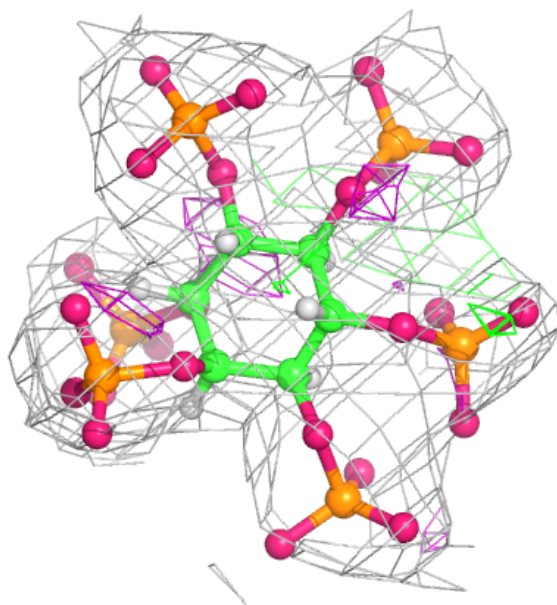
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	KGN	B	501	36/36	0.88	0.20	53,78,100,102	0
4	MG	A	503	1/1	0.91	0.56	53,53,53,53	0
2	KGN	A	501	36/36	0.91	0.20	51,73,85,87	42
4	MG	B	504	1/1	0.92	0.51	43,43,43,43	0
3	ADP	A	502	27/27	0.94	0.24	45,55,66,66	0
3	ADP	B	502	27/27	0.94	0.28	36,46,57,57	39
4	MG	A	504	1/1	0.97	0.27	53,53,53,53	0
5	ZN	B	505	1/1	0.98	0.07	45,45,45,45	0
4	MG	B	503	1/1	0.98	0.36	45,45,45,45	0
5	ZN	A	505	1/1	1.00	0.05	42,42,42,42	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.

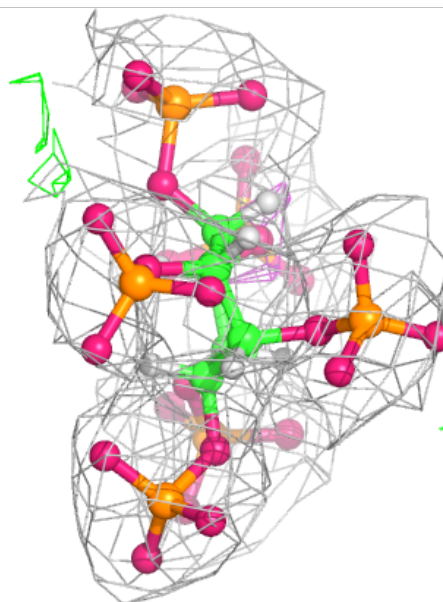
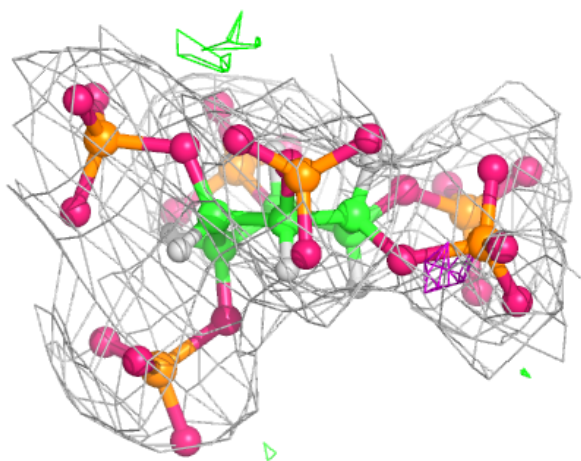
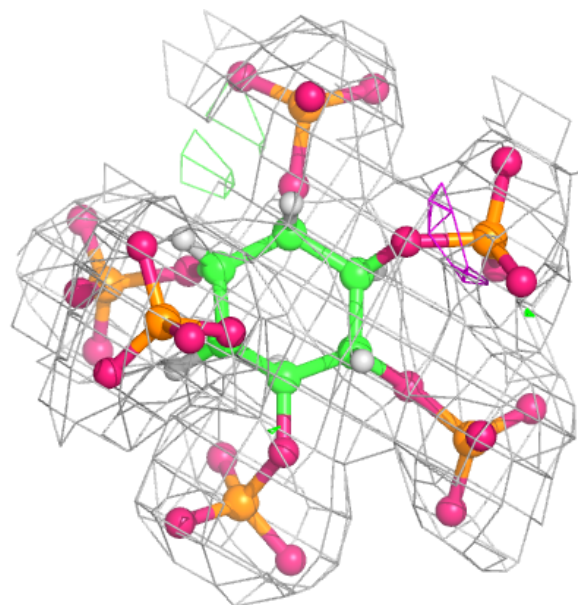
Electron density around KGN B 501:

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



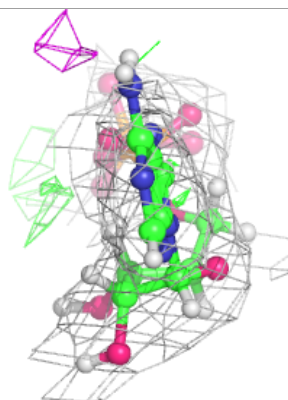
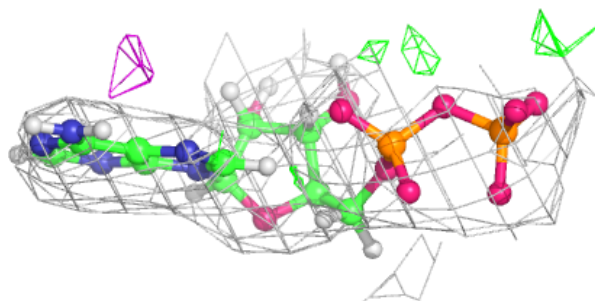
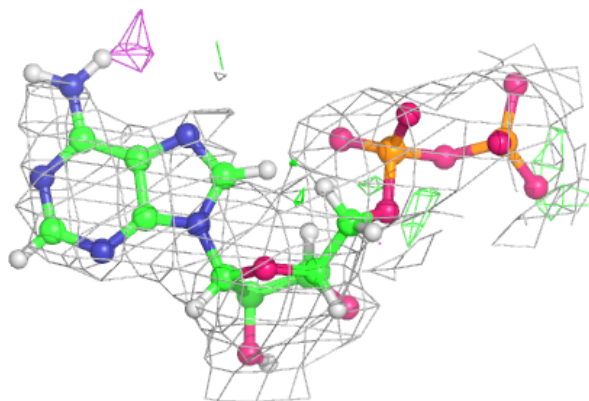
Electron density around KGN A 501:

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

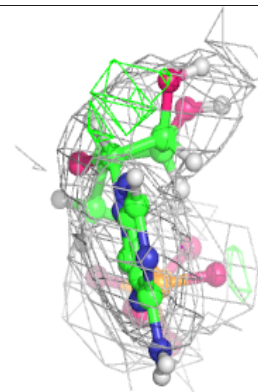
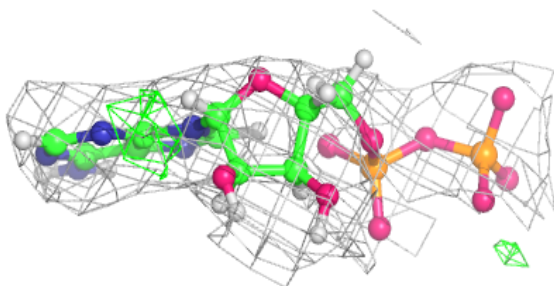
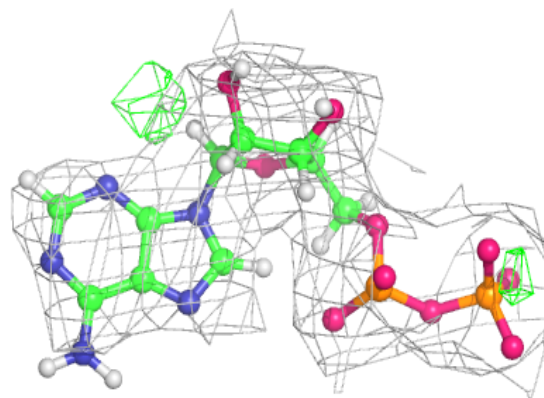


Electron density around ADP A 502:

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

**Electron density around ADP B 502:**

$2mF_o-DF_c$ (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.