wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 06:00 PM EDT

PDB ID	:	1RFU
Title	:	Crystal structure of pyridoxal kinase complexed with ADP and PLP
Authors	:	Liang, D.-C.; Jiang, T.; Li, M.-H.
Deposited on	:	2003-11-10
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

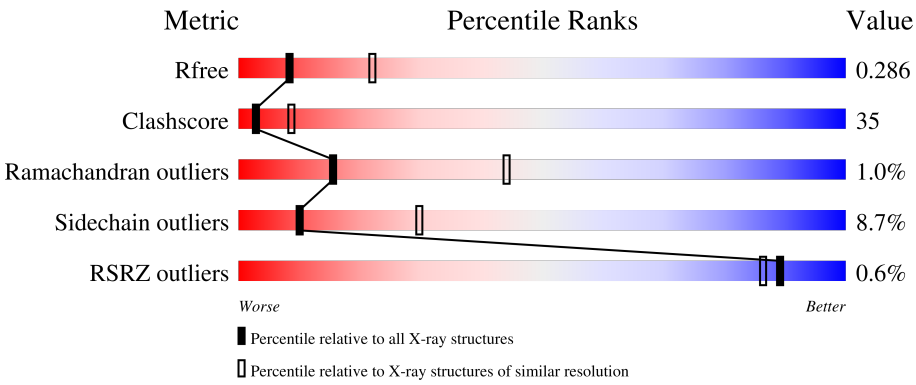
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	312	46% 49% 5%
1	B	312	39% 54% 7%
1	C	312	.% 41% 52% 7%
1	D	312	2% 40% 54% 6%
1	E	312	42% 53% 5%

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Mol	Chain	Length	Quality of chain
1	F	312	44% 51% •
1	G	312	42% 53% 5%
1	H	312	% 37% 58% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20123 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 pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	312	2439	1532	427	463	17	0	0	0
1	B	312	2439	1532	427	463	17	0	0	0
1	C	312	2439	1532	427	463	17	0	0	0
1	D	312	2439	1532	427	463	17	0	0	0
1	E	312	2439	1532	427	463	17	0	0	0
1	F	312	2439	1532	427	463	17	0	0	0
1	G	312	2439	1532	427	463	17	0	0	0
1	H	312	2439	1532	427	463	17	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

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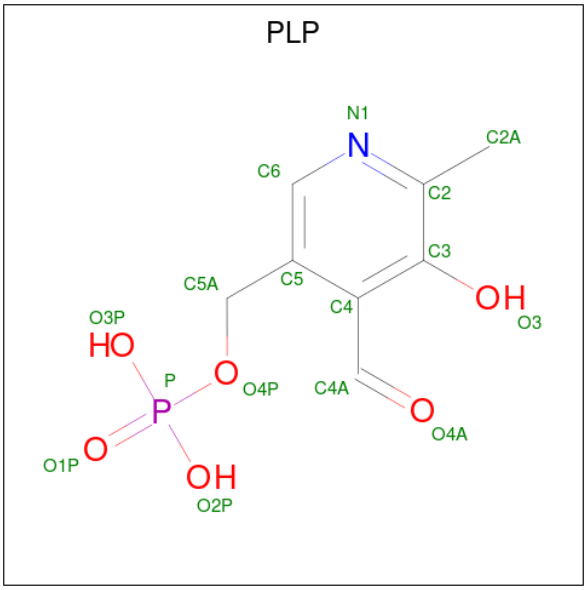
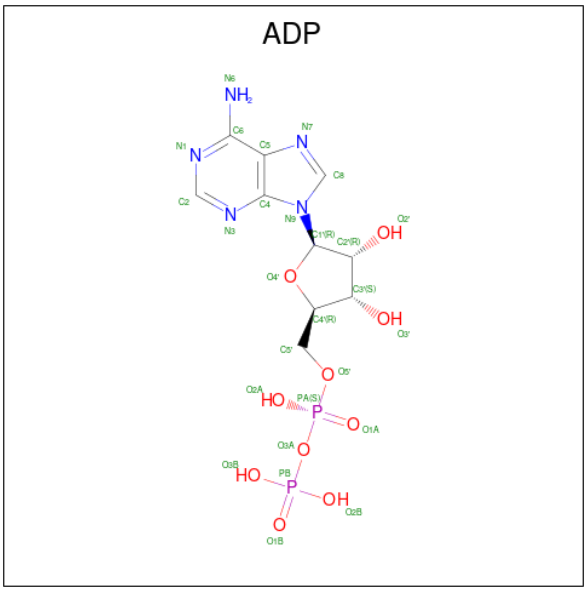
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 15 8 1 5 1	0	0
3	B	1	Total C N O P 15 8 1 5 1	0	0
3	C	1	Total C N O P 15 8 1 5 1	0	0
3	D	1	Total C N O P 15 8 1 5 1	0	0
3	E	1	Total C N O P 15 8 1 5 1	0	0
3	F	1	Total C N O P 15 8 1 5 1	0	0
3	G	1	Total C N O P 15 8 1 5 1	0	0
3	H	1	Total C N O P 15 8 1 5 1	0	0

- 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
			Total	C	N	O	P		
4	A	1	27	10	5	10	2	0	0
4	B	1	27	10	5	10	2	0	0
4	C	1	27	10	5	10	2	0	0
4	D	1	27	10	5	10	2	0	0
4	E	1	27	10	5	10	2	0	0
4	F	1	27	10	5	10	2	0	0
4	G	1	27	10	5	10	2	0	0
4	H	1	27	10	5	10	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	73	73	73	0	0
5	B	54	54	54	0	0
5	C	20	20	20	0	0
5	D	9	9	9	0	0

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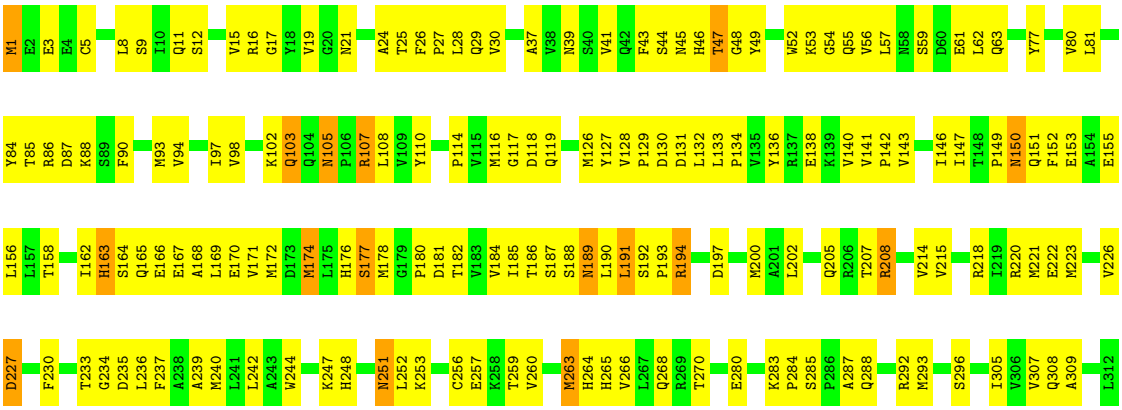
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	41	41	41	0	0
			Total	O		
5	F	37	37	37	0	0
			Total	O		
5	G	21	21	21	0	0
			Total	O		
5	H	12	12	12	0	0

3 Residue-property plots (i)

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.

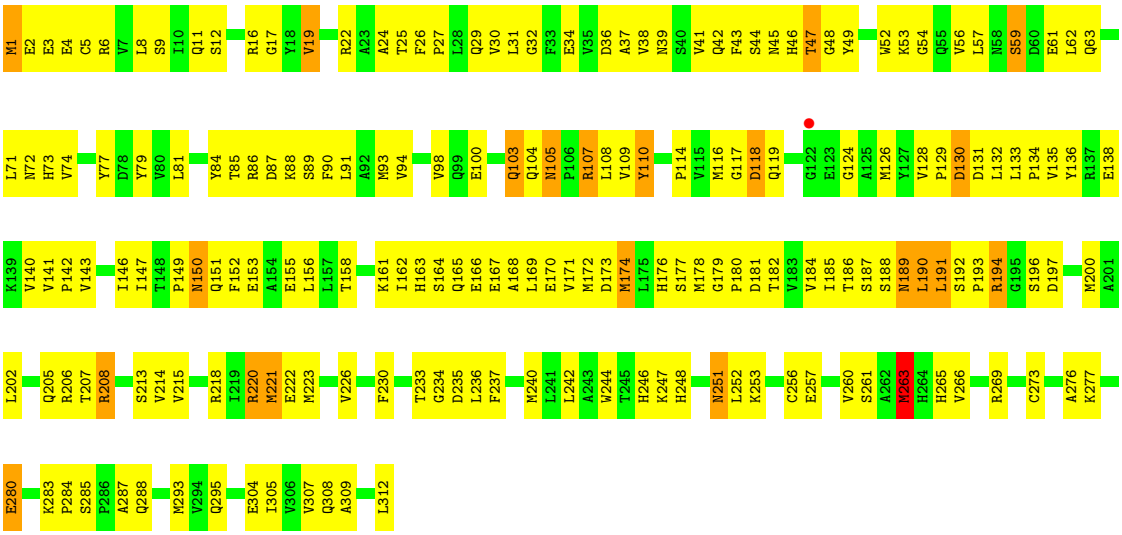
- Molecule 1: pyridoxal kinase

Chain A: 46% 49% 5%



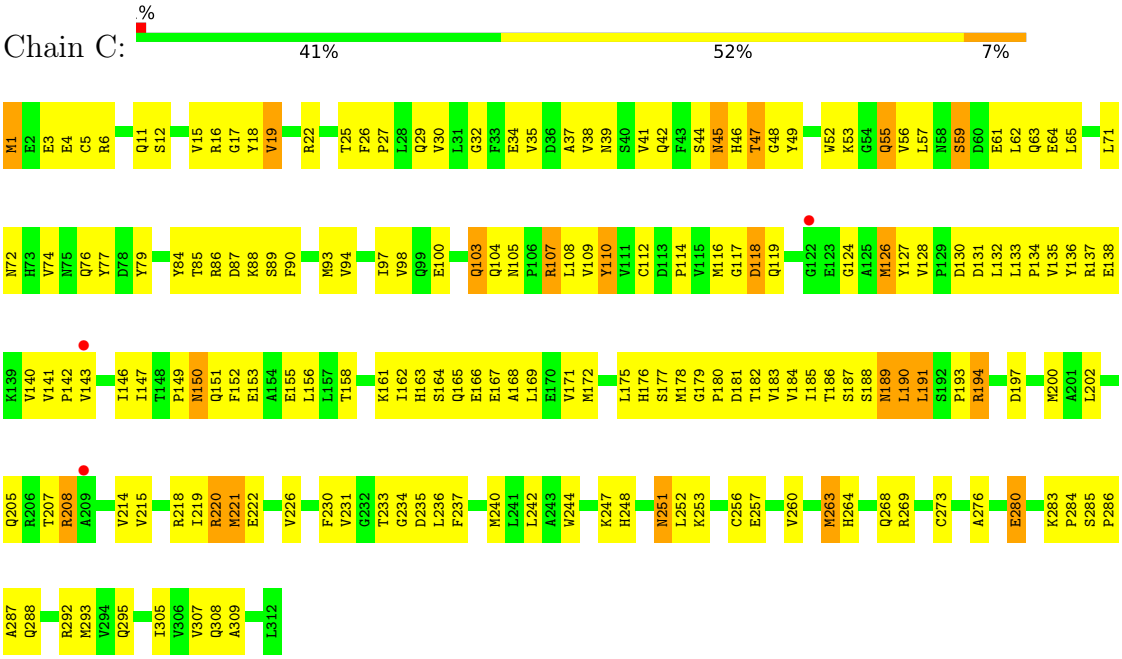
- Molecule 1: pyridoxal kinase

Chain B: 39% 54% 7%



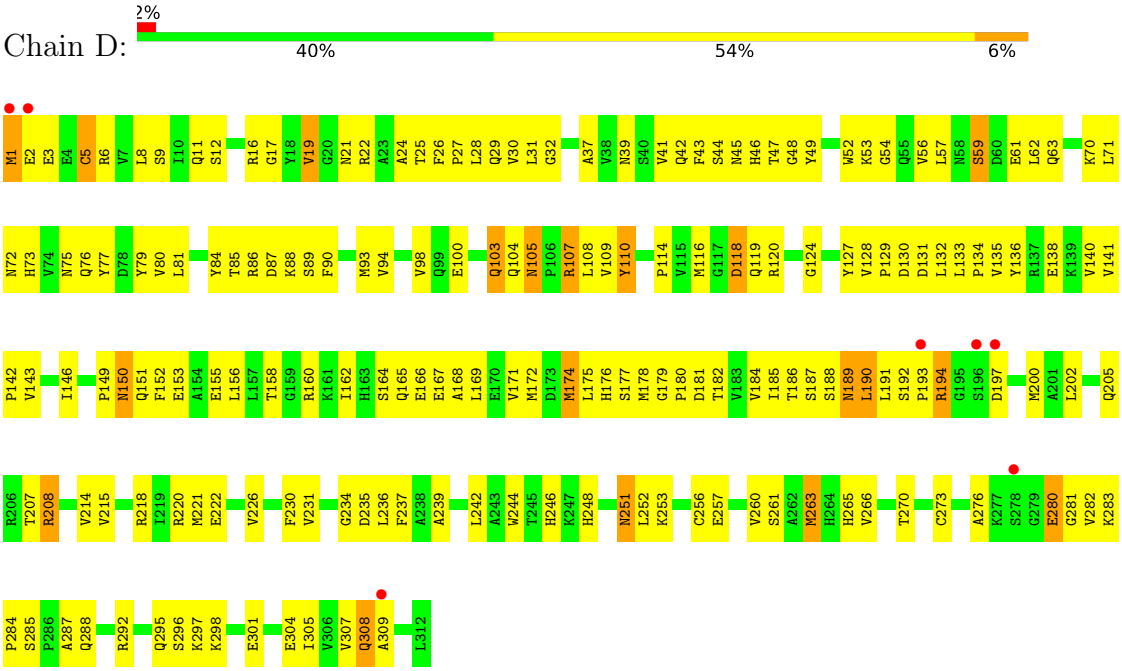
- Molecule 1: pyridoxal kinase

Chain C:



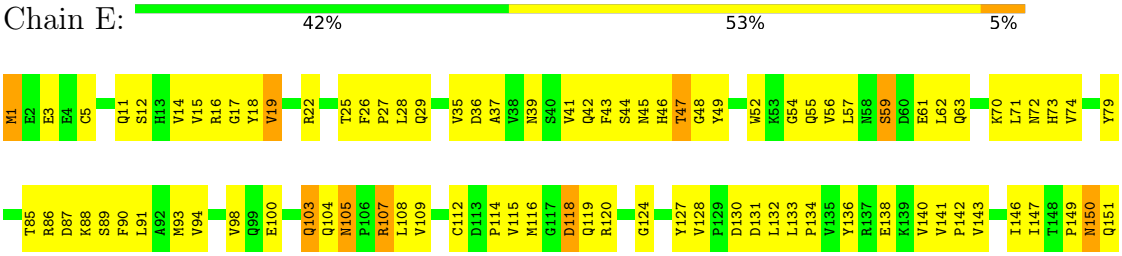
• Molecule 1: pyridoxal kinase

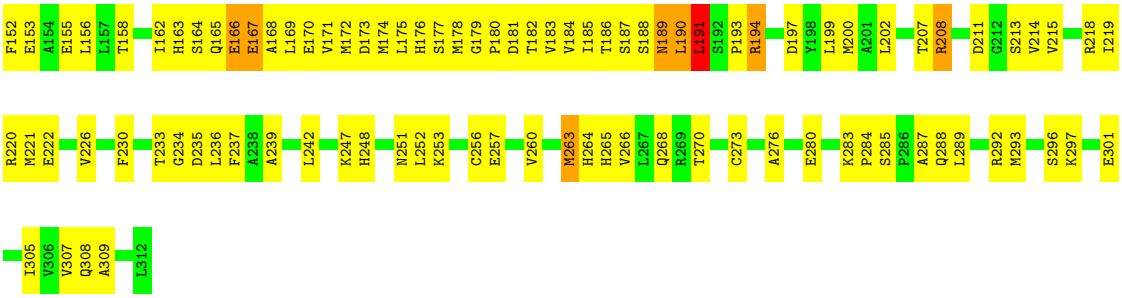
Chain D:



• Molecule 1: pyridoxal kinase

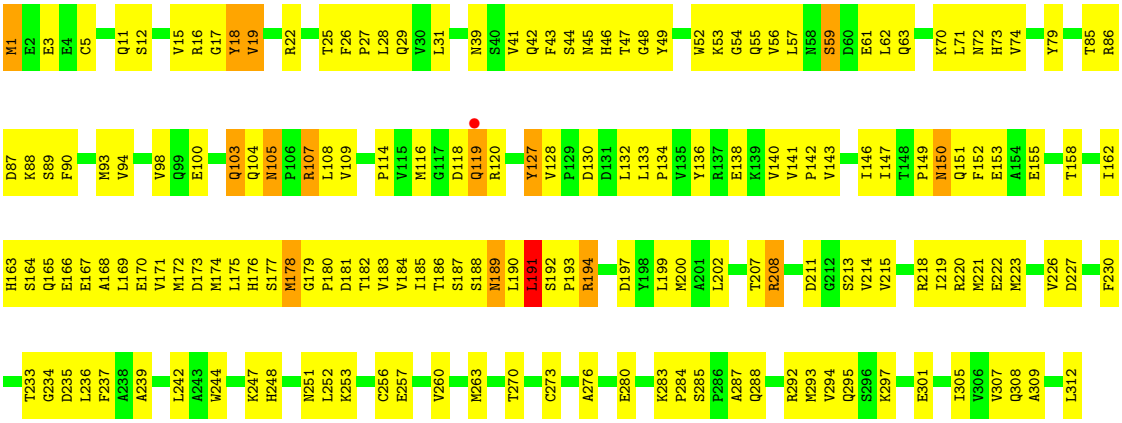
Chain E:





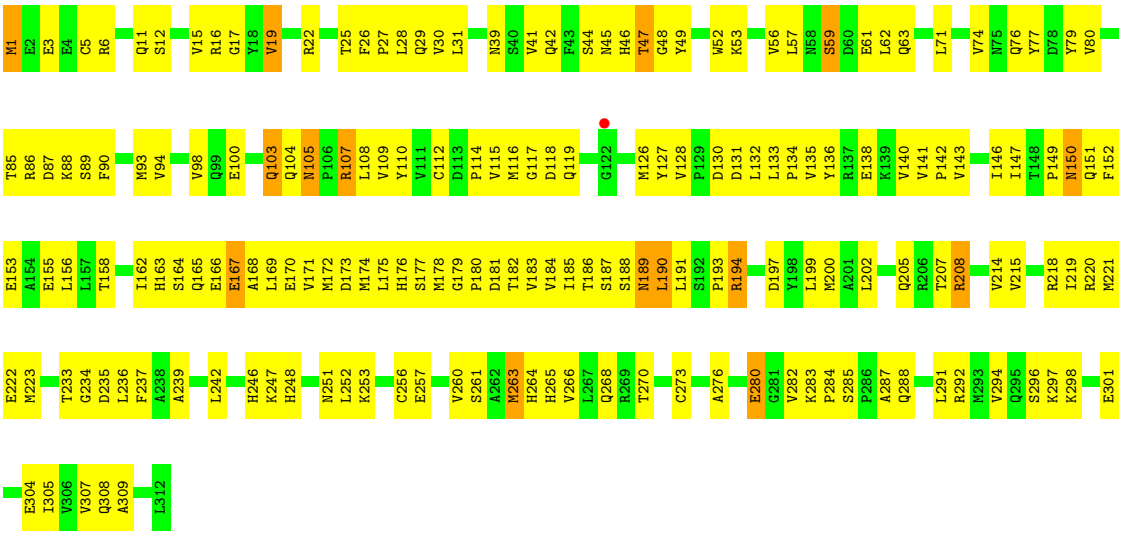
- Molecule 1: pyridoxal kinase

Chain F:



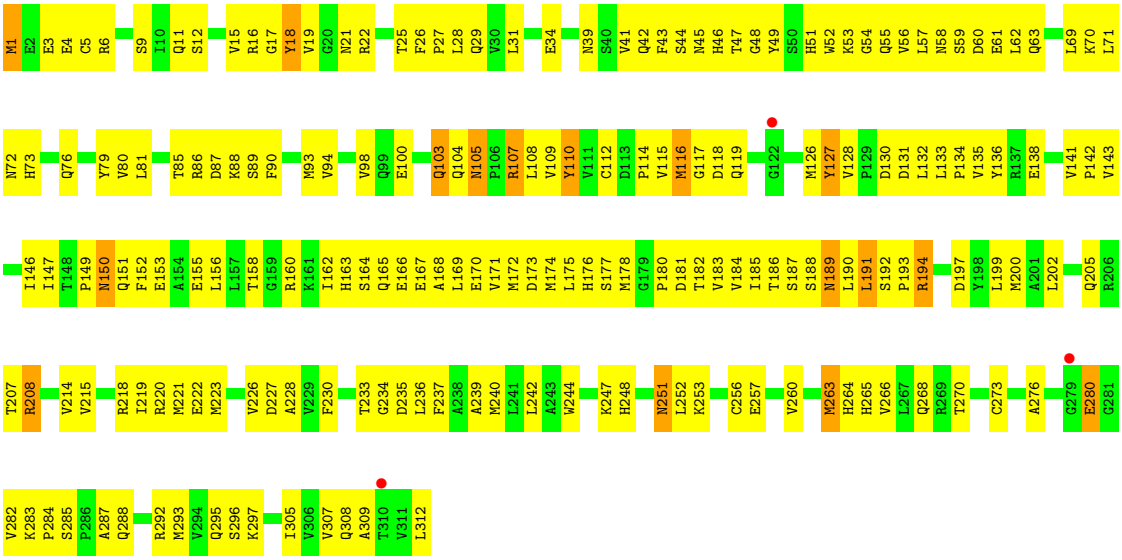
- Molecule 1: pyridoxal kinase

Chain G:



- Molecule 1: pyridoxal kinase

Chain H:


M1 E2 E3 E4 C5 R6 S9 I10 Q11 S12 V15 R16 G17 Y18 V19 G20 N21 R22 T25 F26 P27 L28 Q29 V30 L31 E34 N39 S40 V41 Q42 F43 S44 M45 H46 T47 G48 Y49 S50 H51 W52 K53 G54 Q55 V56 L57 N58 S59 D60 E61 L62 Q63 L69 K70 L71
N72 H73 Q76 Y79 V80 L81 T85 R86 D87 K88 S89 F90 M93 V94 V98 Q99 E100 Q103 Q104 N105 P106 R107 L108 V109 Y110 V111 C112 D113 P114 V115 M116 G117 D118 Q119 G122 M126 Y127 V128 P129 D130 D131 L132 L133 P134 V135 Y136 R137 E138 V141 P142 V143
I146 I147 T148 P149 N150 Q151 F152 E153 A154 E155 L156 L157 T158 G159 R160 K161 I162 H163 S164 Q165 E166 E167 A168 L169 E170 V171 M172 D173 L174 M174 L175 H176 S177 M178 G179 P180 D181 T182 V183 V184 I185 T186 S187 S188 N189 L190 L191 S192 P193 R194 D197 Y198 L199 M200 A201 L202 Q205 R206
T207 R208 V214 V215 R218 I219 R220 M221 E222 M223 V226 D227 A228 V229 F230 T233 G234 D235 L236 F237 A238 A239 M240 L241 L242 A243 W244 K247 H248 N251 L252 K253 C256 E257 V260 M263 H264 H265 V266 L267 Q268 R269 T270 C273 A276 G279 E280 G281
V282 K283 P284 S285 P286 A287 Q288 R292 M293 V294 Q295 S296 K297 I305 V306 V307 Q308 A309 T310 V311 L312

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	109.09Å 109.09Å 284.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.5 (20.00-2.80) 56.7 (19.94-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.238 , 0.286	Depositor DCC
R_{free} test set	3623 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20123	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5074e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PLP, ADP, ZN

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	0.51	0/2484	0.74	1/3367 (0.0%)
1	B	0.54	0/2484	0.79	5/3367 (0.1%)
1	C	0.47	0/2484	0.74	3/3367 (0.1%)
1	D	0.45	0/2484	0.71	1/3367 (0.0%)
1	E	0.54	0/2484	0.76	1/3367 (0.0%)
1	F	0.55	0/2484	0.76	1/3367 (0.0%)
1	G	0.45	0/2484	0.71	1/3367 (0.0%)
1	H	0.44	0/2484	0.71	1/3367 (0.0%)
All	All	0.50	0/19872	0.74	14/26936 (0.1%)

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	E	0	1
1	F	0	2
1	H	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	C	220	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	F	178	MET	CG-SD-CE	6.12	110.00	100.20
1	B	221	MET	CG-SD-CE	6.12	109.99	100.20
1	C	126	MET	CG-SD-CE	6.12	109.99	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	18	TYR	Sidechain
1	F	127	TYR	Sidechain
1	F	18	TYR	Sidechain
1	H	127	TYR	Sidechain
1	H	18	TYR	Sidechain

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	2439	0	2442	176	0
1	B	2439	0	2442	200	0
1	C	2439	0	2442	198	0
1	D	2439	0	2442	182	0
1	E	2439	0	2442	172	0
1	F	2439	0	2442	180	0
1	G	2439	0	2442	163	0
1	H	2439	0	2442	209	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	15	0	7	2	0
3	B	15	0	6	1	0
3	C	15	0	6	1	0
3	D	15	0	7	1	0
3	E	15	0	6	1	0
3	F	15	0	7	2	0
3	G	15	0	6	1	0
3	H	15	0	7	1	0
4	A	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	2	0
4	G	27	0	12	1	0
4	H	27	0	12	2	0
5	A	73	0	0	4	0
5	B	54	0	0	5	0
5	C	20	0	0	2	0
5	D	9	0	0	2	0
5	E	41	0	0	3	0
5	F	37	0	0	5	0
5	G	21	0	0	2	0
5	H	12	0	0	3	0
All	All	20123	0	19684	1390	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 35.

The worst 5 of 1390 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:129:PRO:HG3	1:B:191:LEU:HB2	1.22	1.19
1:B:39:ASN:H	1:F:42:GLN:HE22	1.07	0.95
1:A:191:LEU:HB2	1:D:129:PRO:HG3	1.50	0.93
1:H:208:ARG:HH11	1:H:208:ARG:HG3	1.31	0.93
1:A:39:ASN:H	1:E:42:GLN:HE22	1.05	0.92

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	310/312 (99%)	279 (90%)	29 (9%)	2 (1%)	25	56
1	B	310/312 (99%)	276 (89%)	30 (10%)	4 (1%)	12	36
1	C	310/312 (99%)	272 (88%)	34 (11%)	4 (1%)	12	36
1	D	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	25	56
1	E	310/312 (99%)	274 (88%)	31 (10%)	5 (2%)	9	31
1	F	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	25	56
1	G	310/312 (99%)	275 (89%)	32 (10%)	3 (1%)	15	44
1	H	310/312 (99%)	271 (87%)	36 (12%)	3 (1%)	15	44
All	All	2480/2496 (99%)	2195 (88%)	260 (10%)	25 (1%)	15	44

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	D	191	LEU
1	H	191	LEU
1	B	191	LEU
1	C	191	LEU

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	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	B	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	C	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	D	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	E	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	F	273/273 (100%)	251 (92%)	22 (8%)	11	33
1	G	273/273 (100%)	250 (92%)	23 (8%)	11	31
1	H	273/273 (100%)	248 (91%)	25 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2184/2184 (100%)	1994 (91%)	190 (9%)	10 30

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	197	ASP
1	G	3	GLU
1	E	308	GLN
1	F	127	TYR
1	G	112	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	308	GLN
1	H	55	GLN
1	G	21	ASN
1	G	105	ASN
1	H	150	ASN

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 (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	PLP	D	3401	2	15,15,16	1.62	2 (13%)	20,22,23	2.16	4 (20%)
4	ADP	C	2402	2	24,29,29	1.72	6 (25%)	29,45,45	1.55	2 (6%)
3	PLP	F	5401	2	15,15,16	1.65	2 (13%)	20,22,23	2.07	4 (20%)
4	ADP	D	3402	2	24,29,29	1.68	6 (25%)	29,45,45	1.57	3 (10%)
4	ADP	H	7402	2	24,29,29	1.68	6 (25%)	29,45,45	1.55	3 (10%)
3	PLP	G	6401	2	15,15,16	1.73	3 (20%)	20,22,23	2.05	5 (25%)
3	PLP	H	7401	2	15,15,16	1.55	3 (20%)	20,22,23	2.01	4 (20%)
4	ADP	E	4402	2	24,29,29	1.64	6 (25%)	29,45,45	1.53	3 (10%)
4	ADP	A	402	2	24,29,29	1.19	2 (8%)	29,45,45	1.60	4 (13%)
3	PLP	A	401	2	15,15,16	2.02	3 (20%)	20,22,23	2.32	6 (30%)
4	ADP	B	1402	2	24,29,29	1.72	7 (29%)	29,45,45	1.55	3 (10%)
4	ADP	G	6402	2	24,29,29	1.67	6 (25%)	29,45,45	1.53	3 (10%)
3	PLP	B	1401	2	15,15,16	1.59	3 (20%)	20,22,23	2.09	6 (30%)
3	PLP	E	4401	2	15,15,16	1.54	2 (13%)	20,22,23	2.09	5 (25%)
4	ADP	F	5402	2	24,29,29	1.71	7 (29%)	29,45,45	1.57	3 (10%)
3	PLP	C	2401	2	15,15,16	1.69	3 (20%)	20,22,23	2.01	5 (25%)

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	PLP	D	3401	2	-	2/6/6/8	0/1/1/1
4	ADP	C	2402	2	-	2/12/32/32	0/3/3/3
3	PLP	F	5401	2	-	2/6/6/8	0/1/1/1
4	ADP	D	3402	2	-	2/12/32/32	0/3/3/3
4	ADP	H	7402	2	-	2/12/32/32	0/3/3/3
3	PLP	G	6401	2	-	2/6/6/8	0/1/1/1
3	PLP	H	7401	2	-	2/6/6/8	0/1/1/1
4	ADP	E	4402	2	-	3/12/32/32	0/3/3/3
4	ADP	A	402	2	-	7/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	401	2	-	4/6/6/8	0/1/1/1
4	ADP	B	1402	2	-	2/12/32/32	0/3/3/3
4	ADP	G	6402	2	-	2/12/32/32	0/3/3/3
3	PLP	B	1401	2	-	1/6/6/8	0/1/1/1
3	PLP	E	4401	2	-	1/6/6/8	0/1/1/1
4	ADP	F	5402	2	-	2/12/32/32	0/3/3/3
3	PLP	C	2401	2	-	2/6/6/8	0/1/1/1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PLP	C5-C4	5.56	1.46	1.40
3	C	2401	PLP	C5-C4	4.35	1.45	1.40
3	D	3401	PLP	C5-C4	4.26	1.45	1.40
3	G	6401	PLP	C5-C4	4.12	1.45	1.40
3	B	1401	PLP	C5-C4	4.01	1.44	1.40

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3401	PLP	O4P-C5A-C5	6.99	122.67	109.35
4	D	3402	ADP	N3-C2-N1	-6.31	118.81	128.68
3	A	401	PLP	O4P-C5A-C5	6.29	121.33	109.35
3	G	6401	PLP	O4P-C5A-C5	6.25	121.27	109.35
4	A	402	ADP	N3-C2-N1	-6.25	118.91	128.68

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	PLP	C4-C5-C5A-O4P
3	A	401	PLP	C6-C5-C5A-O4P
3	A	401	PLP	C5A-O4P-P-O1P
3	C	2401	PLP	C4-C5-C5A-O4P
3	D	3401	PLP	C4-C5-C5A-O4P

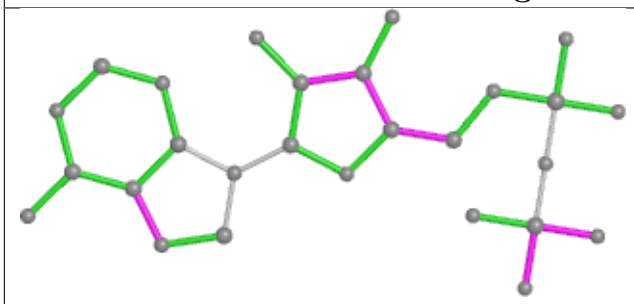
There are no ring outliers.

16 monomers are involved in 22 short contacts:

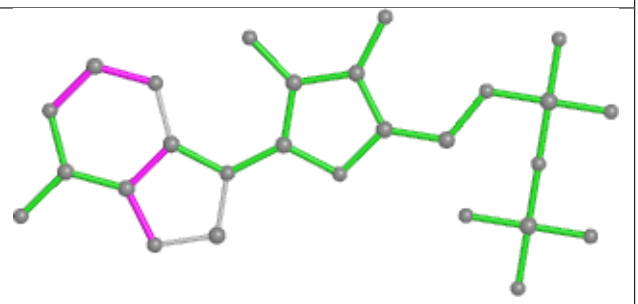
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3401	PLP	1	0
4	C	2402	ADP	1	0
3	F	5401	PLP	2	0
4	D	3402	ADP	1	0
4	H	7402	ADP	2	0
3	G	6401	PLP	1	0
3	H	7401	PLP	1	0
4	E	4402	ADP	1	0
4	A	402	ADP	3	0
3	A	401	PLP	2	0
4	B	1402	ADP	2	0
4	G	6402	ADP	1	0
3	B	1401	PLP	1	0
3	E	4401	PLP	1	0
4	F	5402	ADP	2	0
3	C	2401	PLP	1	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 then 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.

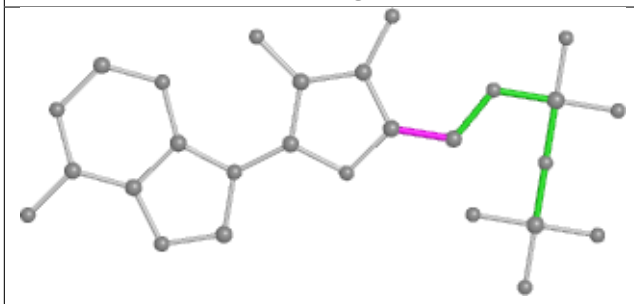
Ligand ADP C 2402



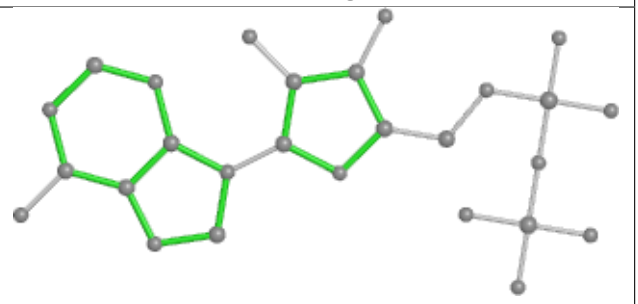
Bond lengths



Bond angles

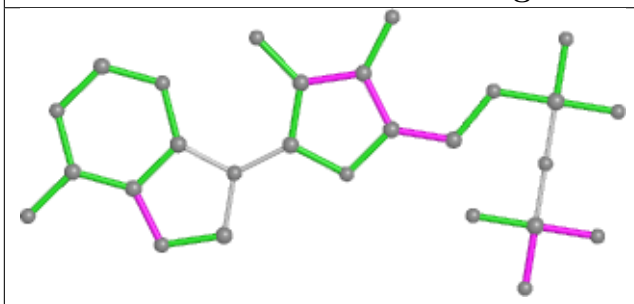


Torsions

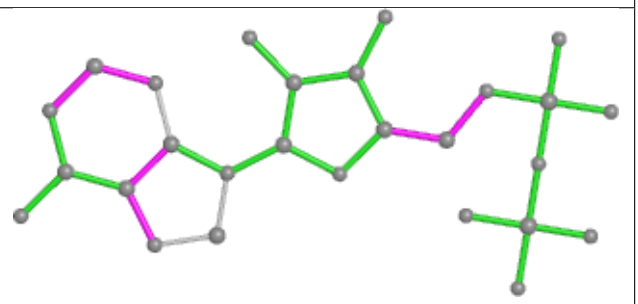


Rings

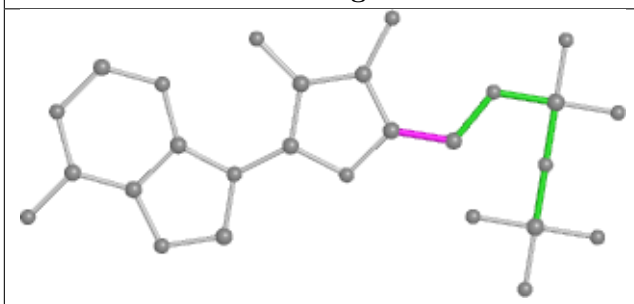
Ligand ADP D 3402



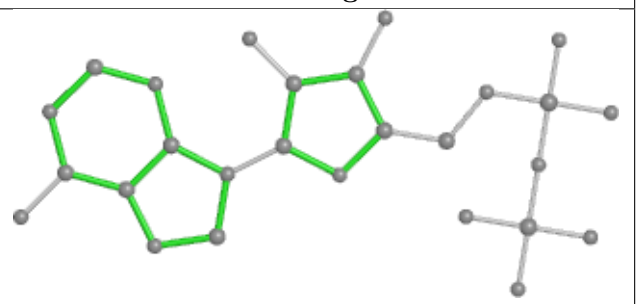
Bond lengths



Bond angles

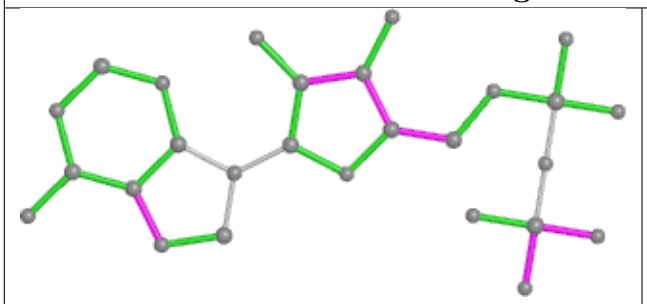


Torsions

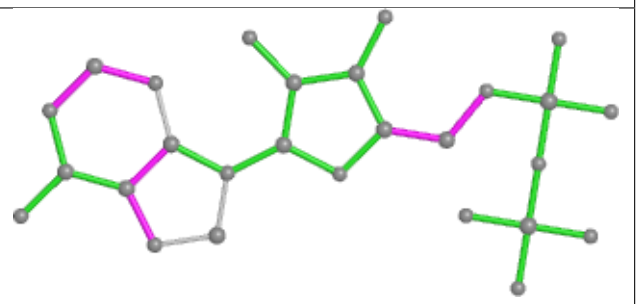


Rings

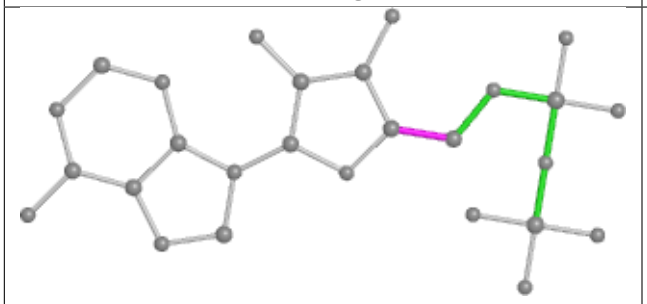
Ligand ADP H 7402



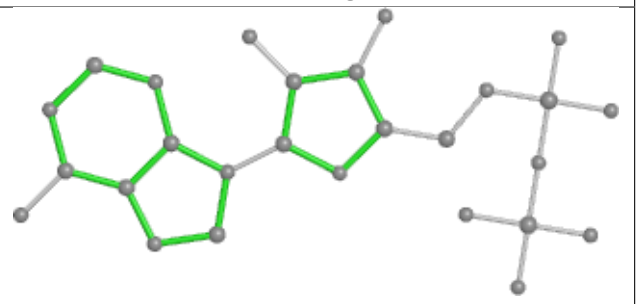
Bond lengths



Bond angles

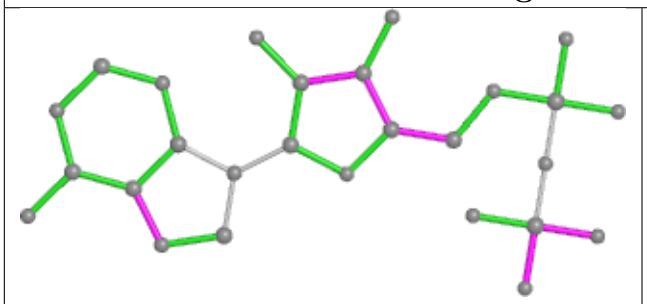


Torsions

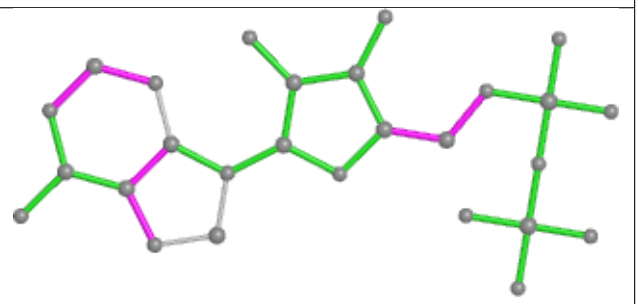


Rings

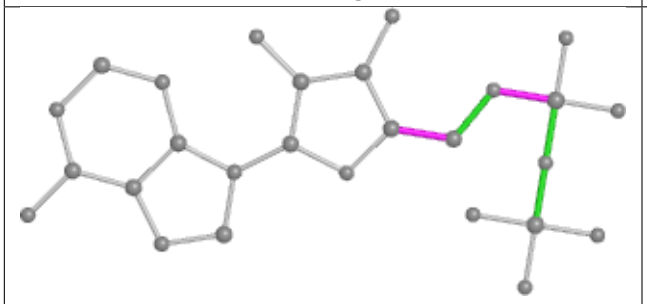
Ligand ADP E 4402



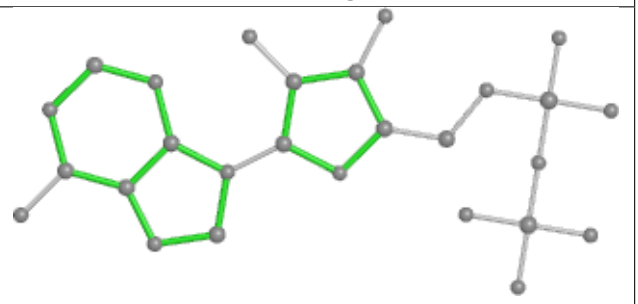
Bond lengths



Bond angles

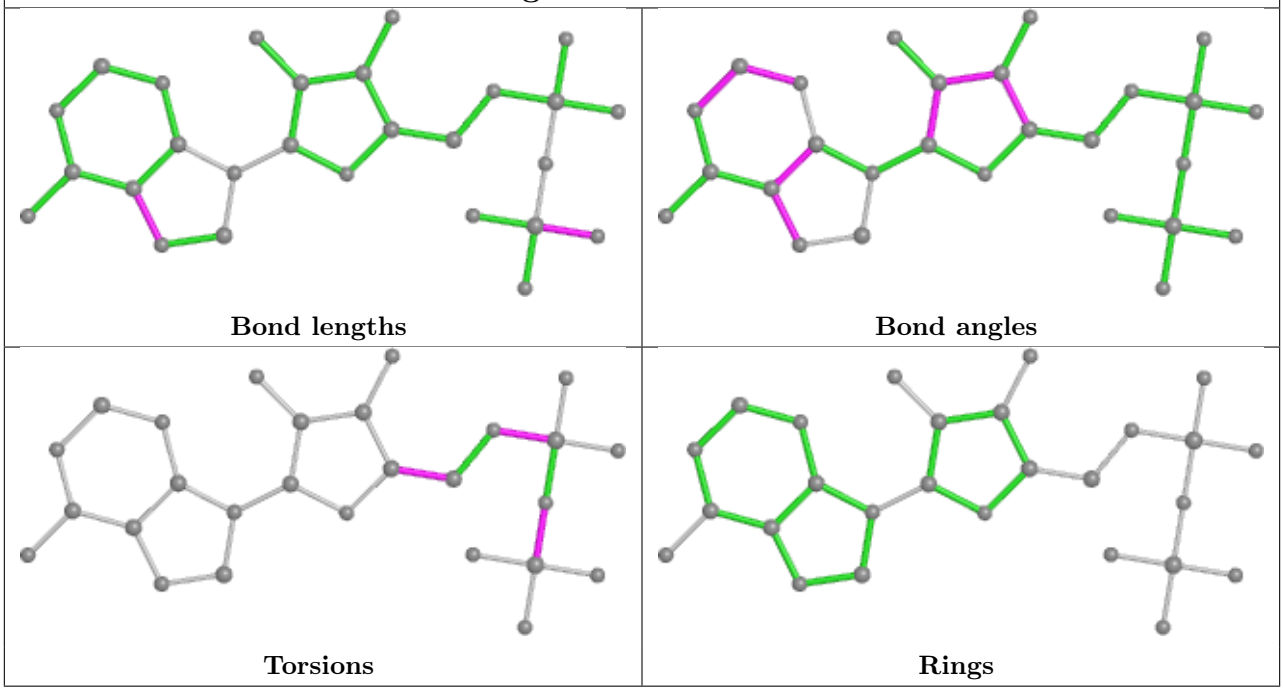


Torsions

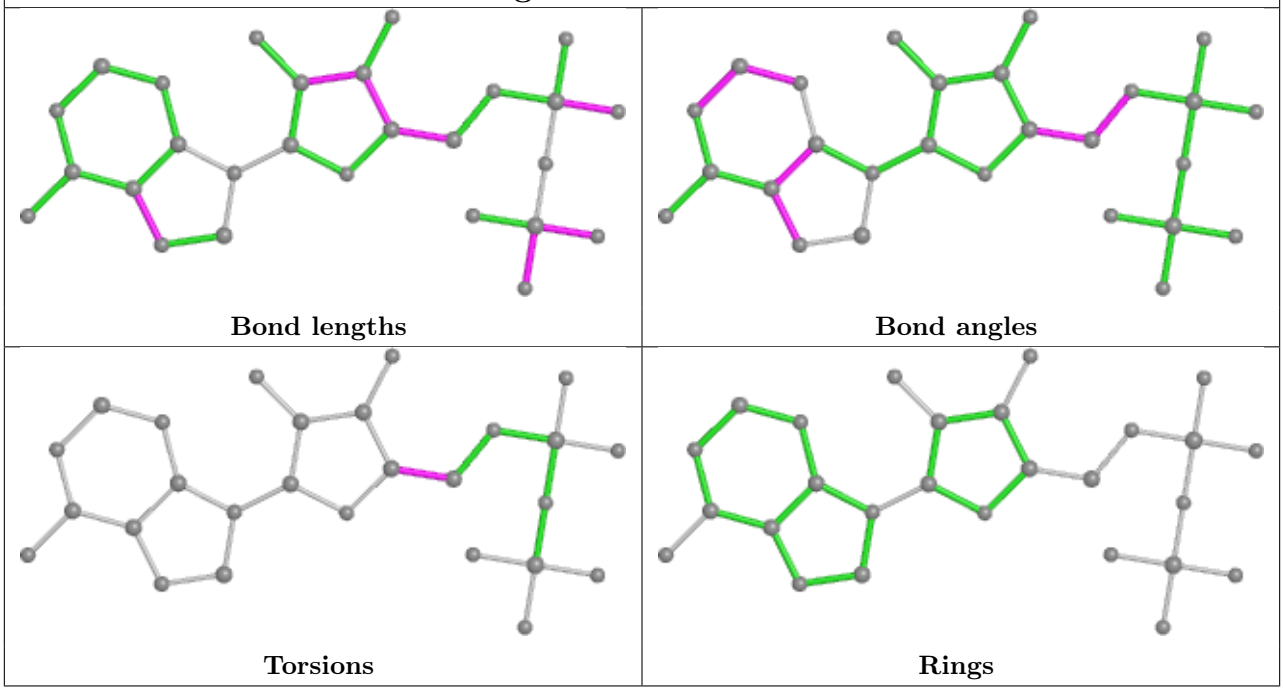


Rings

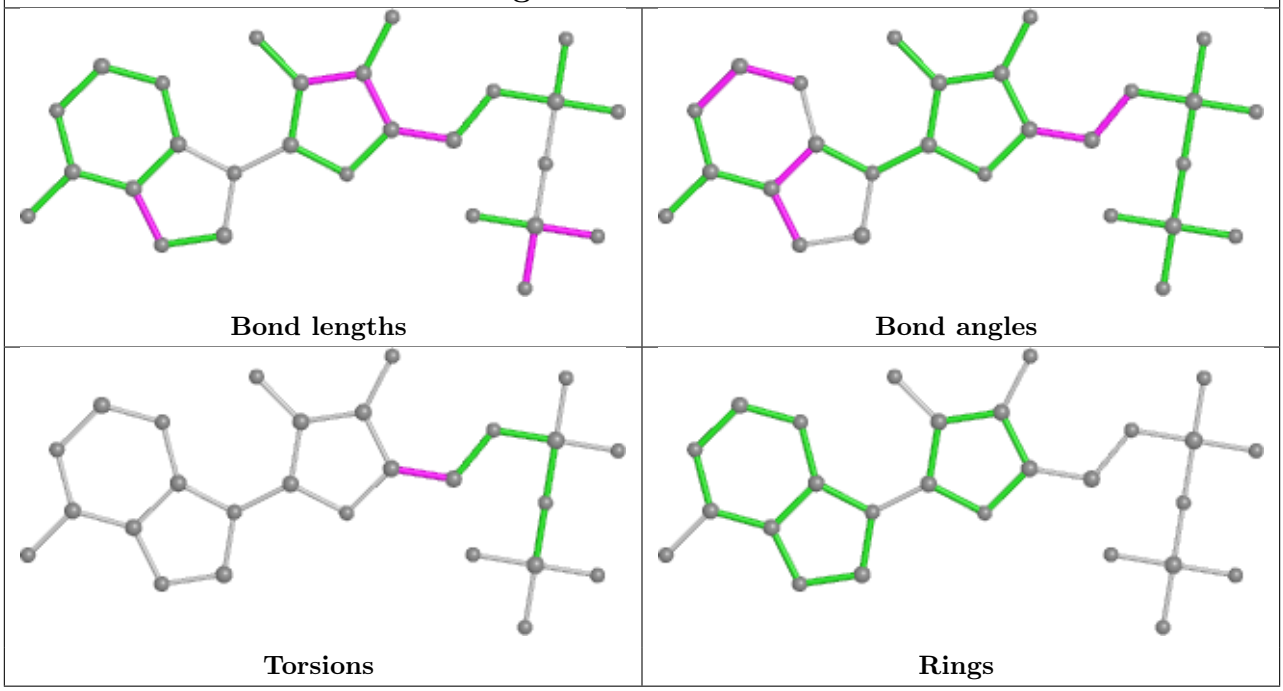
Ligand ADP A 402



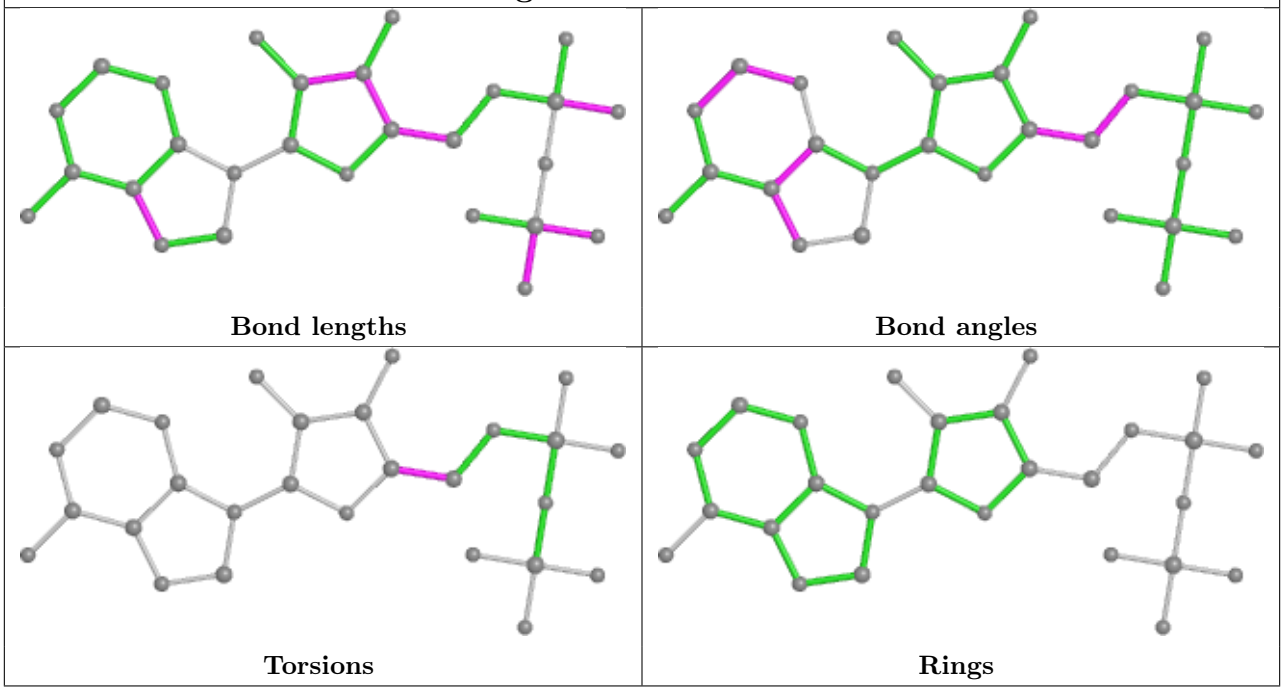
Ligand ADP B 1402



Ligand ADP G 6402



Ligand ADP F 5402



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	312/312 (100%)	-0.16	0	100	100	13, 35, 55, 69	0
1	B	312/312 (100%)	-0.22	1 (0%)	94	93	15, 32, 49, 66	0
1	C	312/312 (100%)	-0.19	3 (0%)	82	77	19, 36, 50, 65	0
1	D	312/312 (100%)	-0.13	7 (2%)	62	52	23, 40, 54, 65	0
1	E	312/312 (100%)	-0.26	0	100	100	9, 31, 47, 61	0
1	F	312/312 (100%)	-0.20	1 (0%)	94	93	7, 32, 49, 65	0
1	G	312/312 (100%)	-0.24	1 (0%)	94	93	20, 37, 53, 63	0
1	H	312/312 (100%)	-0.16	3 (0%)	82	77	24, 39, 52, 61	0
All	All	2496/2496 (100%)	-0.19	16 (0%)	89	86	7, 35, 52, 69	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	SER	4.5
1	C	209	ALA	4.3
1	H	310	THR	3.5
1	D	1	MET	3.1
1	D	309	ALA	2.9

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

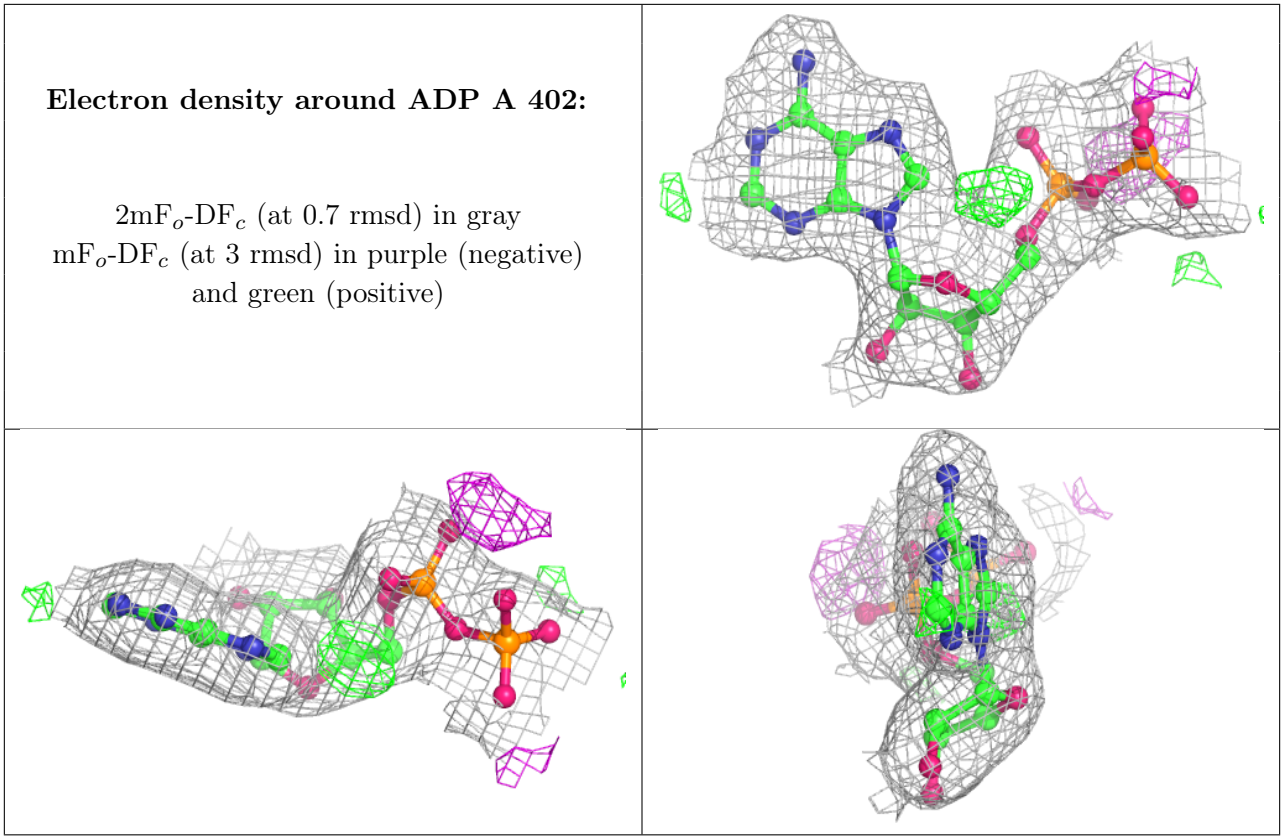
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	E	4403	1/1	0.94	0.14	59,59,59,59	0
3	PLP	A	401	15/16	0.95	0.16	17,21,44,44	0
3	PLP	D	3401	15/16	0.95	0.16	40,42,55,56	0
2	ZN	B	1403	1/1	0.96	0.17	54,54,54,54	0
3	PLP	C	2401	15/16	0.96	0.20	44,45,55,55	0
2	ZN	G	6403	1/1	0.96	0.12	85,85,85,85	0
4	ADP	A	402	27/27	0.96	0.17	19,26,32,33	0
4	ADP	D	3402	27/27	0.96	0.17	32,42,50,51	0
4	ADP	E	4402	27/27	0.96	0.18	17,27,32,35	0
4	ADP	H	7402	27/27	0.96	0.15	41,43,53,54	0
2	ZN	A	403	1/1	0.97	0.14	48,48,48,48	0
2	ZN	F	5403	1/1	0.97	0.15	52,52,52,52	0
3	PLP	F	5401	15/16	0.97	0.17	14,17,29,31	0
3	PLP	G	6401	15/16	0.97	0.17	29,32,41,42	0
3	PLP	H	7401	15/16	0.97	0.16	25,26,32,33	0
2	ZN	C	2403	1/1	0.97	0.10	49,49,49,49	0
4	ADP	C	2402	27/27	0.97	0.16	30,33,37,39	0
2	ZN	H	7403	1/1	0.97	0.12	59,59,59,59	0
2	ZN	D	3403	1/1	0.97	0.09	45,45,45,45	0
4	ADP	F	5402	27/27	0.97	0.16	26,31,36,37	0
3	PLP	B	1401	15/16	0.97	0.17	19,24,39,40	0
4	ADP	B	1402	27/27	0.98	0.17	17,25,32,32	0
4	ADP	G	6402	27/27	0.98	0.15	30,34,38,39	0
3	PLP	E	4401	15/16	0.98	0.17	11,13,25,26	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

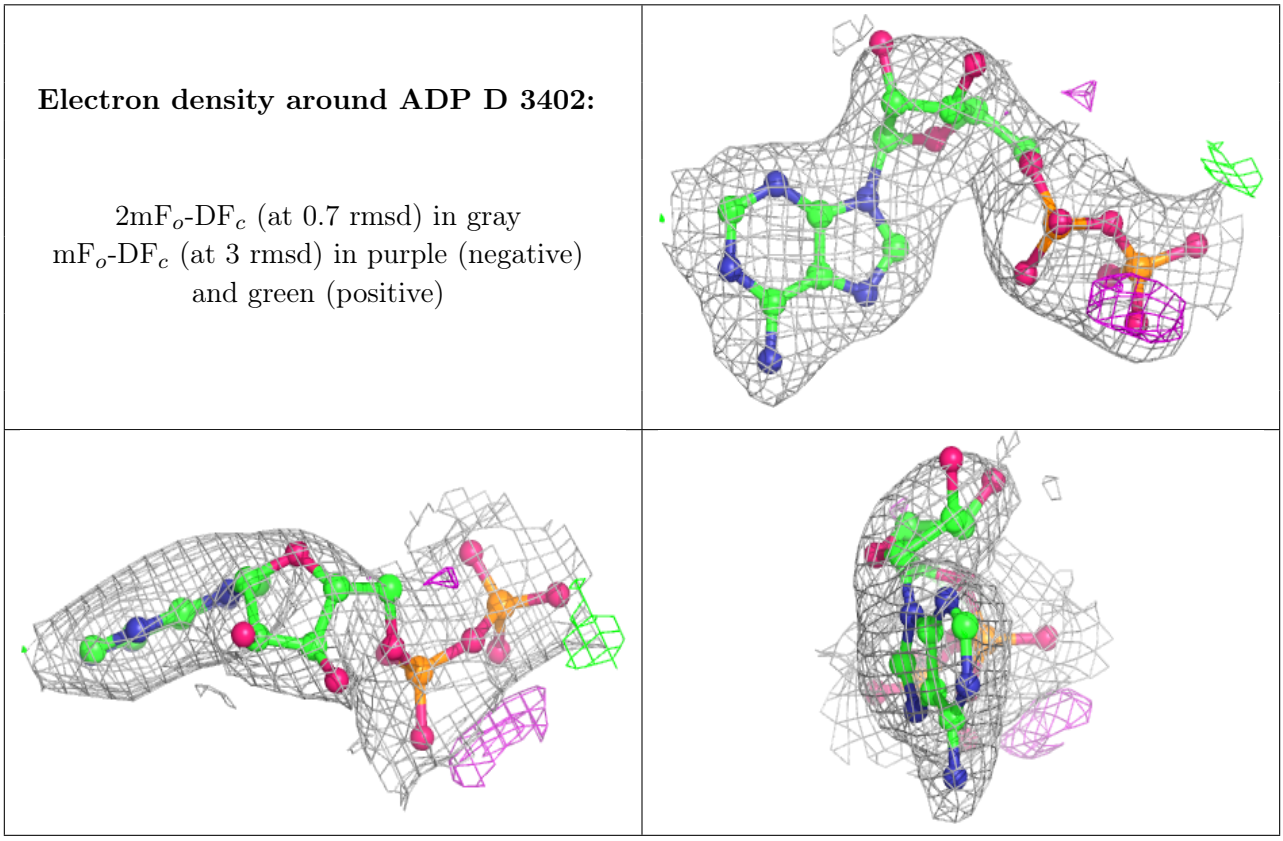
Electron density around ADP A 402:

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



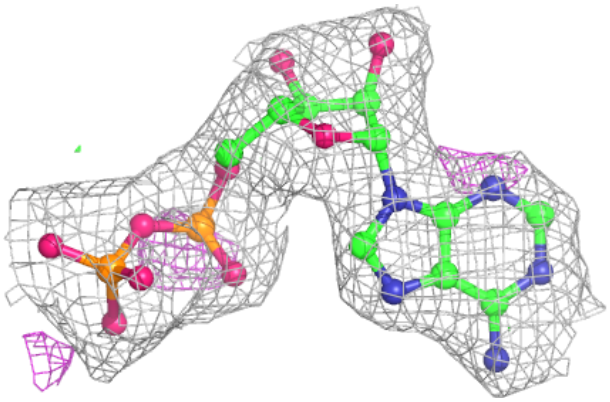
Electron density around ADP D 3402:

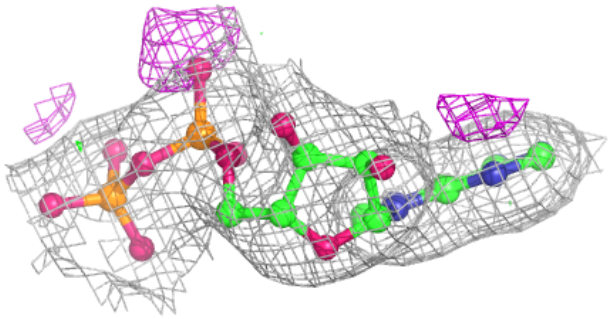
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

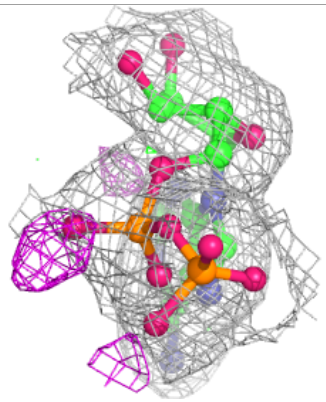


Electron density around ADP E 4402:

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

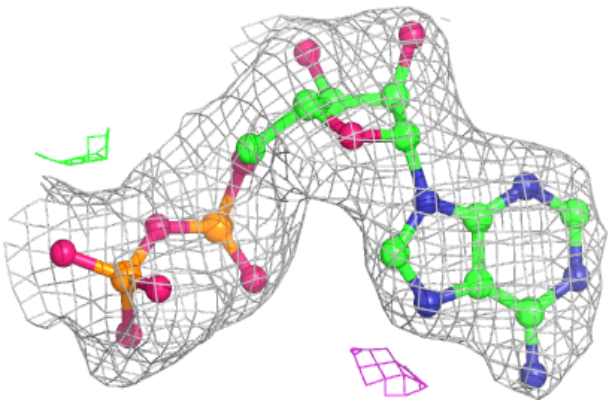


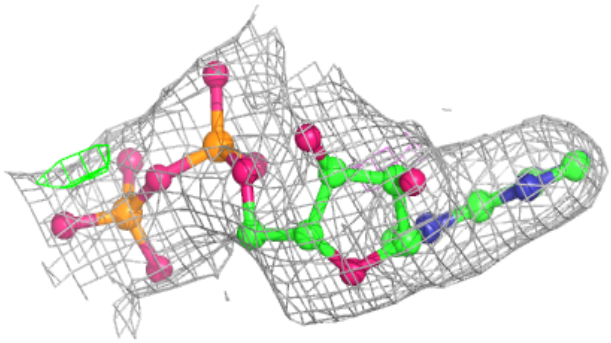


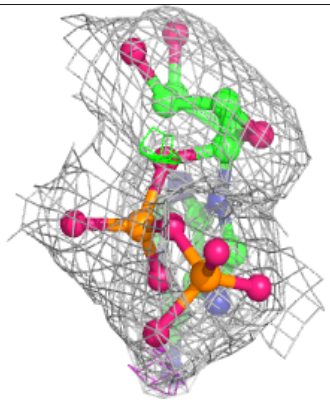


Electron density around ADP H 7402:

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

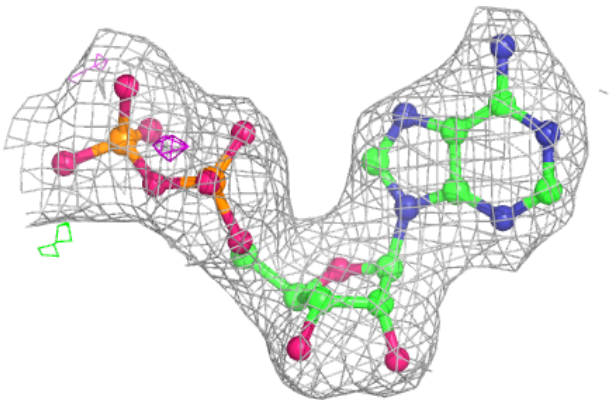


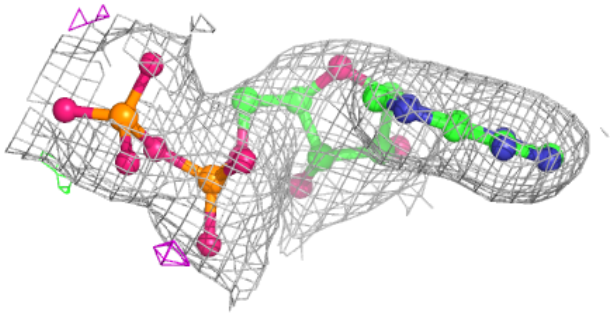


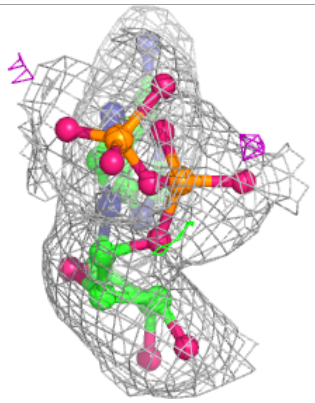


Electron density around ADP C 2402:

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

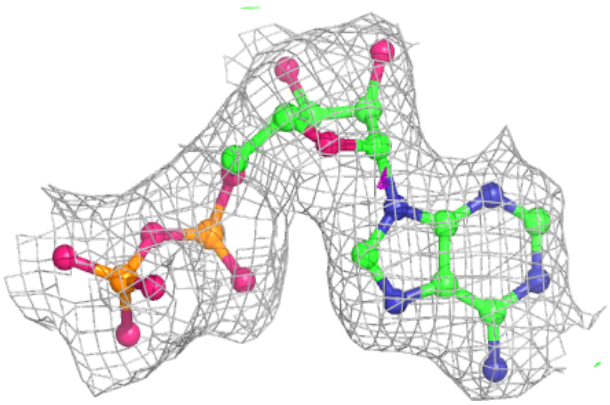


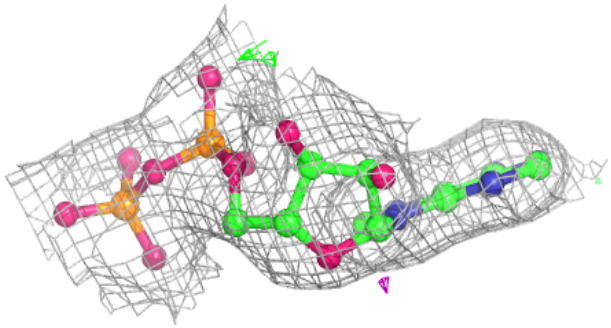


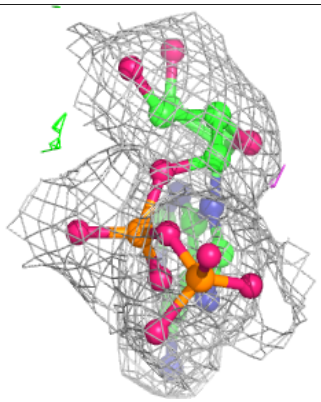


Electron density around ADP F 5402:

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

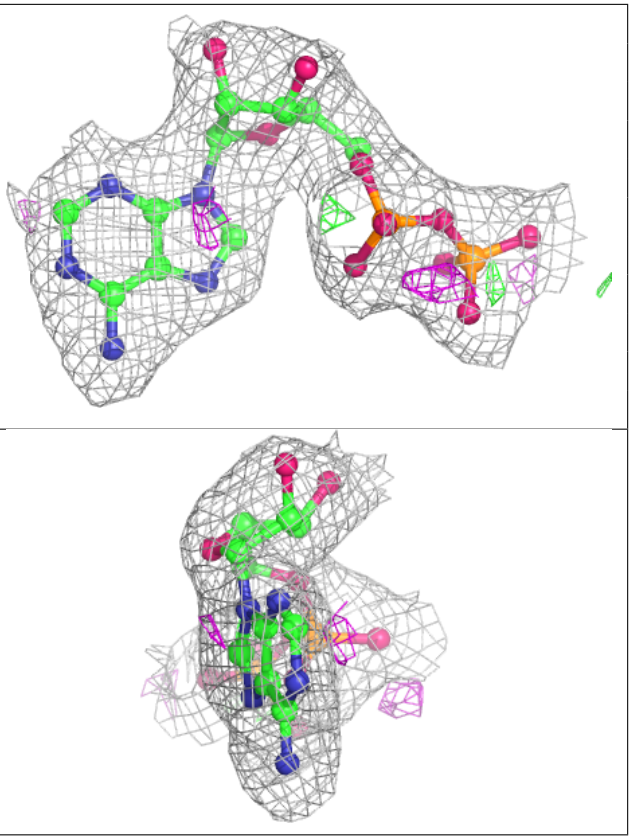


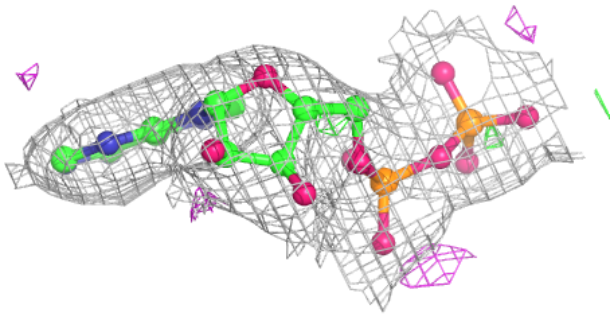




Electron density around ADP B 1402:

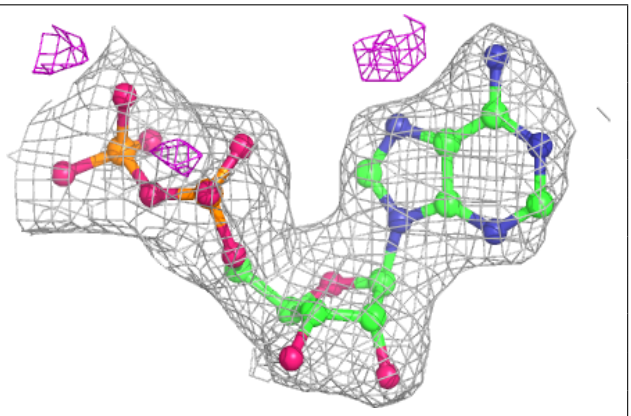
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

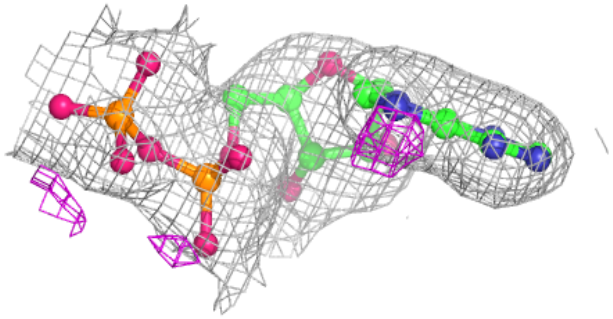


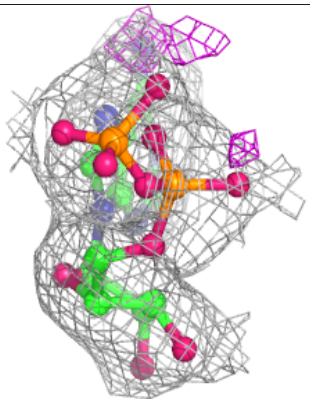


Electron density around ADP G 6402:

$2mF_o$-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.