wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2024 – 12:06 PM EST

PDB ID	:	3K5I
Title	:	Crystal structure of N5-carboxyaminoimidazole synthase from aspergillus clavatus in complex with ADP and 5-aminoimadazole ribonucleotide
Authors	:	Thoden, J.B.; Holden, H.M.; Paritala, H.; Firestine, S.M.
Deposited on	:	2009-10-07
Resolution	:	2.00 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 (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:

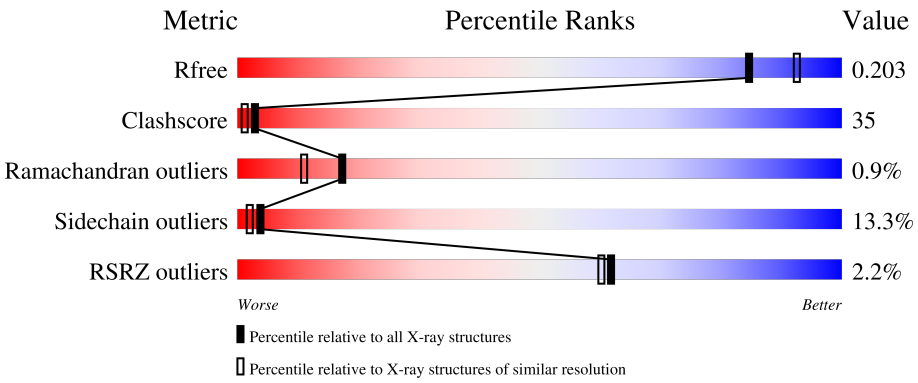
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	403	47% 39% 7% 5%
1	B	403	4% 37% 40% 13% • 7%
1	C	403	% 41% 42% 10% • 5%
1	D	403	3% 35% 43% 12% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AIR	A	402	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13147 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 Phosphoribosyl-aminoimidazole carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2975	1870	523	566	16	0	5	0
1	B	376	2944	1850	516	563	15	0	6	0
1	C	382	2995	1881	529	569	16	0	6	0
1	D	373	2888	1816	506	550	16	0	1	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	HIS	-	expression tag	UNP A1CII2
A	-18	GLY	-	expression tag	UNP A1CII2
A	-17	SER	-	expression tag	UNP A1CII2
A	-16	SER	-	expression tag	UNP A1CII2
A	-15	HIS	-	expression tag	UNP A1CII2
A	-14	HIS	-	expression tag	UNP A1CII2
A	-13	HIS	-	expression tag	UNP A1CII2
A	-12	HIS	-	expression tag	UNP A1CII2
A	-11	HIS	-	expression tag	UNP A1CII2
A	-10	HIS	-	expression tag	UNP A1CII2
A	-9	SER	-	expression tag	UNP A1CII2
A	-8	SER	-	expression tag	UNP A1CII2
A	-7	GLU	-	expression tag	UNP A1CII2
A	-6	ASN	-	expression tag	UNP A1CII2
A	-5	LEU	-	expression tag	UNP A1CII2
A	-4	TYR	-	expression tag	UNP A1CII2
A	-3	PHE	-	expression tag	UNP A1CII2
A	-2	GLN	-	expression tag	UNP A1CII2
A	-1	GLY	-	expression tag	UNP A1CII2
A	0	HIS	-	expression tag	UNP A1CII2
B	-19	HIS	-	expression tag	UNP A1CII2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A1CII2
B	-17	SER	-	expression tag	UNP A1CII2
B	-16	SER	-	expression tag	UNP A1CII2
B	-15	HIS	-	expression tag	UNP A1CII2
B	-14	HIS	-	expression tag	UNP A1CII2
B	-13	HIS	-	expression tag	UNP A1CII2
B	-12	HIS	-	expression tag	UNP A1CII2
B	-11	HIS	-	expression tag	UNP A1CII2
B	-10	HIS	-	expression tag	UNP A1CII2
B	-9	SER	-	expression tag	UNP A1CII2
B	-8	SER	-	expression tag	UNP A1CII2
B	-7	GLU	-	expression tag	UNP A1CII2
B	-6	ASN	-	expression tag	UNP A1CII2
B	-5	LEU	-	expression tag	UNP A1CII2
B	-4	TYR	-	expression tag	UNP A1CII2
B	-3	PHE	-	expression tag	UNP A1CII2
B	-2	GLN	-	expression tag	UNP A1CII2
B	-1	GLY	-	expression tag	UNP A1CII2
B	0	HIS	-	expression tag	UNP A1CII2
C	-19	HIS	-	expression tag	UNP A1CII2
C	-18	GLY	-	expression tag	UNP A1CII2
C	-17	SER	-	expression tag	UNP A1CII2
C	-16	SER	-	expression tag	UNP A1CII2
C	-15	HIS	-	expression tag	UNP A1CII2
C	-14	HIS	-	expression tag	UNP A1CII2
C	-13	HIS	-	expression tag	UNP A1CII2
C	-12	HIS	-	expression tag	UNP A1CII2
C	-11	HIS	-	expression tag	UNP A1CII2
C	-10	HIS	-	expression tag	UNP A1CII2
C	-9	SER	-	expression tag	UNP A1CII2
C	-8	SER	-	expression tag	UNP A1CII2
C	-7	GLU	-	expression tag	UNP A1CII2
C	-6	ASN	-	expression tag	UNP A1CII2
C	-5	LEU	-	expression tag	UNP A1CII2
C	-4	TYR	-	expression tag	UNP A1CII2
C	-3	PHE	-	expression tag	UNP A1CII2
C	-2	GLN	-	expression tag	UNP A1CII2
C	-1	GLY	-	expression tag	UNP A1CII2
C	0	HIS	-	expression tag	UNP A1CII2
D	-19	HIS	-	expression tag	UNP A1CII2
D	-18	GLY	-	expression tag	UNP A1CII2
D	-17	SER	-	expression tag	UNP A1CII2

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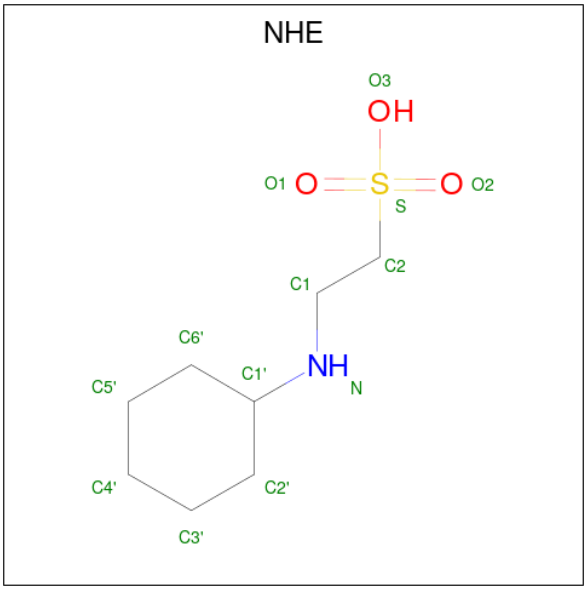
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A1CII2
D	-15	HIS	-	expression tag	UNP A1CII2
D	-14	HIS	-	expression tag	UNP A1CII2
D	-13	HIS	-	expression tag	UNP A1CII2
D	-12	HIS	-	expression tag	UNP A1CII2
D	-11	HIS	-	expression tag	UNP A1CII2
D	-10	HIS	-	expression tag	UNP A1CII2
D	-9	SER	-	expression tag	UNP A1CII2
D	-8	SER	-	expression tag	UNP A1CII2
D	-7	GLU	-	expression tag	UNP A1CII2
D	-6	ASN	-	expression tag	UNP A1CII2
D	-5	LEU	-	expression tag	UNP A1CII2
D	-4	TYR	-	expression tag	UNP A1CII2
D	-3	PHE	-	expression tag	UNP A1CII2
D	-2	GLN	-	expression tag	UNP A1CII2
D	-1	GLY	-	expression tag	UNP A1CII2
D	0	HIS	-	expression tag	UNP A1CII2

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

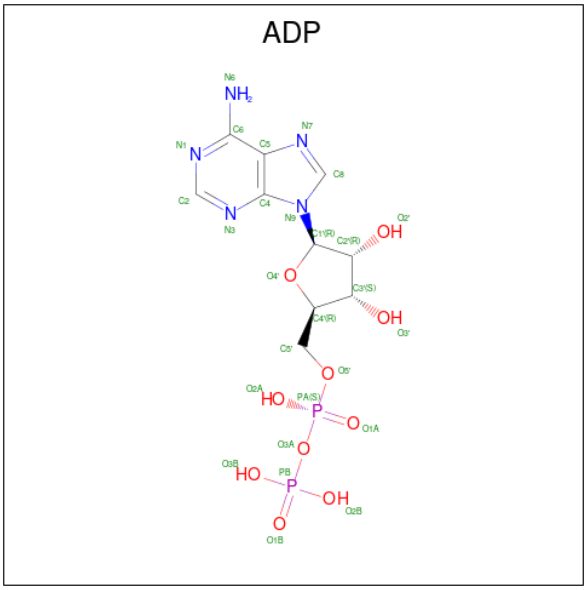
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	13	8	1	3	1	0	0
			Total	C	N	O	S		
3	C	1	13	8	1	3	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
			Total	C	N	O	P		
4	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
4	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
4	D	1	27	10	5	10	2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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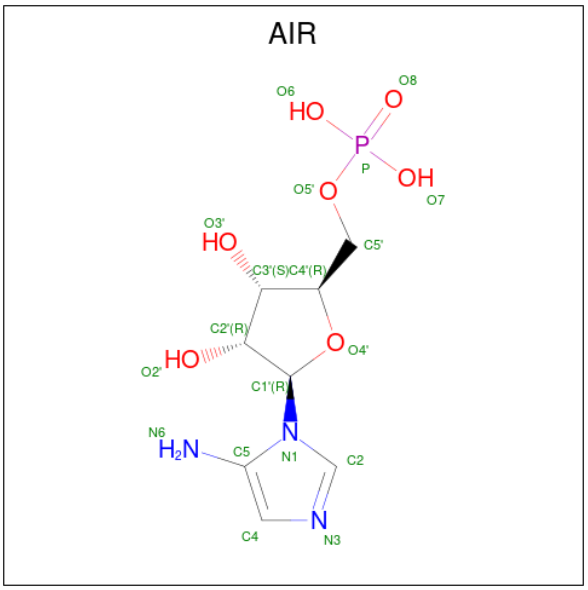
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	D	1	1	1	0	0

- Molecule 6 is 5-AMINOIMIDAZOLE RIBONUCLEOTIDE (three-letter code: AIR) (formula: $C_8H_{14}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	19	8	3	7	1	0	0
			Total	C	N	O	P		
6	B	1	19	8	3	7	1	0	0
			Total	C	N	O	P		
6	C	1	19	8	3	7	1	0	0
			Total	C	N	O	P		
6	D	1	19	8	3	7	1	0	0

- Molecule 7 is water.

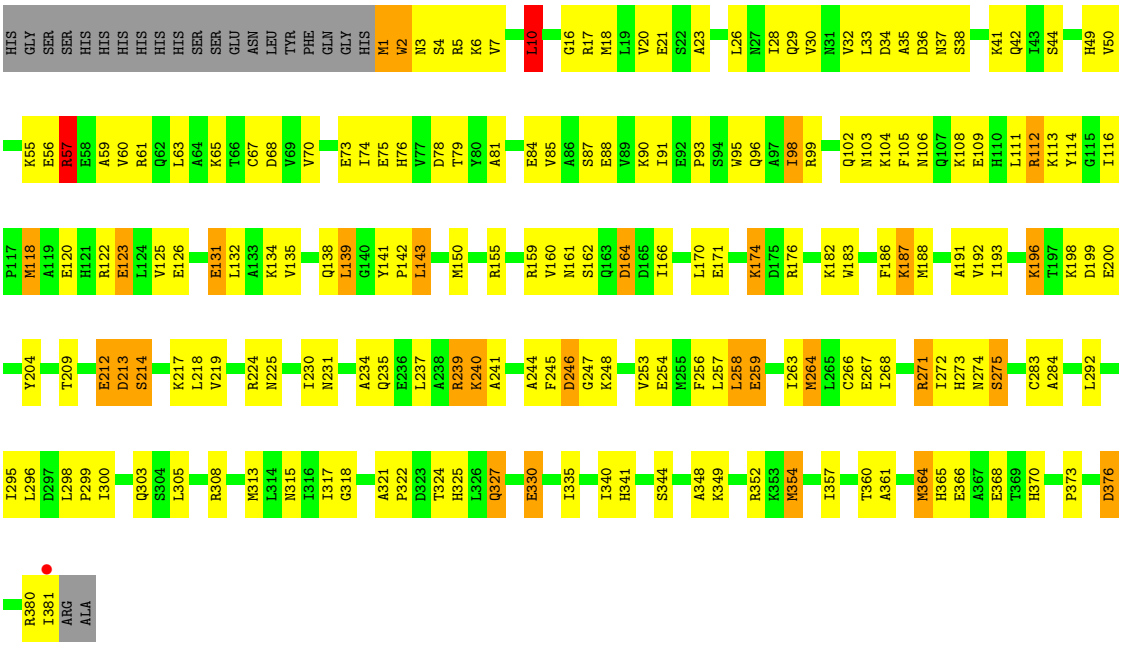
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	322	322	322	0	0
			Total	O		
7	B	266	266	266	0	0
			Total	O		
7	C	299	299	299	0	0
			Total	O		
7	D	243	243	243	0	0

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.

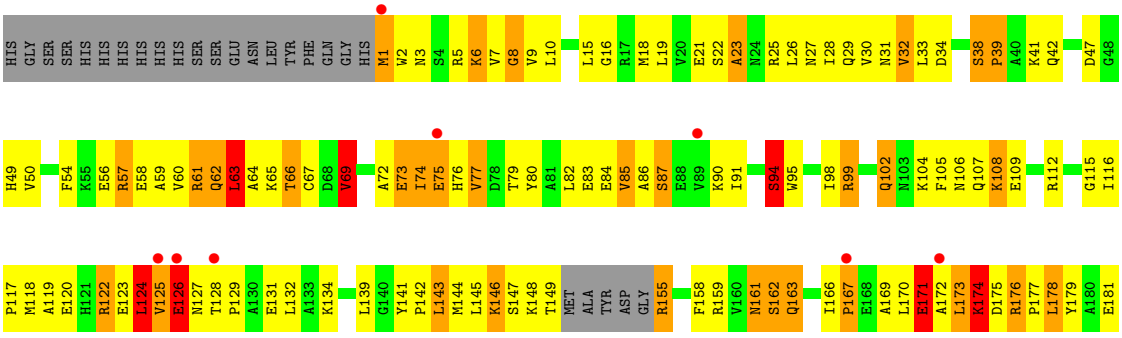
• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

Chain A: 47% 39% 7% 5%



• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

Chain B: 4% 37% 40% 13% • 7%



K182 K187 M188 E189 L190 V195 K196 T197 K198 D199 E200 T206 V207 E208 T209 V210 Q211 E212 D213 S214 I215 C216 K217 L218 V219 Y220 A221 P222 A223 R224 N225 V226 N231 Q232 K233 A234 Q235 E236 L237 K240 D246 G247 K248 G249 V250 L257 L258 E259 D260 D261 S262 I263 M264

R271 I272 H273 N274 S275 G276 T279 I280 E281 G282 L285 S286 D289 L292 R293 A294 I295 L296 D297 L298 P299 I300 S304 L305 R308 S311 I316 I317 G318 G319 A320 A321 P322 D323 T324 H325 L326 Q327 E330 C331 A332 L333 S334 N337 A338 S339 Y343

A347 A348 K349 P350 G351 R352 I357 A361 P362 T363 M364 H365 E366 A367 E368 T369 H370 I371 Q372 P373 L374 I375 D376 V377 V378 D379 R380 I381 ARG ALA

• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

Chain C: % 41% 42% 10% • 5%

HIS GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLU ASN LEU TYR PHE GLN GLY HIS M1 W2 N3 S4 R5 K6 V7 G8 V9 L10 G11 G12 G13 Q14 L15 G16 R17 R25 L26 N27 I28 Q29 V32 L33 D34 A35 D36 N37 S38 P39 A40 K41 Q42 I43 H46 D47 G48

H49 K55 E56 R57 E58 A59 V60 R61 Q62 L63 A64 K65 T66 C67 D68 V69 V70 E73 I74 E75 A81 L82 V85 A86 S87 E88 V89 K90 P93 S94 W95 Q96 A97 I98 R99 T100 I101 F105 N106 Q107 K108 E109 H110 L111 R112 K113 I116 P117 E120 H121 R122 E123

L124 V125 E126 N127 T128 P129 A130 E131 L132 A133 K134 Q138 L139 G140 Y141 P142 L145 K146 S147 K148 T149 M150 R155 G156 N157 F158 R159 V160 N161 S162 Q163 D164 D165 I166 P167 E168 E171 A172 L173 K174 D175 R176 P177 L178 Y179 A180 E181 K182 W183 A184 Y185 F186 K187 M188 E189

I193 K196 T197 K198 D199 P205 T209 V210 Q211 E212 D213 S214 L218 V219 R224 N225 V226 A229 I230 N231 Q232 K233 E236 L237 A238 R239 K240 A241 V242 A243 A244 F245 V250 E254 M255 F256 L257 L258 E259 D260 D261 S262 I263 M264 L265 C266 E267 I268 A269 S270 R271

I272 H273 N274 H277 I280 A284 L285 S286 H291 L292 R293 A294 I295 L298 P299 I300 S304 I307 R308 S311 L314 N315 I316 I317 A321 P322 D323 T324 H325 L326 A329 E330 C331 A332 L333 N337 A338 S339 L342 Y343 S344 K345 G346 A347 A348 G351

R352 K353 M354 I357 T358 V359 T360 A361 P362 T363 M364 H365 E366 A367 E368 Q372 P373 L374 I375 D376 V377 V378 D379 R380 I381 R382 ALA

• Molecule 1: Phosphoribosyl-aminoimidazole carboxylase

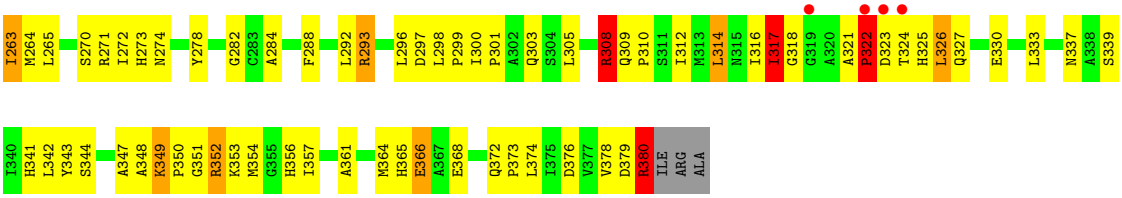
Chain D: 3% 35% 43% 12% • 7%

HIS GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLU ASN LEU TYR PHE GLN GLY HIS M1 R5 K6 V7 G8 V9 G12 G13 Q14 L15 G16 L19 L26 N27 I28 Q29 V30 N31 V32 L33 D34 A35 D36 N37 S38 P39 A40 K41 Q42 I43 S44 D47 G48 H49 V50

T51 G52 S53 F54 K55 E56 R57 E58 A59 V60 R61 Q62 L63 A64 K65 T66 C67 D68 E73 I74 GLU HIS V77 D78 T79 Y80 A81 L82 E83 E84 V85 A86 S87 E88 V89 E92 P93 S94 W95 Q96 A97 I98 R99 Q102 N103 K104 F105 N106 Q107 K108 E109 H110 L111 R112 K113 Y114 G115

I116 P117 M118 A119 E120 H121 R122 E123 L124 V125 E126 N127 T128 P129 A130 E131 L132 A133 K134 V135 G136 E137 Q138 L139 G140 Y141 P142 L143 M144 L145 K146 S147 K148 T149 M150 ALA TYR ASP GLY ARG G156 N157 F158 R159 V160 N161 S162 Q163 D164 D165 I166 P167 E168 A169 L170 E171 A172 L173 K174 D175

R176 P177 L178 Y179 A180 E181 K182 A191 K196 T197 K198 D199 E200 V201 L202 S203 Y204 P205 T206 V207 E208 E212 D213 S214 I215 C216 K217 L218 V219 Y220 A221 P222 A223 R224 N225 D228 A229 Q232 K233 L237 A244 F245 D246 G247 K248 F251 F256 L257 D261 S262


I263
M264
L265
S270
R271
I272
H273
N274
Y278
G282
C283
A284
F288
L292
R293
L296
D297
L298
P299
I300
P301
A302
Q303
S304
L305
R308
Q309
P310
S311
I312
M313
L314
N315
I316
I317
G318
G319
A320
A321
P322
D323
T324
H325
L326
Q327
E330
L333
N337
A338
S339
I340
H341
L342
Y343
S344
A347
A348
K349
P350
G351
R352
K353
M354
G355
H356
I357
A361
M364
H365
E366
A367
E368
Q372
P373
L374
I375
D376
V377
V378
D379
R380
ILE
ARG
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.50Å 134.20Å 98.50Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 44.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.00) 91.9 (44.73-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.62 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , 0.269 0.207 , 0.203	Depositor DCC
R_{free} test set	11671 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å^2)	14.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 135.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13147	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NHE, AIR, MG, ADP, NA

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	0.85	2/3049 (0.1%)	1.67	38/4128 (0.9%)
1	B	0.80	0/3019	1.68	58/4086 (1.4%)
1	C	0.83	0/3072	1.69	47/4157 (1.1%)
1	D	0.81	0/2941	1.68	48/3980 (1.2%)
All	All	0.83	2/12081 (0.0%)	1.68	191/16351 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ALA	CA-CB	6.50	1.66	1.52
1	A	192	VAL	CB-CG1	5.80	1.65	1.52

The worst 5 of 191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	308	ARG	NE-CZ-NH1	-22.98	108.81	120.30
1	A	57	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	C	308	ARG	NE-CZ-NH2	14.93	127.77	120.30
1	A	57	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	B	352	ARG	NE-CZ-NH1	12.95	126.77	120.30

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	2975	0	2984	162	0
1	B	2944	0	2953	200	0
1	C	2995	0	3008	208	0
1	D	2888	0	2908	278	0
2	A	1	0	0	0	0
3	A	13	0	17	1	0
3	C	13	0	17	5	0
4	A	27	0	10	1	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	19	0	11	0	0
6	B	19	0	11	2	0
6	C	19	0	12	2	0
6	D	19	0	12	2	0
7	A	322	0	0	18	0
7	B	266	0	0	22	0
7	C	299	0	0	18	0
7	D	243	0	0	26	0
All	All	13147	0	11979	841	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 841 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:THR:HG23	1:C:381:ILE:HG21	1.25	1.17
1:D:53:SER:HB3	1:D:56:GLU:HG3	1.20	1.16
1:C:62:GLN:HE22	1:C:65[A]:LYS:HE3	1.09	1.12
1:A:116:ILE:HD11	1:A:240:LYS:HD3	1.28	1.12
1:A:187:LYS:HE2	1:A:259:GLU:HA	1.35	1.08

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	384/403 (95%)	365 (95%)	18 (5%)	1 (0%)	41	37
1	B	378/403 (94%)	346 (92%)	28 (7%)	4 (1%)	14	8
1	C	386/403 (96%)	368 (95%)	16 (4%)	2 (0%)	29	23
1	D	368/403 (91%)	344 (94%)	18 (5%)	6 (2%)	9	4
All	All	1516/1612 (94%)	1423 (94%)	80 (5%)	13 (1%)	17	11

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ALA
1	B	174	LYS
1	C	322	PRO
1	D	171	GLU
1	D	172	ALA

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	322/336 (96%)	295 (92%)	27 (8%)	11	7
1	B	320/336 (95%)	260 (81%)	60 (19%)	1	0
1	C	324/336 (96%)	286 (88%)	38 (12%)	5	3
1	D	312/336 (93%)	265 (85%)	47 (15%)	3	1
All	All	1278/1344 (95%)	1106 (86%)	172 (14%)	4	2

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	265	LEU
1	D	129	PRO
1	C	307	ILE
1	D	54	PHE
1	D	150	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	211	GLN
1	D	110	HIS
1	C	327	GLN
1	D	106	ASN
1	C	232	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 (i)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	ADP	B	400	5	24,29,29	1.05	2 (8%)	29,45,45	1.86	8 (27%)
4	ADP	D	400	5	24,29,29	1.05	2 (8%)	29,45,45	2.41	8 (27%)
6	AIR	C	402	-	16,20,20	0.80	0	20,30,30	1.77	6 (30%)
6	AIR	D	402	-	16,20,20	0.83	0	20,30,30	1.66	4 (20%)
6	AIR	A	402	-	16,20,20	0.85	1 (6%)	20,30,30	2.29	8 (40%)
4	ADP	A	400	5	24,29,29	1.12	2 (8%)	29,45,45	3.21	13 (44%)
3	NHE	C	384	-	13,13,13	1.07	1 (7%)	16,17,17	3.48	5 (31%)
3	NHE	A	385	-	13,13,13	1.16	1 (7%)	16,17,17	2.41	6 (37%)
4	ADP	C	400	5	24,29,29	0.92	2 (8%)	29,45,45	1.97	6 (20%)
6	AIR	B	402	-	16,20,20	0.64	0	20,30,30	2.08	7 (35%)

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
4	ADP	B	400	5	-	0/12/32/32	0/3/3/3
4	ADP	D	400	5	-	0/12/32/32	0/3/3/3
6	AIR	C	402	-	-	0/6/26/26	0/2/2/2
6	AIR	D	402	-	-	0/6/26/26	0/2/2/2
6	AIR	A	402	-	1/1/5/5	5/6/26/26	0/2/2/2
4	ADP	A	400	5	-	2/12/32/32	0/3/3/3
3	NHE	C	384	-	-	5/7/15/15	0/1/1/1
3	NHE	A	385	-	-	2/7/15/15	0/1/1/1
4	ADP	C	400	5	-	2/12/32/32	0/3/3/3
6	AIR	B	402	-	-	5/6/26/26	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ADP	C6-N6	-3.43	1.21	1.34
3	A	385	NHE	C2-S	3.30	1.82	1.77
4	B	400	ADP	C2-N1	3.11	1.39	1.33
4	D	400	ADP	C2-N1	2.78	1.39	1.33
4	A	400	ADP	C2-N1	2.74	1.39	1.33

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	384	NHE	O1-S-C2	11.27	120.48	106.92
4	A	400	ADP	C5-C6-N6	10.17	135.81	120.35
4	D	400	ADP	C5-C6-N1	-6.94	104.61	120.35
6	A	402	AIR	C5'-C4'-C3'	6.01	137.71	115.18
4	A	400	ADP	O3B-PB-O1B	5.96	134.00	110.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	402	AIR	C4'

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	385	NHE	C6'-C1'-N-C1
3	C	384	NHE	N-C1-C2-S
3	C	384	NHE	C1-C2-S-O2
4	A	400	ADP	PA-O3A-PB-O3B
6	A	402	AIR	C3'-C4'-C5'-O5'

There are no ring outliers.

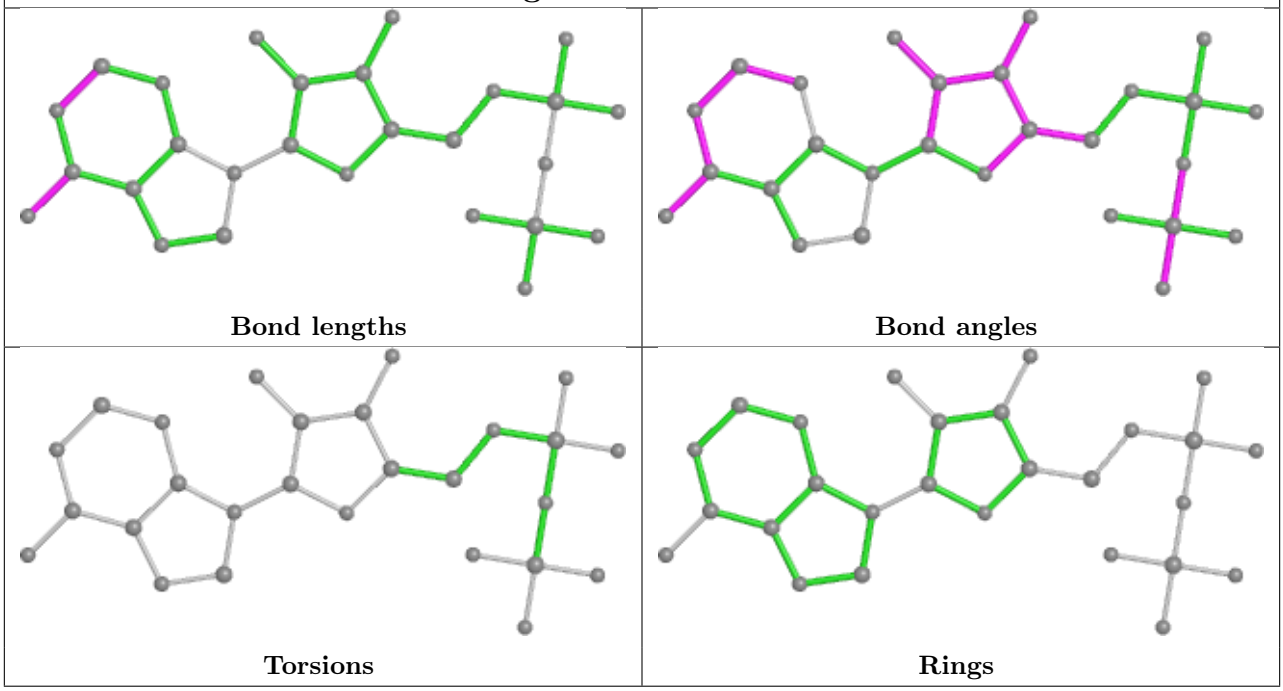
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	400	ADP	1	0
4	D	400	ADP	2	0
6	C	402	AIR	2	0
6	D	402	AIR	2	0
4	A	400	ADP	1	0
3	C	384	NHE	5	0
3	A	385	NHE	1	0
4	C	400	ADP	2	0
6	B	402	AIR	2	0

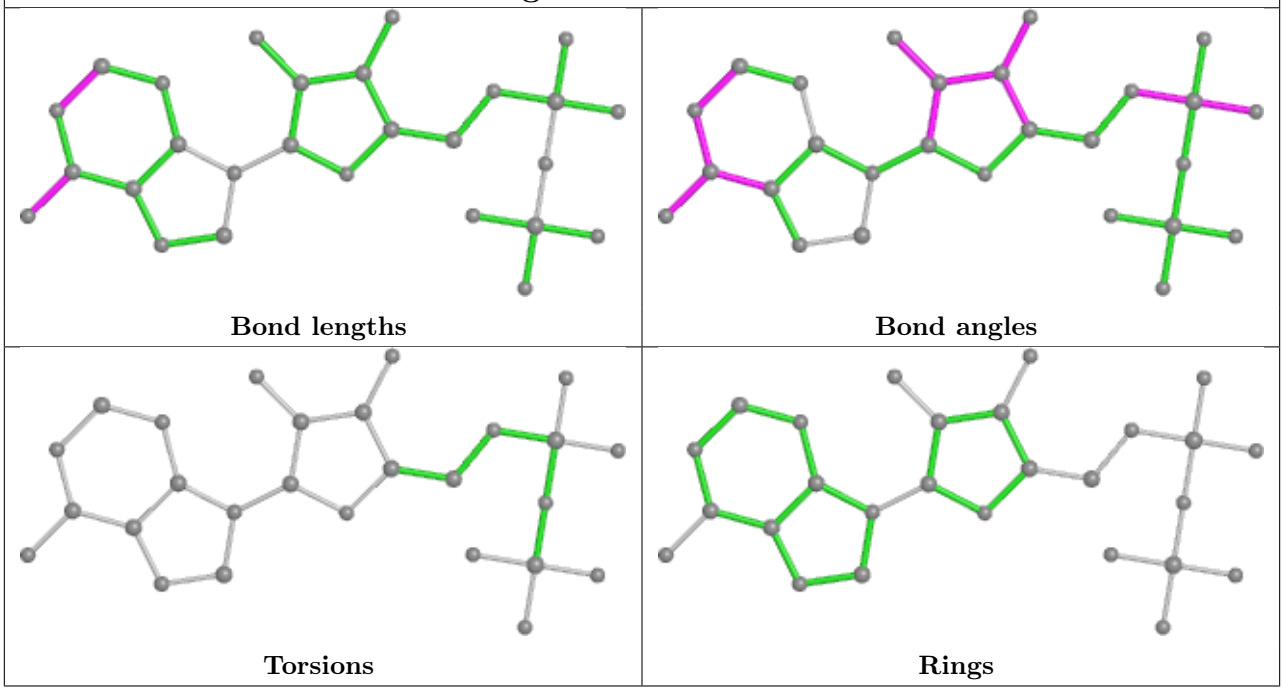
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

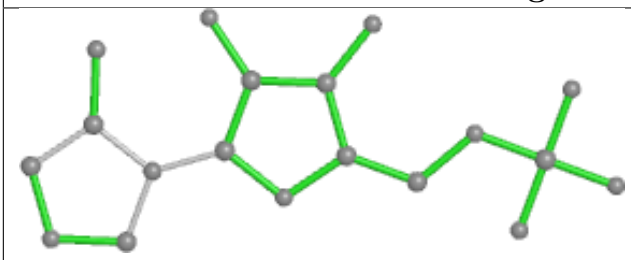
Ligand ADP B 400



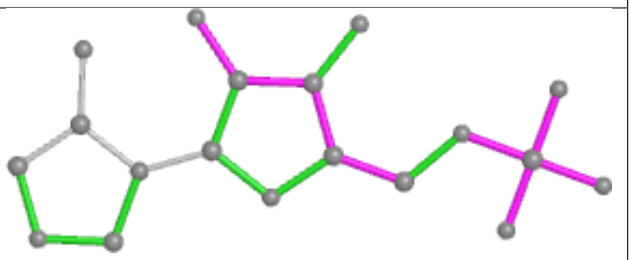
Ligand ADP D 400



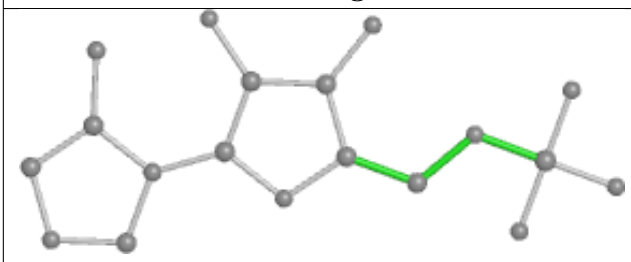
Ligand AIR C 402



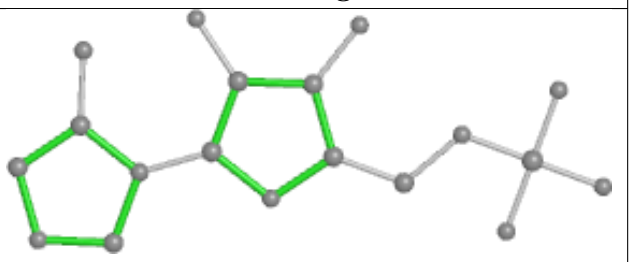
Bond lengths



Bond angles

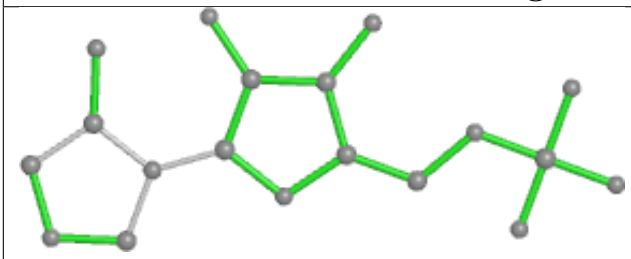


Torsions



Rings

Ligand AIR D 402



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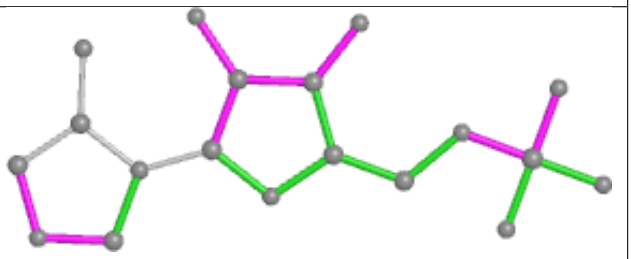

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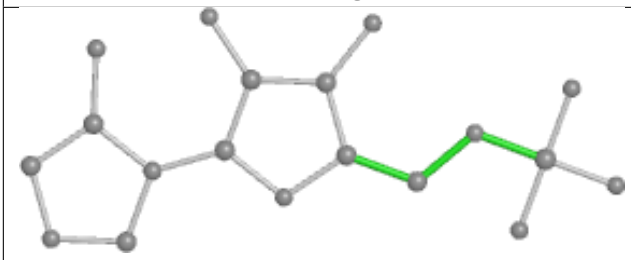

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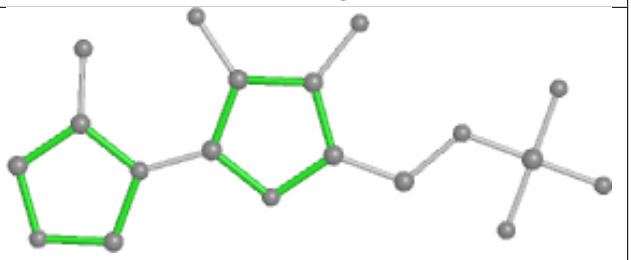
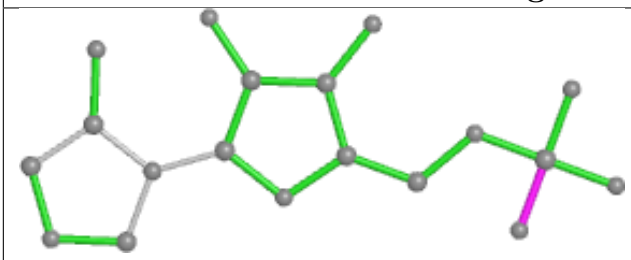
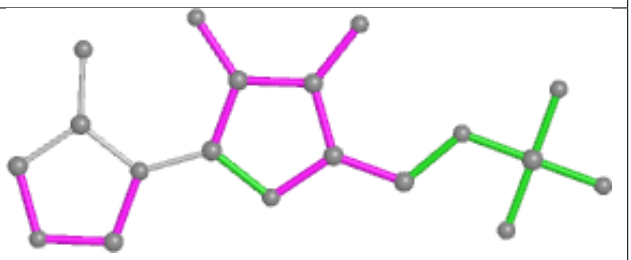


Rings

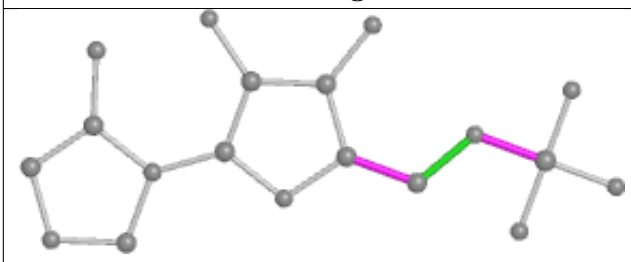
Ligand AIR A 402



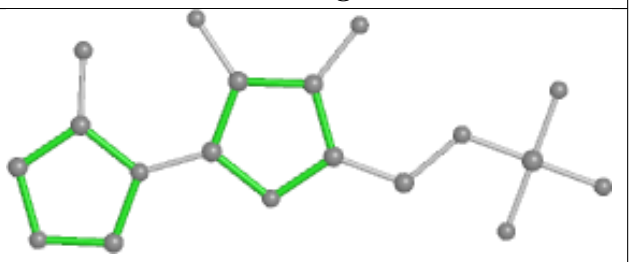
Bond lengths



Bond angles

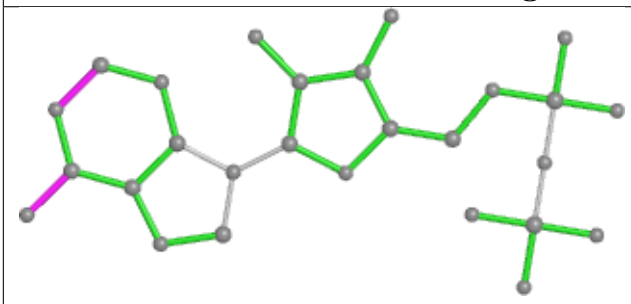


Torsions

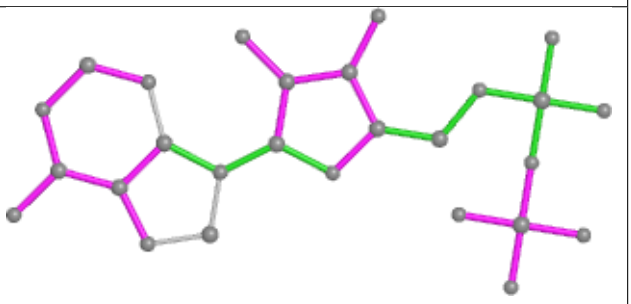


Rings

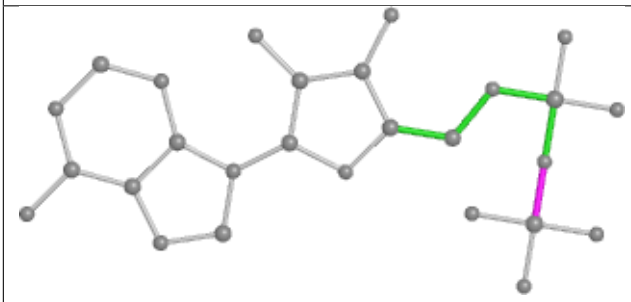
Ligand ADP A 400



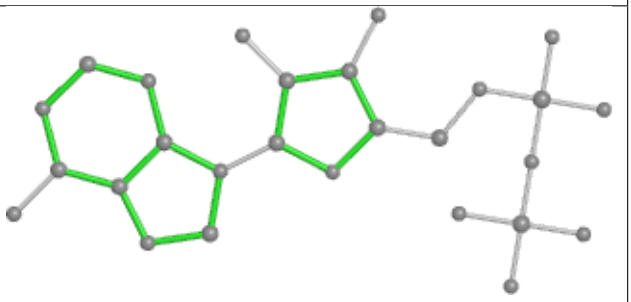
Bond lengths



Bond angles

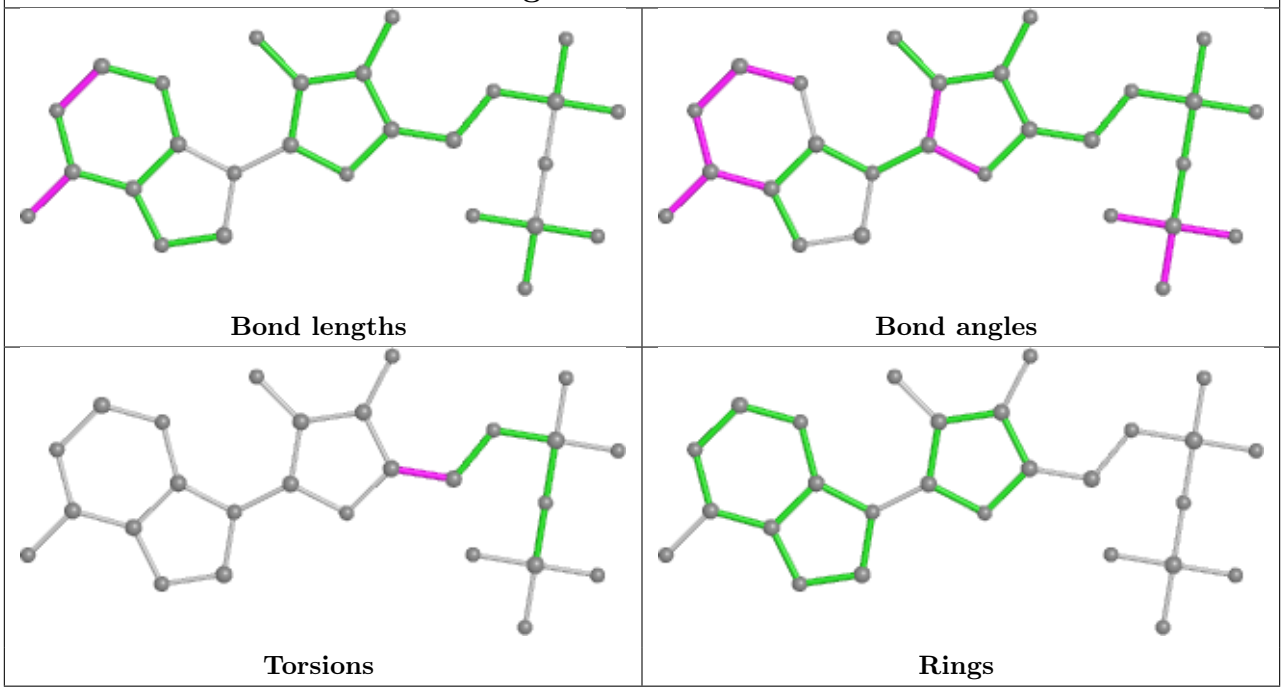


Torsions

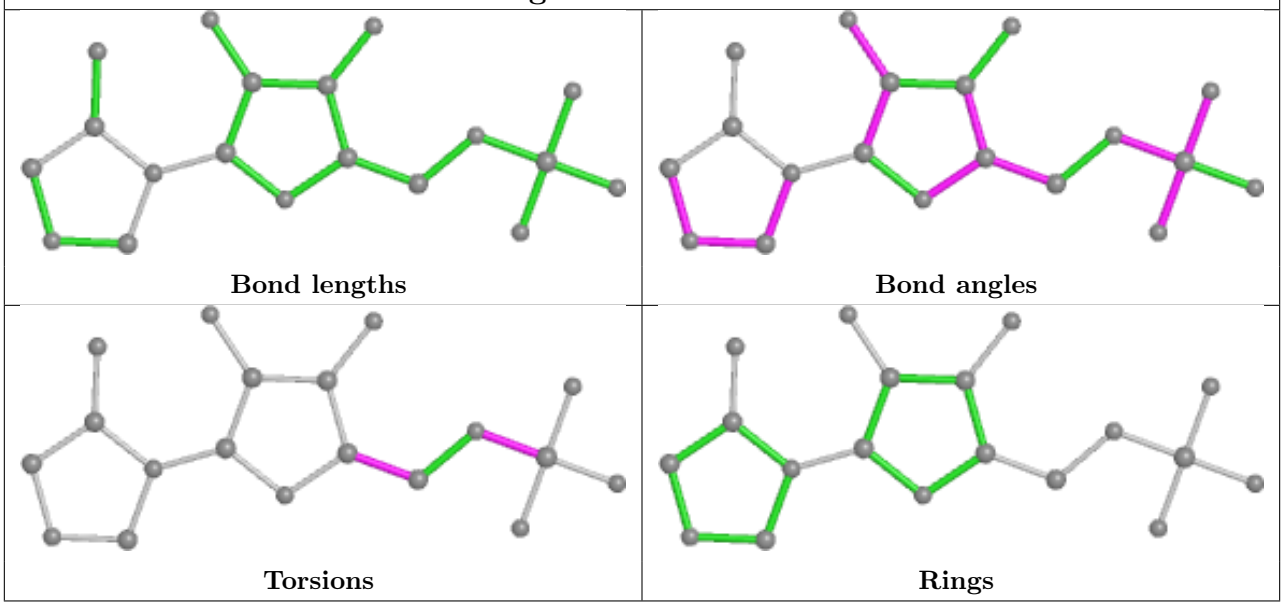


Rings

Ligand ADP C 400



Ligand AIR B 402



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	381/403 (94%)	-0.24	1 (0%)	94	93	7, 25, 59, 79	0
1	B	376/403 (93%)	0.03	15 (3%)	38	37	8, 28, 72, 93	0
1	C	382/403 (94%)	-0.24	3 (0%)	86	85	10, 27, 61, 84	0
1	D	373/403 (92%)	0.04	14 (3%)	40	39	10, 29, 71, 90	0
All	All	1512/1612 (93%)	-0.11	33 (2%)	62	60	7, 27, 67, 93	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.4
1	D	322	PRO	5.3
1	B	323	ASP	3.8
1	B	172	ALA	3.6
1	D	324	THR	3.6

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)

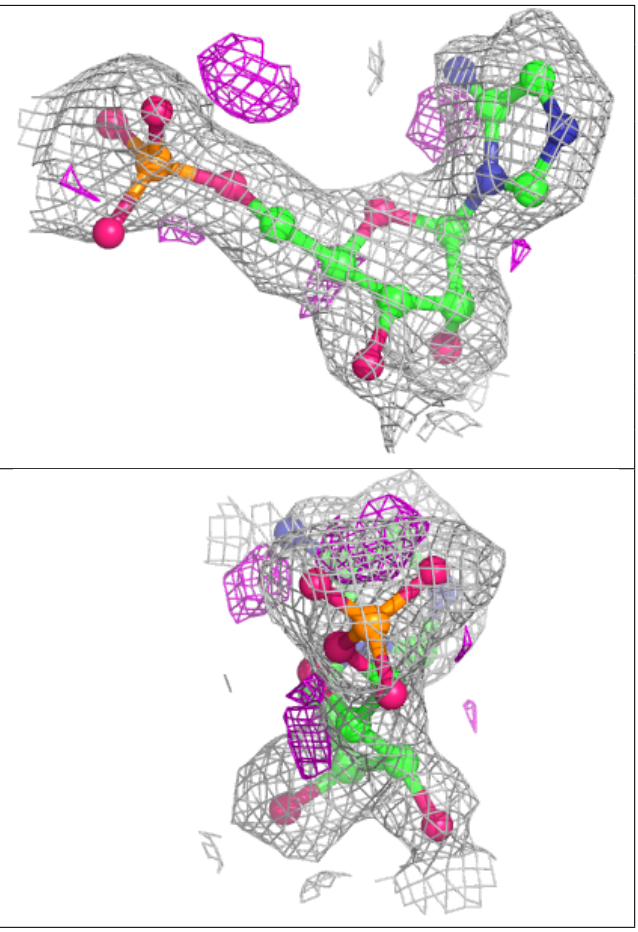
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	401	1/1	0.84	0.10	31,31,31,31	0
2	NA	A	384	1/1	0.88	0.13	37,37,37,37	0
6	AIR	D	402	19/19	0.88	0.17	14,45,99,99	0
5	MG	B	401	1/1	0.93	0.05	27,27,27,27	0
4	ADP	D	400	27/27	0.94	0.10	8,29,56,98	0
4	ADP	B	400	27/27	0.94	0.10	4,35,63,99	0
6	AIR	B	402	19/19	0.95	0.11	2,34,99,99	0
6	AIR	A	402	19/19	0.95	0.10	1,15,23,23	0
6	AIR	C	402	19/19	0.96	0.10	4,13,32,38	0
3	NHE	C	384	13/13	0.96	0.13	17,37,56,77	0
4	ADP	C	400	27/27	0.97	0.09	4,21,41,47	0
4	ADP	A	400	27/27	0.97	0.08	6,19,31,99	0
5	MG	A	401	1/1	0.97	0.04	14,14,14,14	0
3	NHE	A	385	13/13	0.97	0.12	15,30,99,99	0
5	MG	C	401	1/1	0.97	0.03	18,18,18,18	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.

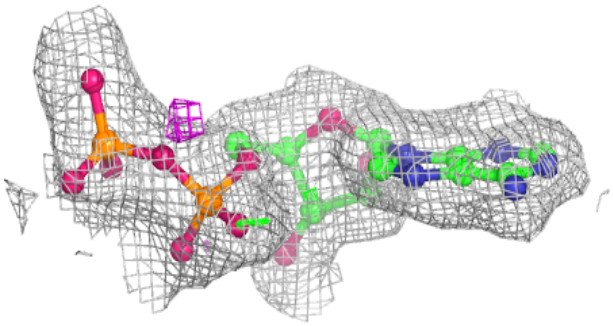
Electron density around AIR D 402:

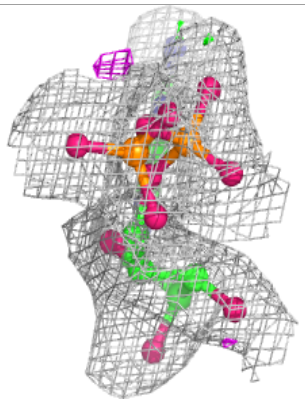
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP D 400:

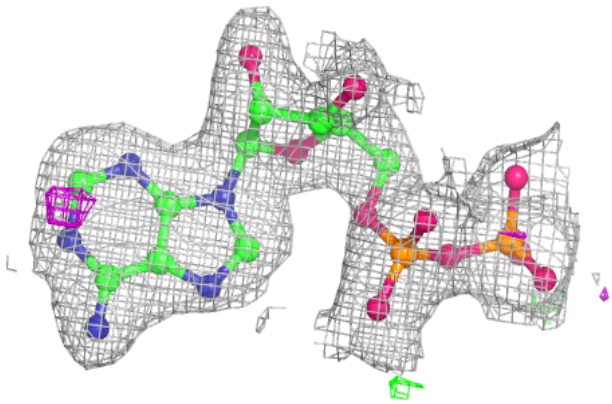
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

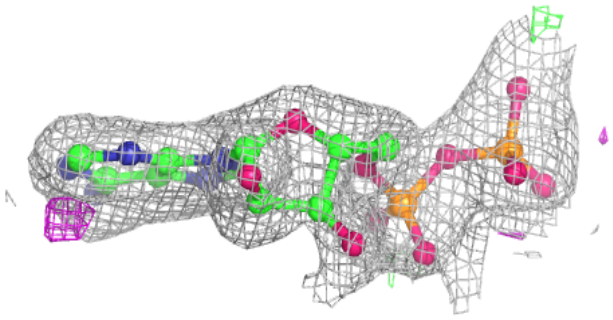




Electron density around ADP B 400:

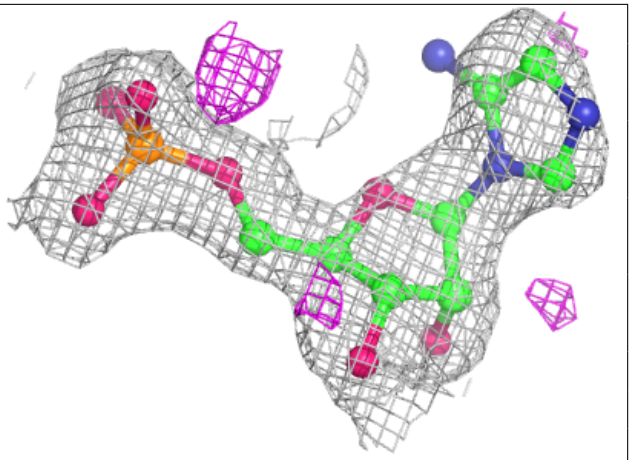
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

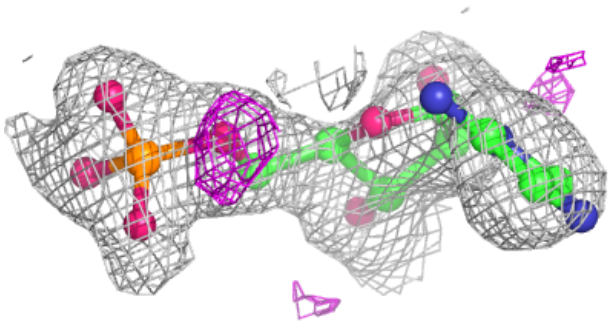


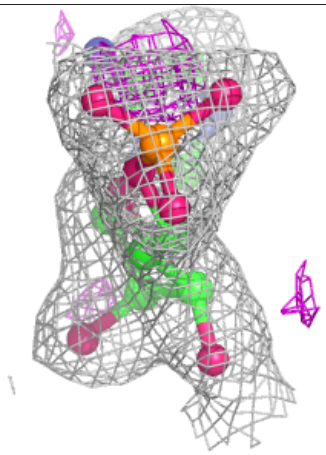


Electron density around AIR B 402:

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

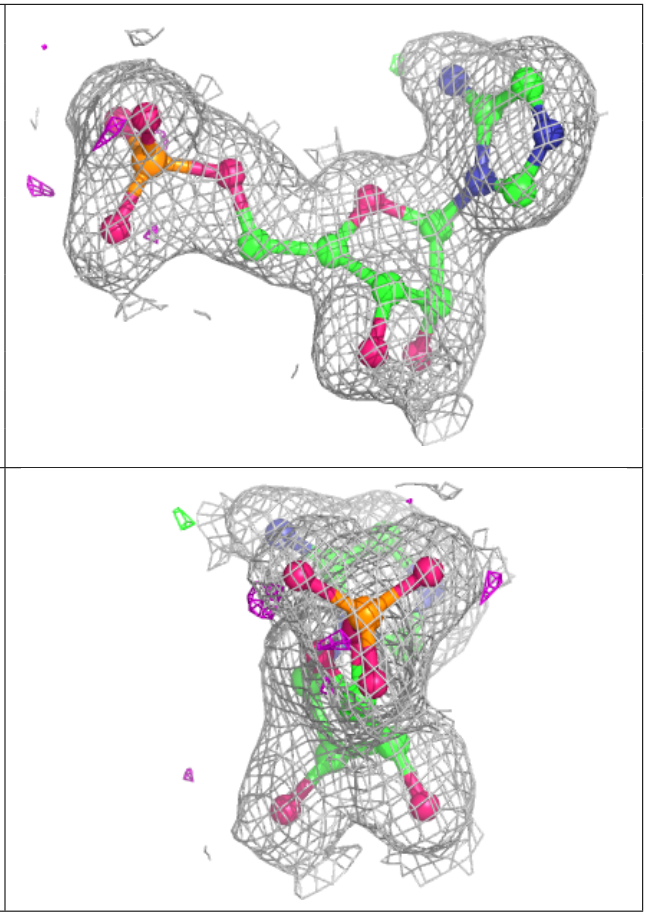






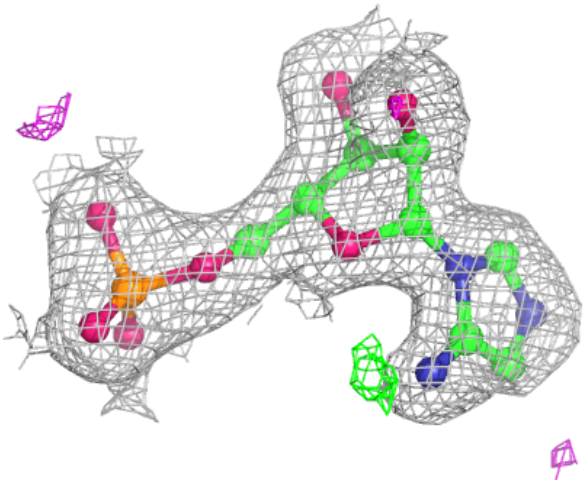
Electron density around AIR A 402:

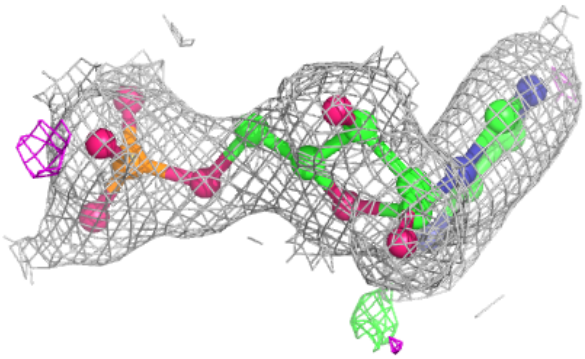
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

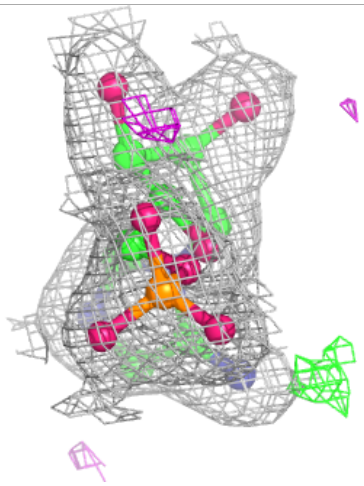


Electron density around AIR C 402:

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

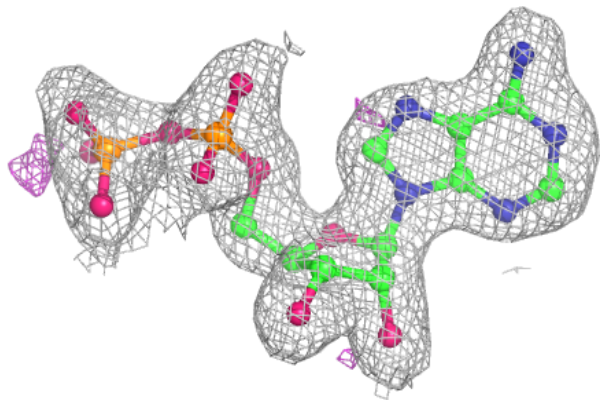


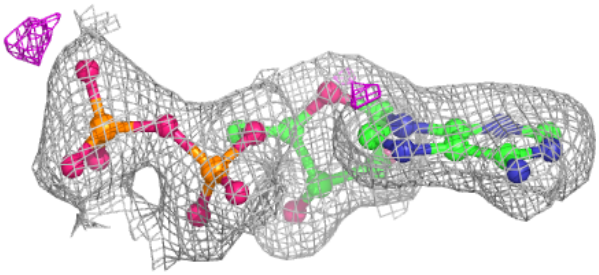


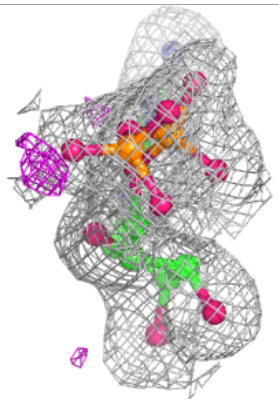


Electron density around ADP C 400:

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

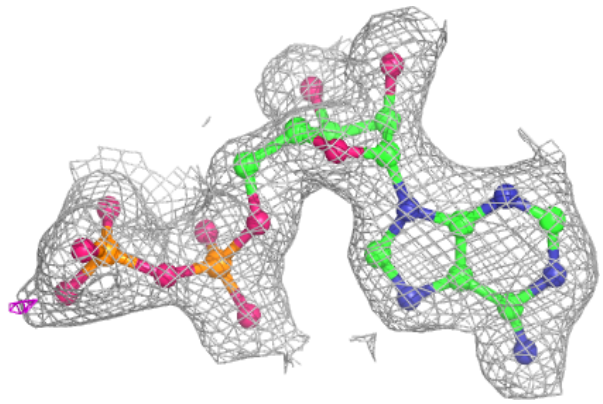


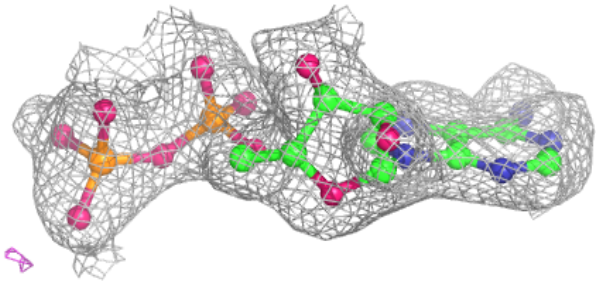


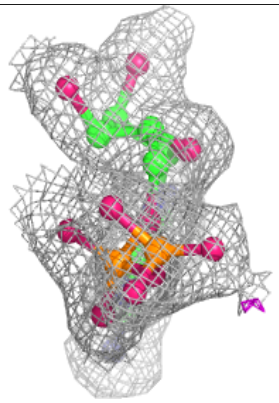


Electron density around ADP A 400:

$2mF_o$-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.