



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:54 PM UTC

PDB ID : 1JM6 / pdb_00001jm6
Title : Pyruvate dehydrogenase kinase, isozyme 2, containing ADP
Authors : Steussy, C.N.; Popov, K.M.; Bowker-Kinley, M.M.; Sloan, R.B.; Harris, R.A.;
Hamilton, J.A.
Deposited on : 2001-07-17
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

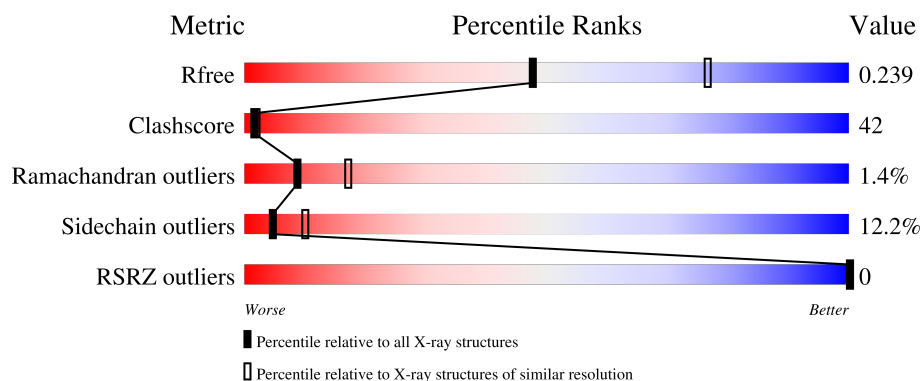
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

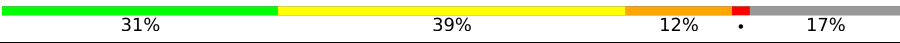
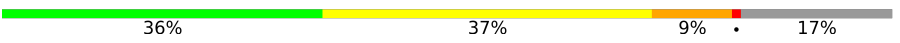
The reported resolution of this entry is 2.50 Å.

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	
1	B	407	

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
3	ADP	B	3510	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5677 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.

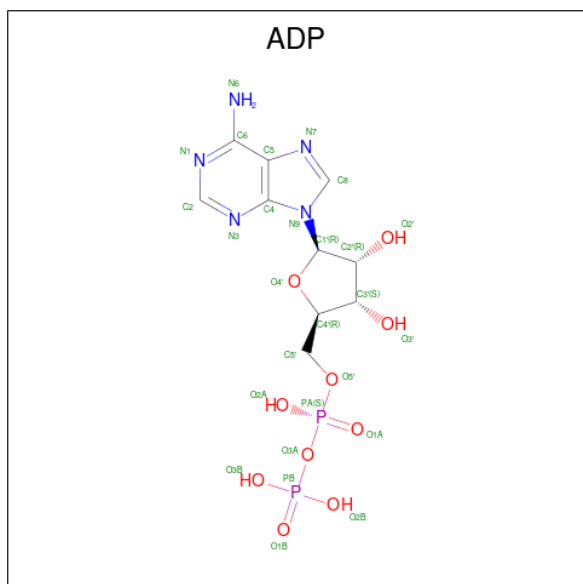
- Molecule 1 is a protein called Pyruvate dehydrogenase kinase, isozyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2709	1743	444	505	17			
1	B	336	Total	C	N	O	S	0	0	0
			2684	1728	441	498	17			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

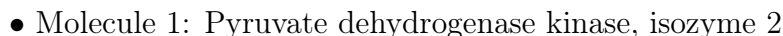


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	109	Total	O	0	0
			109	109		

- Molecule 1: Pyruvate dehydrogenase kinase, isozyme 2



V1360	K1201
E1361	L1202
R1362	L1203
L1363	C1204
P1364	D1205
V1365	K1206
TYR	Y1207
ASN	L1208
LYS	Y1209
SER	M1209
ALA	P1212
TRP	
ARG	Q1217
HIS	E1218
TYR	Y1219
GLN	N1220
THR	
ILE	N1223
GLN	A1224
GLU	T1225
ALA	Q1226
GLY	P1227
ASP	I1228
TRP	
CYS	Y1232
VAL	V1233
PRO	P1234
SER	S1235
THR	H1236
GLU	L1237
PRO	Y1238
LYS	
ASN	F1245
THR	K1246
SER	N1247
THR	A1248
TYR	M1249
ARG	R1250
VAL	
SER	V1253
	S1258
	T1261
	L1262
	P1263
	P1264
	I1265
	K1266
	I1267
	M1268
	V1269
	A1270
	L1271
	L1276
	K1279
	R1283

V1287
R1290
K1291
R1294
L1295
F1296
S1297
Y1298
T1302
A1303
P1304
T1305
P1306
GLN
PRO
GLY
THR
GLY
GLY
THR
P1314
L1315
A1316
G1317
F1318
G1319
Y1320
G1321
L1322
P1323
I1324
S1325
R1326
L1327
K1330
Y1331
F1332
Q1333
G1334
D1335
L1338
F1339
S1340
M1341
E1342
G1343
F1344
G1345
T1346
D1347
T1357
D1358
S1359

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.42Å 109.87Å 71.41Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 6.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.2 (6.00-2.50) 88.4 (6.00-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.202 , 0.262 0.187 , 0.239	Depositor DCC
R_{free} test set	1626 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5677	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.07	24/2771 (0.9%)	1.66	72/3752 (1.9%)
1	B	0.85	12/2745 (0.4%)	1.34	26/3715 (0.7%)
All	All	0.96	36/5516 (0.7%)	1.51	98/7467 (1.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1178	LYS	C-N	-12.33	1.16	1.33
1	B	1115	HIS	CA-C	-9.02	1.40	1.52
1	A	1096	GLU	C-O	8.29	1.34	1.24
1	B	1027	GLN	C-N	-7.50	1.23	1.33
1	A	1090	PHE	C-N	-7.48	1.14	1.33

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	PHE	O-C-N	-15.69	102.73	122.34
1	A	1137	PRO	CA-C-N	14.68	148.39	121.97
1	A	1137	PRO	C-N-CA	14.68	148.39	121.97
1	A	1138	VAL	N-CA-C	13.88	138.22	109.34
1	A	1077	GLN	OE1-CD-NE2	-10.78	111.82	122.60

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	2709	0	2692	263	0
1	B	2684	0	2679	197	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	1	0
3	B	27	0	12	9	0
4	A	119	0	0	19	0
4	B	109	0	0	16	0
All	All	5677	0	5395	455	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 42.

The worst 5 of 455 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:1042:PHE:CE2	1:A:1095:PRO:HG3	1.64	1.33
1:A:1138:VAL:O	1:A:1138:VAL:CG1	1.75	1.29
1:A:1223:ASN:HD22	1:A:1226:GLN:CB	1.58	1.16
1:A:1031:PHE:HA	1:A:1036:ALA:N	1.60	1.15
1:A:1177:PRO:HD2	1:A:1179:HIS:NE2	1.62	1.14

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	329/407 (81%)	290 (88%)	32 (10%)	7 (2%)	5 9
1	B	326/407 (80%)	306 (94%)	18 (6%)	2 (1%)	21 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	655/814 (80%)	596 (91%)	50 (8%)	9 (1%)	9	17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1138	VAL
1	A	1224	ALA
1	A	1295	LEU
1	A	1039	LYS
1	B	1199	MET

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	305/363 (84%)	266 (87%)	39 (13%)	4	9
1	B	302/363 (83%)	267 (88%)	35 (12%)	5	11
All	All	607/726 (84%)	533 (88%)	74 (12%)	5	10

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1188	SER
1	B	1360	VAL
1	B	1217	GLN
1	B	1318	PHE
1	A	1257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1115	HIS
1	B	1162	ASN
1	B	1256	HIS

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Mol	Chain	Res	Type
1	B	1144	GLN
1	A	1223	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	3510	2	28,29,29	1.58	6 (21%)	43,45,45	2.25	11 (25%)
3	ADP	A	3500	2	28,29,29	1.57	5 (17%)	43,45,45	2.25	11 (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	ADP	B	3510	2	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	3500	2	-	7/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3500	ADP	PA-O3A	-3.87	1.55	1.59
3	B	3510	ADP	PA-O3A	-3.85	1.55	1.59
3	B	3510	ADP	C5-N7	-2.80	1.34	1.39
3	A	3500	ADP	C5-N7	-2.78	1.34	1.39
3	B	3510	ADP	PB-O2B	2.77	1.65	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3510	ADP	C5-C4-N3	-6.42	117.87	126.72
3	A	3500	ADP	C5-C4-N3	-6.41	117.89	126.72
3	A	3500	ADP	N3-C2-N1	-6.15	119.27	128.58
3	B	3510	ADP	N3-C2-N1	-6.15	119.27	128.58
3	A	3500	ADP	C4-C5-N7	-5.12	104.73	110.58

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3500	ADP	PA-O3A-PB-O3B
3	A	3500	ADP	C5'-O5'-PA-O1A
3	A	3500	ADP	C5'-O5'-PA-O3A
3	B	3510	ADP	PA-O3A-PB-O3B
3	B	3510	ADP	C5'-O5'-PA-O1A

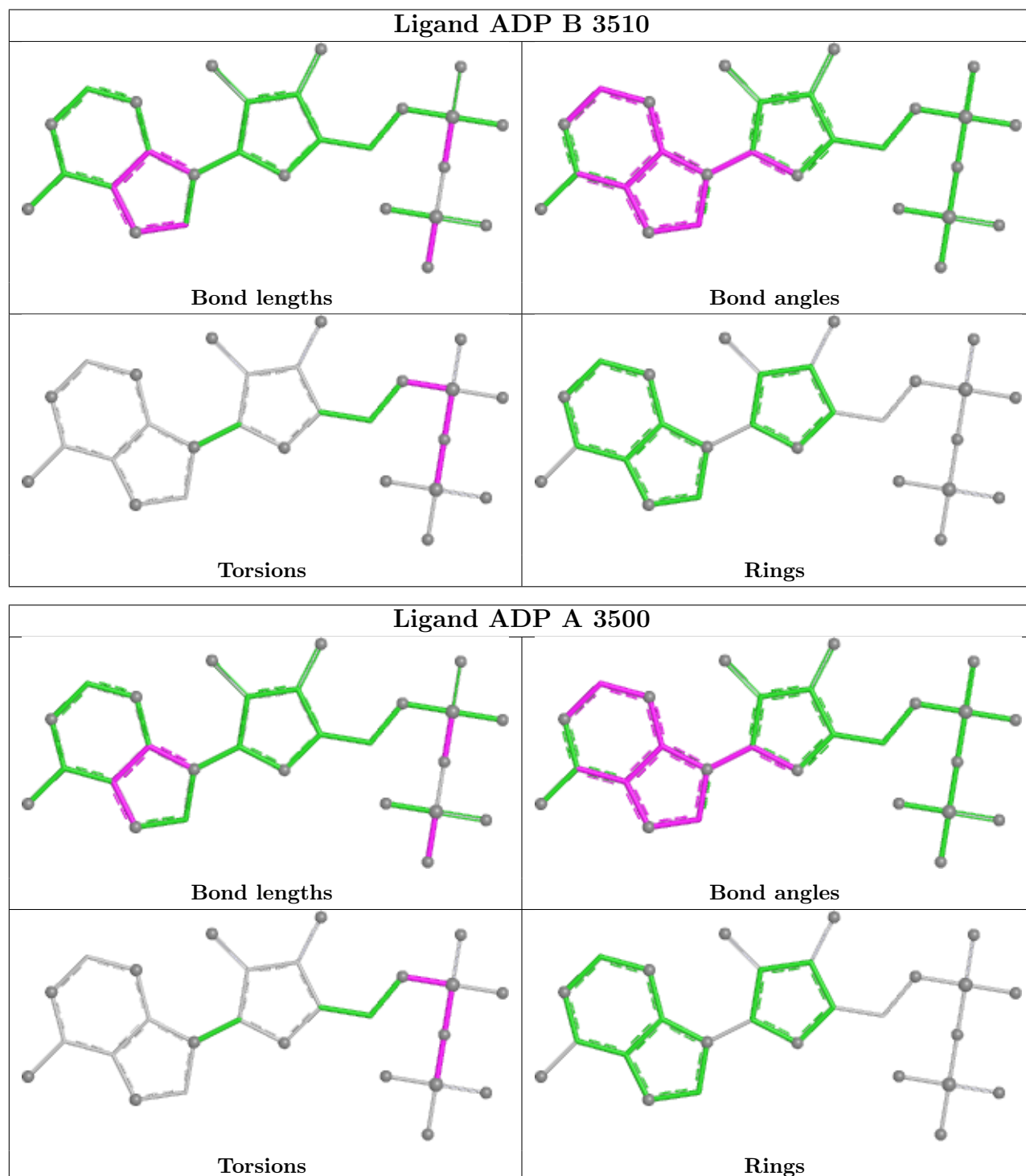
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3510	ADP	9	0
3	A	3500	ADP	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1178:LYS	C	1179:HIS	N	1.16
1	A	1090:PHE	C	1091:LEU	N	1.14

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	339/407 (83%)	-1.37	0 100 100	19, 41, 80, 117	0
1	B	336/407 (82%)	-1.41	0 100 100	20, 40, 70, 107	0
All	All	675/814 (82%)	-1.39	0 100 100	19, 41, 74, 117	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.

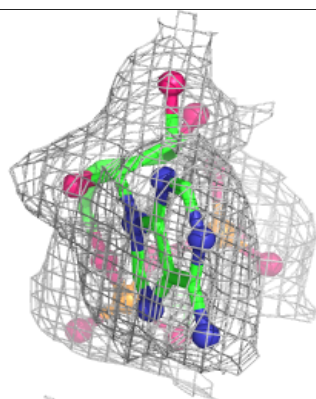
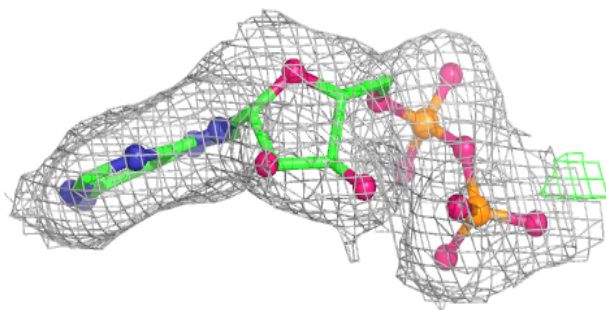
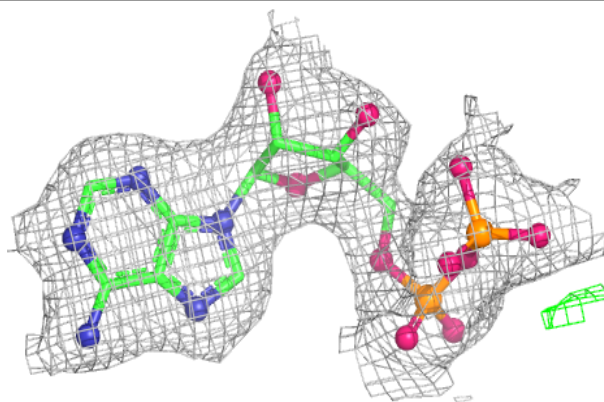
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	4601	1/1	0.99	0.02	44,44,44,44	0
2	MG	B	4611	1/1	0.99	0.04	47,47,47,47	0
3	ADP	A	3500	27/27	1.00	0.02	16,26,35,38	0
3	ADP	B	3510	27/27	1.00	0.02	16,26,35,38	0

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.

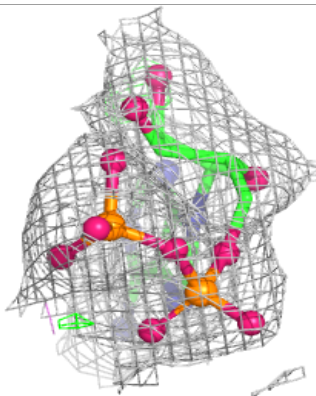
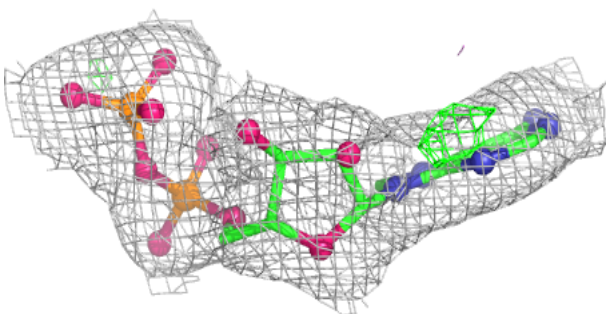
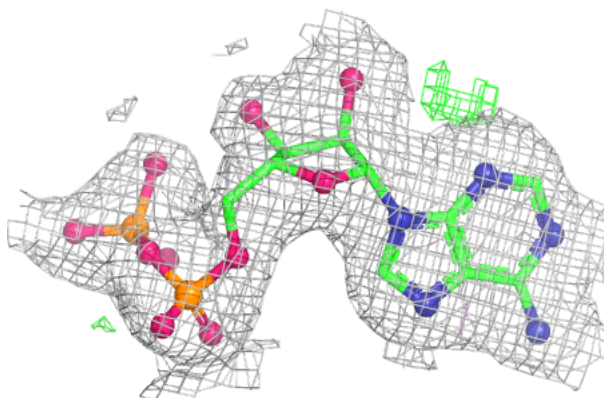
Electron density around ADP A 3500:

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



Electron density around ADP B 3510:

$2mF_o-DF_c$ (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.