



wwPDB X-ray Structure Validation Summary Report

Aug 16, 2023 – 07:34 AM EDT

PDB ID : 1Y8P
Title : Crystal structure of the PDK3-L2 complex
Authors : Kato, M.; Chuang, J.L.; Wynn, R.M.; Chuang, D.T.
Deposited on : 2004-12-13
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

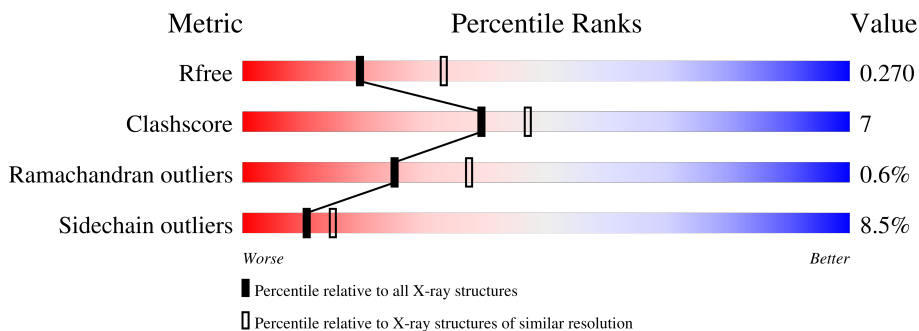
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	419	 71% 16% • 9%
2	B	128	 63% 11% • 24%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3949 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 [lipoamide]] kinase isozyme 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	3112	2005	520	574	13	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	cloning artifact	UNP Q15120
A	-11	GLY	-	cloning artifact	UNP Q15120
A	-10	SER	-	cloning artifact	UNP Q15120
A	-9	HIS	-	expression tag	UNP Q15120
A	-8	HIS	-	expression tag	UNP Q15120
A	-7	HIS	-	expression tag	UNP Q15120
A	-6	HIS	-	expression tag	UNP Q15120
A	-5	HIS	-	expression tag	UNP Q15120
A	-4	HIS	-	expression tag	UNP Q15120
A	-3	GLY	-	cloning artifact	UNP Q15120
A	-2	MET	-	cloning artifact	UNP Q15120
A	-1	ALA	-	cloning artifact	UNP Q15120
A	0	ARG	-	cloning artifact	UNP Q15120
A	1	LEU	-	cloning artifact	UNP Q15120
A	2	GLU	-	cloning artifact	UNP Q15120
A	3	ASN	-	cloning artifact	UNP Q15120
A	4	LEU	-	cloning artifact	UNP Q15120
A	5	TYR	-	cloning artifact	UNP Q15120
A	6	PHE	-	cloning artifact	UNP Q15120
A	7	GLN	-	cloning artifact	UNP Q15120
A	8	GLY	-	cloning artifact	UNP Q15120

- Molecule 2 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	97	736	471	115	146	4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	GLY	-	cloning artifact	UNP P10515
B	107	GLY	-	cloning artifact	UNP P10515
B	108	SER	-	cloning artifact	UNP P10515
B	109	HIS	-	expression tag	UNP P10515
B	110	HIS	-	expression tag	UNP P10515
B	111	HIS	-	expression tag	UNP P10515
B	112	HIS	-	expression tag	UNP P10515
B	113	HIS	-	expression tag	UNP P10515
B	114	HIS	-	expression tag	UNP P10515
B	115	GLY	-	cloning artifact	UNP P10515
B	116	MET	-	cloning artifact	UNP P10515
B	117	ALA	-	cloning artifact	UNP P10515
B	118	ARG	-	cloning artifact	UNP P10515
B	119	LEU	-	cloning artifact	UNP P10515
B	120	GLU	-	cloning artifact	UNP P10515
B	121	ASN	-	cloning artifact	UNP P10515
B	122	LEU	-	cloning artifact	UNP P10515
B	123	TYR	-	cloning artifact	UNP P10515
B	124	PHE	-	cloning artifact	UNP P10515
B	125	GLN	-	cloning artifact	UNP P10515

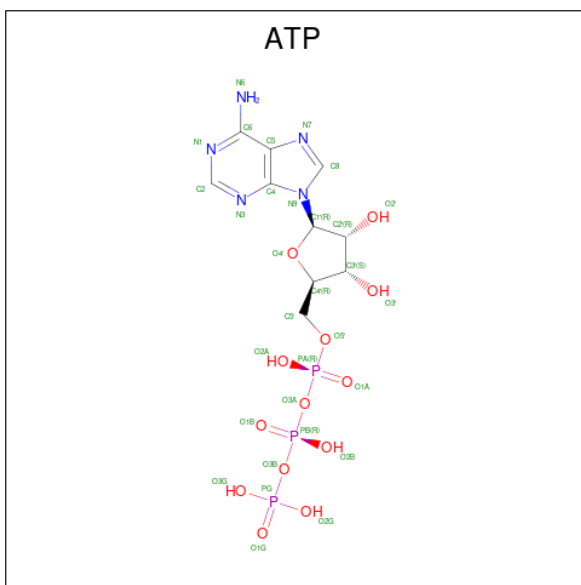
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

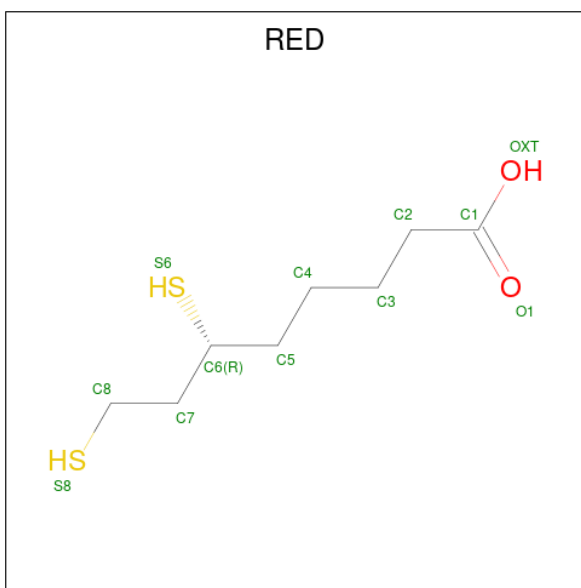
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	2	2	2	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

- Molecule 6 is DIHYDROLIPOIC ACID (three-letter code: RED) (formula: $C_8H_{16}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
6	B	1	11	8	1	2	0	0

- Molecule 7 is water.

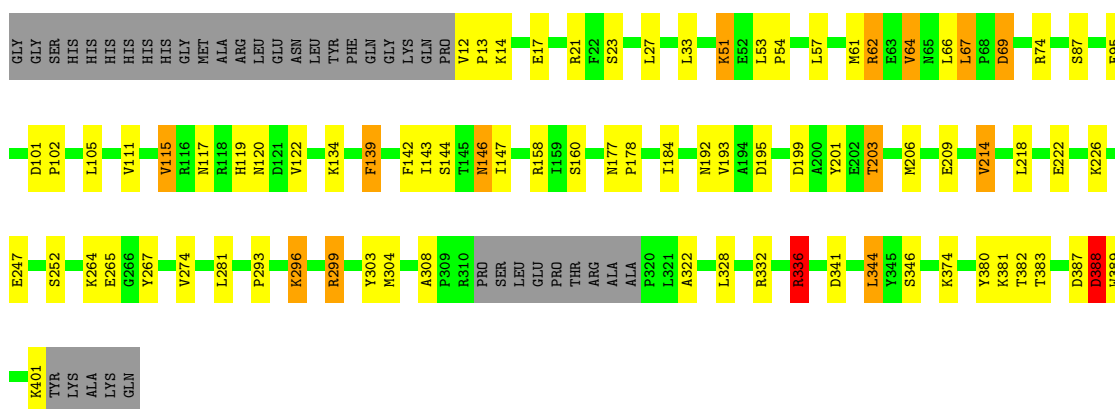
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total 53	O 53	0	0
7	B	3	Total 3	O 3	0	0

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. 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. 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.

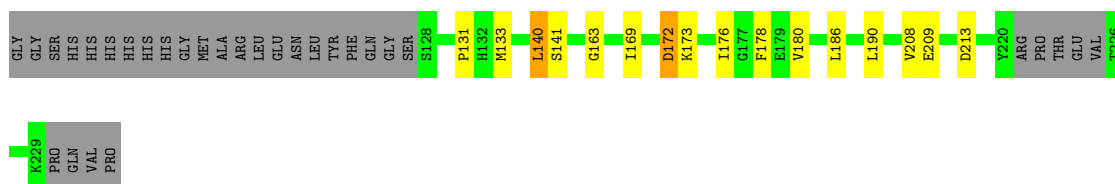
- Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

Chain A:  71% 16% 9%



- Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex

Chain B:  63% 11% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.90Å 120.90Å 240.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.63 48.24 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.63) 98.4 (48.24-2.63)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.230 0.256 , 0.270	Depositor DCC
R_{free} test set	1566 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3949	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: RED, MG, K, ATP

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	0.74	0/3193	0.81	4/4326 (0.1%)
2	B	0.68	0/749	0.76	2/1017 (0.2%)
All	All	0.73	0/3942	0.80	6/5343 (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	A	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	388	ASP	N-CA-CB	-6.26	99.33	110.60
1	A	344	LEU	CA-CB-CG	5.93	128.93	115.30
2	B	172	ASP	N-CA-CB	-5.49	100.73	110.60
2	B	180	VAL	CB-CA-C	-5.31	101.31	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	ASP	Peptide

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	3112	0	3078	47	0
2	B	736	0	727	11	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	31	0	12	0	0
6	B	11	0	15	4	0
7	A	53	0	0	4	0
7	B	3	0	0	0	0
All	All	3949	0	3832	57	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 7.

The worst 5 of 57 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)
2:B:173:LYS:NZ	6:B:373:RED:C1	1.82	1.43
2:B:173:LYS:HZ1	6:B:373:RED:C1	1.40	1.31
2:B:173:LYS:HZ3	6:B:373:RED:C1	1.63	0.89
1:A:303:TYR:O	1:A:304:MET:HG2	1.76	0.85
1:A:87:SER:OG	1:A:119:HIS:HE1	1.60	0.84

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	378/419 (90%)	356 (94%)	19 (5%)	3 (1%)	19	28
2	B	93/128 (73%)	88 (95%)	5 (5%)	0	100	100
All	All	471/547 (86%)	444 (94%)	24 (5%)	3 (1%)	25	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	THR
1	A	388	ASP
1	A	214	VAL

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	345/374 (92%)	314 (91%)	31 (9%)	9	14
2	B	79/109 (72%)	74 (94%)	5 (6%)	18	27
All	All	424/483 (88%)	388 (92%)	36 (8%)	10	15

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	THR
2	B	190	LEU
1	A	388	ASP
2	B	140	LEU
1	A	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	192	ASN
1	A	302	ASN

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Mol	Chain	Res	Type
1	A	240	HIS
1	A	86	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 5 ligands modelled in this entry, 3 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
5	ATP	A	504	4,3	26,33,33	1.07	1 (3%)	31,52,52	1.77	8 (25%)
6	RED	B	373	-	9,10,11	0.35	0	6,10,12	3.61	1 (16%)

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
5	ATP	A	504	4,3	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RED	B	373	-	-	3/7/9/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	ATP	O4'-C1'	3.48	1.45	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	373	RED	C7-C8-S8	-8.15	105.25	113.74
5	A	504	ATP	O3G-PG-O3B	5.53	123.19	104.64
5	A	504	ATP	N3-C2-N1	-3.42	123.33	128.68
5	A	504	ATP	C4-C5-N7	-2.92	106.36	109.40
5	A	504	ATP	PA-O3A-PB	-2.52	124.18	132.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	ATP	PB-O3B-PG-O3G
5	A	504	ATP	C5'-O5'-PA-O1A
6	B	373	RED	C5-C6-C7-C8
6	B	373	RED	C6-C7-C8-S8
5	A	504	ATP	C5'-O5'-PA-O3A

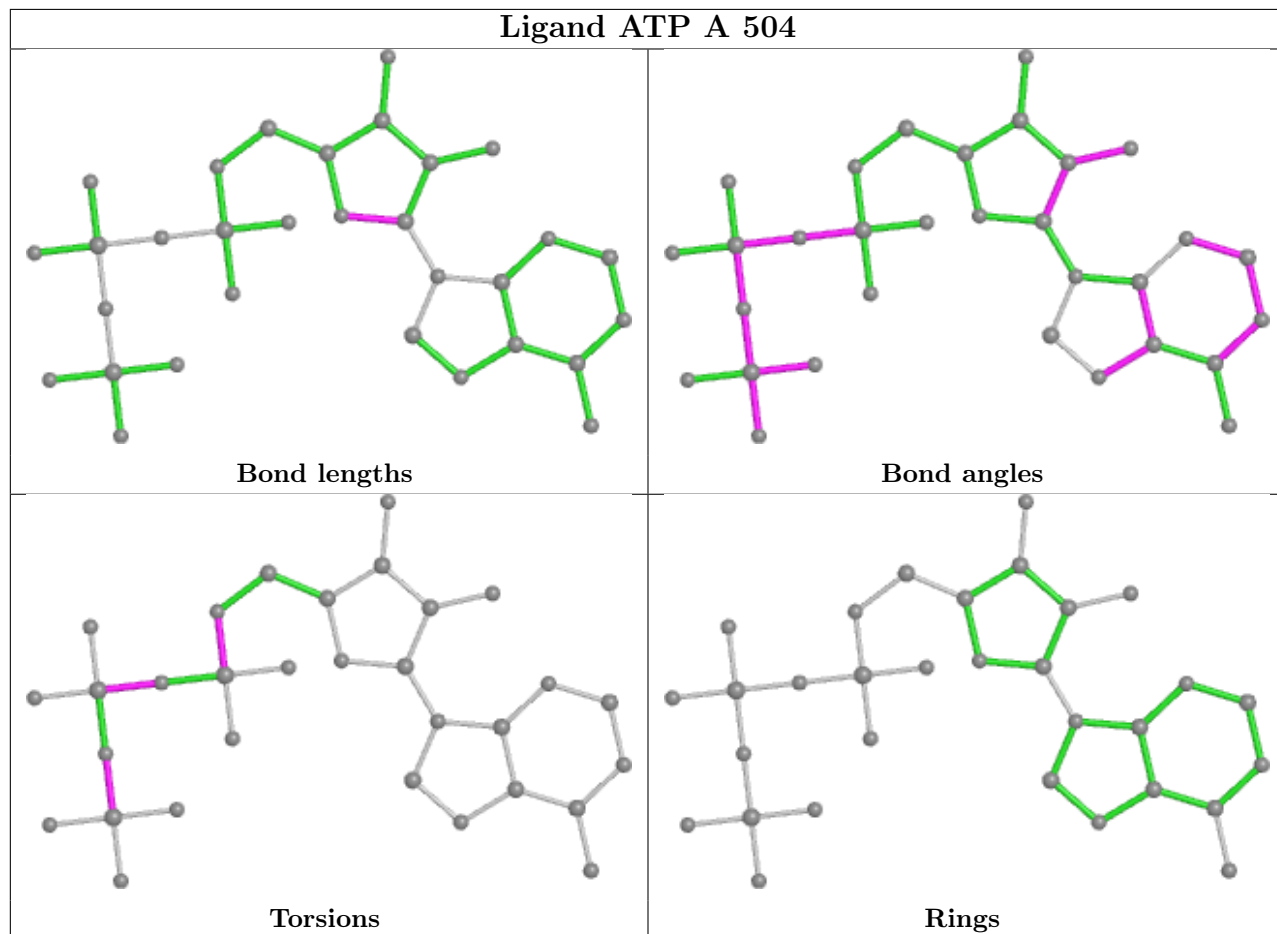
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	373	RED	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

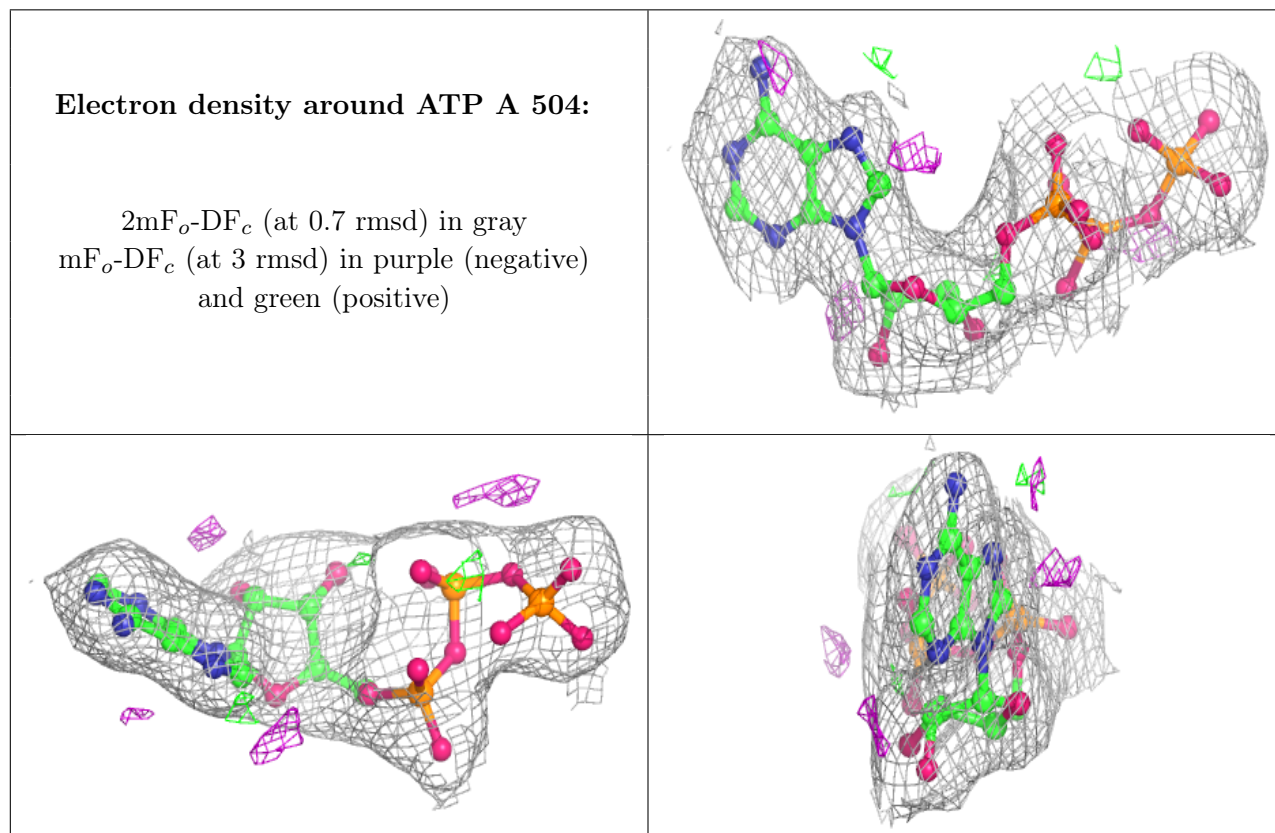
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.