wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 05:30 AM EDT

PDB ID	:	1Y8O
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	:	2.48 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:

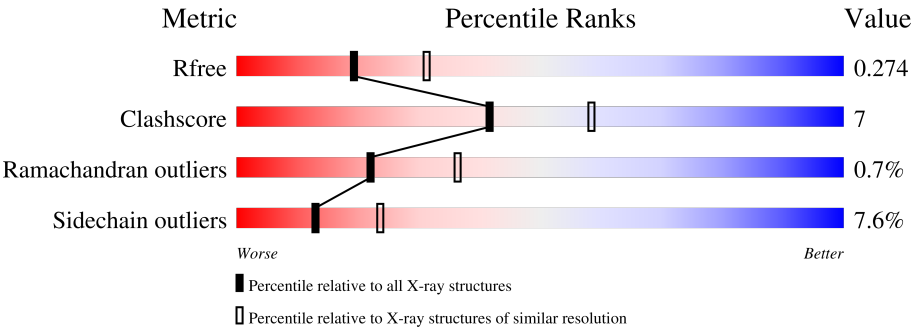
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)

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%

Mol	Chain	Length	Quality of chain
1	A	419	70% 16% · 11%
2	B	128	55% 19% · 24%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3910 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	374	3066	1977	510	566	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
2	B	97	Total	C	N	O	S	0	0	0
			736	471	115	146	4			

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

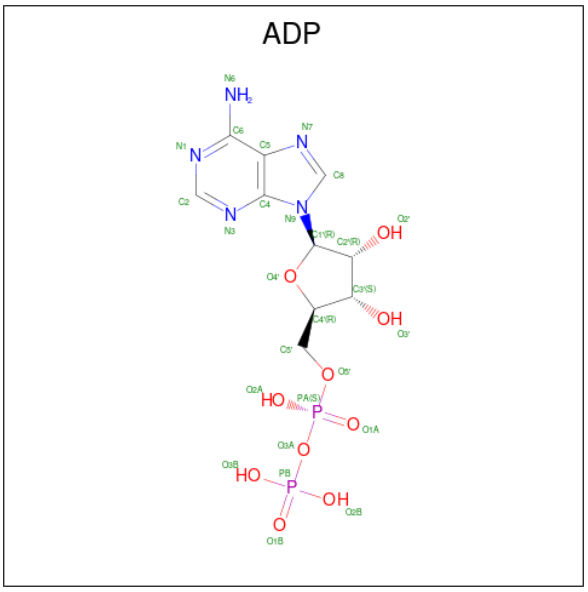
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

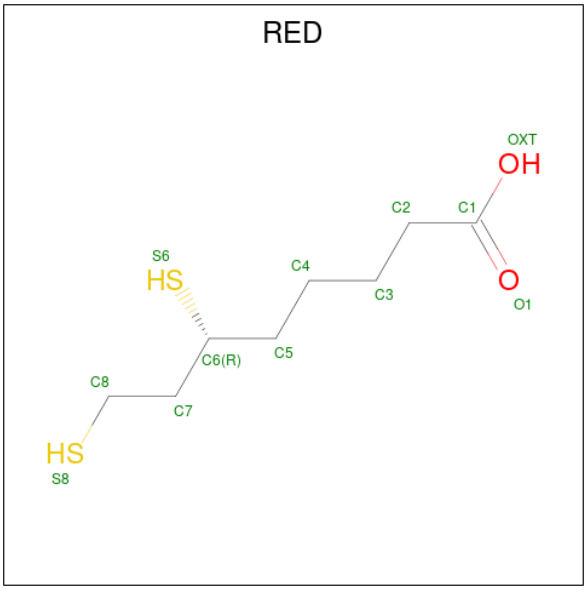
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

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



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

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



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

- Molecule 7 is water.

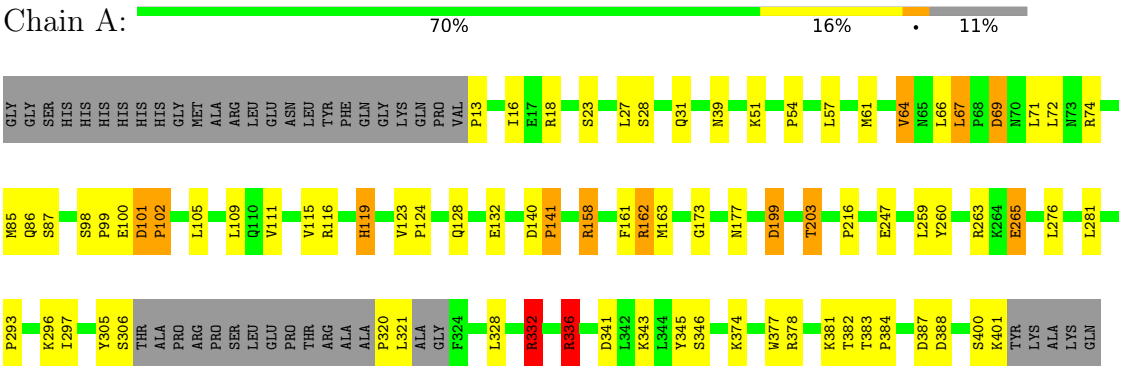
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	63	Total O 63 63	0	0
7	B	4	Total O 4 4	0	0

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.

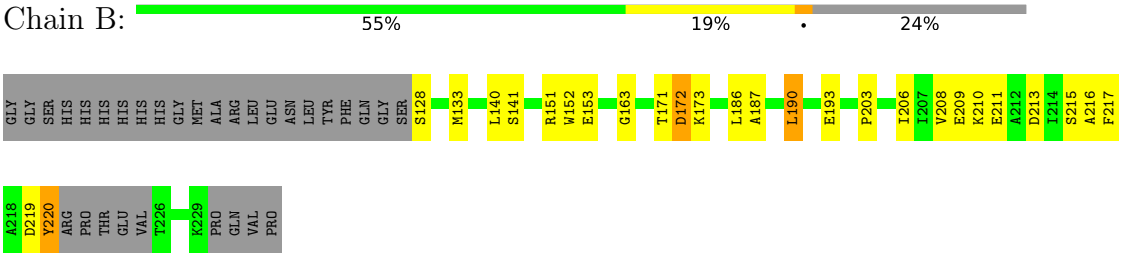
• Molecule 1: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.75Å 120.75Å 239.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.48 48.13 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.48) 99.7 (48.13-2.48)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.234 0.257 , 0.274	Depositor DCC
R_{free} test set	1494 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

5.1 Standard geometry

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

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	0.84	3/3145 (0.1%)	0.85	10/4257 (0.2%)
2	B	1.27	5/749 (0.7%)	0.83	1/1017 (0.1%)
All	All	0.94	8/3894 (0.2%)	0.85	11/5274 (0.2%)

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
2	B	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	ALA	C-N	13.97	1.66	1.34
2	B	215	SER	CB-OG	13.31	1.59	1.42
2	B	220	TYR	C-O	11.16	1.44	1.23
2	B	216	ALA	C-O	-10.40	1.03	1.23
2	B	211	GLU	CD-OE1	6.59	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	336	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	388	ASP	N-CA-CB	-7.08	97.86	110.60
1	A	18	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	199	ASP	CB-CG-OD1	6.09	123.78	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	171	THR	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	3066	0	3029	39	0
2	B	736	0	727	15	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	27	0	12	0	0
6	B	11	0	15	3	0
7	A	63	0	0	3	0
7	B	4	0	0	0	0
All	All	3910	0	3783	53	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 53 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:HZ3	6:B:373:RED:C1	1.14	1.51
2:B:173:LYS:NZ	6:B:373:RED:C1	1.78	1.43
1:A:247:GLU:HG3	7:A:560:HOH:O	1.35	1.21
2:B:173:LYS:HZ1	6:B:373:RED:C1	1.82	0.88
1:A:28:SER:H	1:A:31:GLN:HE21	1.26	0.82

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	369/419 (88%)	361 (98%)	6 (2%)	2 (0%)	29 46
2	B	93/128 (73%)	91 (98%)	1 (1%)	1 (1%)	14 23
All	All	462/547 (84%)	452 (98%)	7 (2%)	3 (1%)	22 40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	ASP
1	A	100	GLU
1	A	141	PRO

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	341/374 (91%)	315 (92%)	26 (8%)	13 24
2	B	79/109 (72%)	73 (92%)	6 (8%)	13 24
All	All	420/483 (87%)	388 (92%)	32 (8%)	13 24

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	140	LEU
2	B	141	SER
1	A	119	HIS

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Mol	Chain	Res	Type
1	A	116	ARG
2	B	186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	240	HIS
1	A	73	ASN
1	A	86	GLN
1	A	119	HIS

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	ADP	A	504	4,3	24,29,29	1.27	3 (12%)	29,45,45	1.47	5 (17%)
6	RED	B	373	-	9,10,11	0.55	0	6,10,12	4.35	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	ADP	A	504	4,3	-	2/12/32/32	0/3/3/3
6	RED	B	373	-	-	3/7/9/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	ADP	O4'-C1'	3.66	1.46	1.41
5	A	504	ADP	C5-C4	2.96	1.48	1.40
5	A	504	ADP	C2-N3	2.13	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	373	RED	C7-C8-S8	-10.33	102.98	113.74
5	A	504	ADP	N3-C2-N1	-3.01	123.98	128.68
5	A	504	ADP	C3'-C2'-C1'	2.49	104.72	100.98
5	A	504	ADP	C2-N1-C6	2.48	123.00	118.75
5	A	504	ADP	C4-C5-N7	-2.27	107.03	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	373	RED	C3-C4-C5-C6
6	B	373	RED	C6-C7-C8-S8
6	B	373	RED	C4-C5-C6-C7
5	A	504	ADP	PB-O3A-PA-O5'
5	A	504	ADP	PA-O3A-PB-O2B

There are no ring outliers.

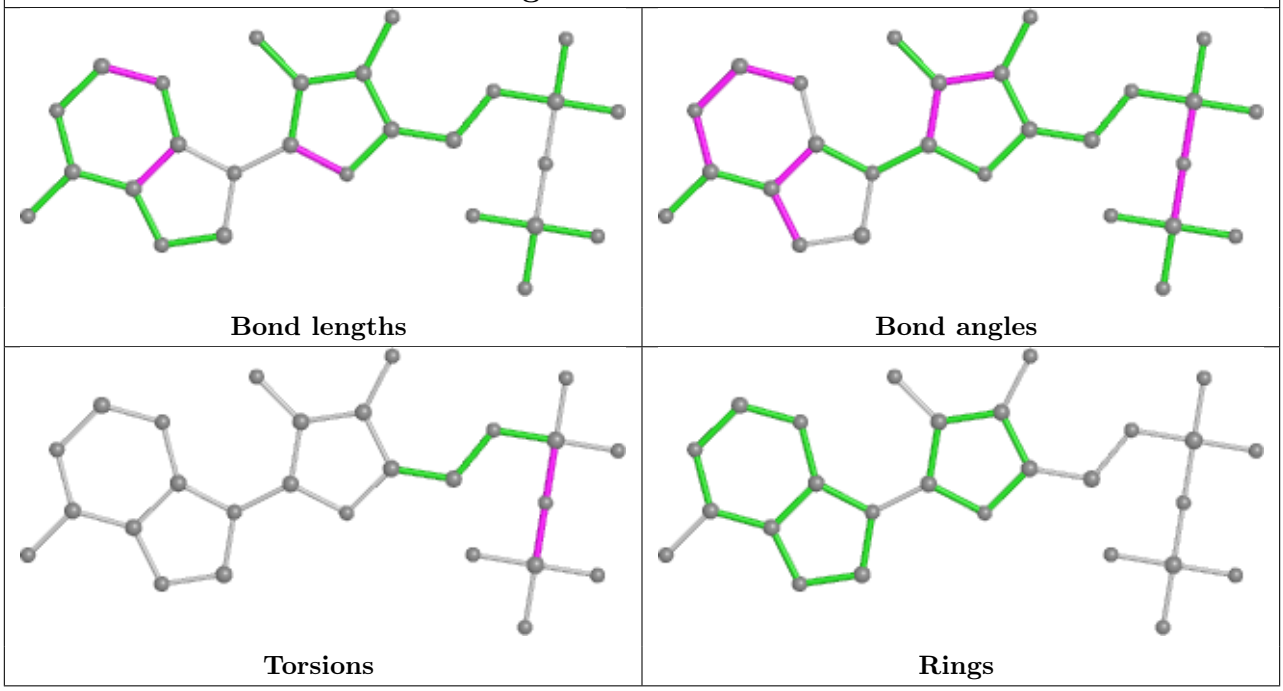
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	373	RED	3	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 A 504



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
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	216:ALA	C	217:PHE	N	1.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

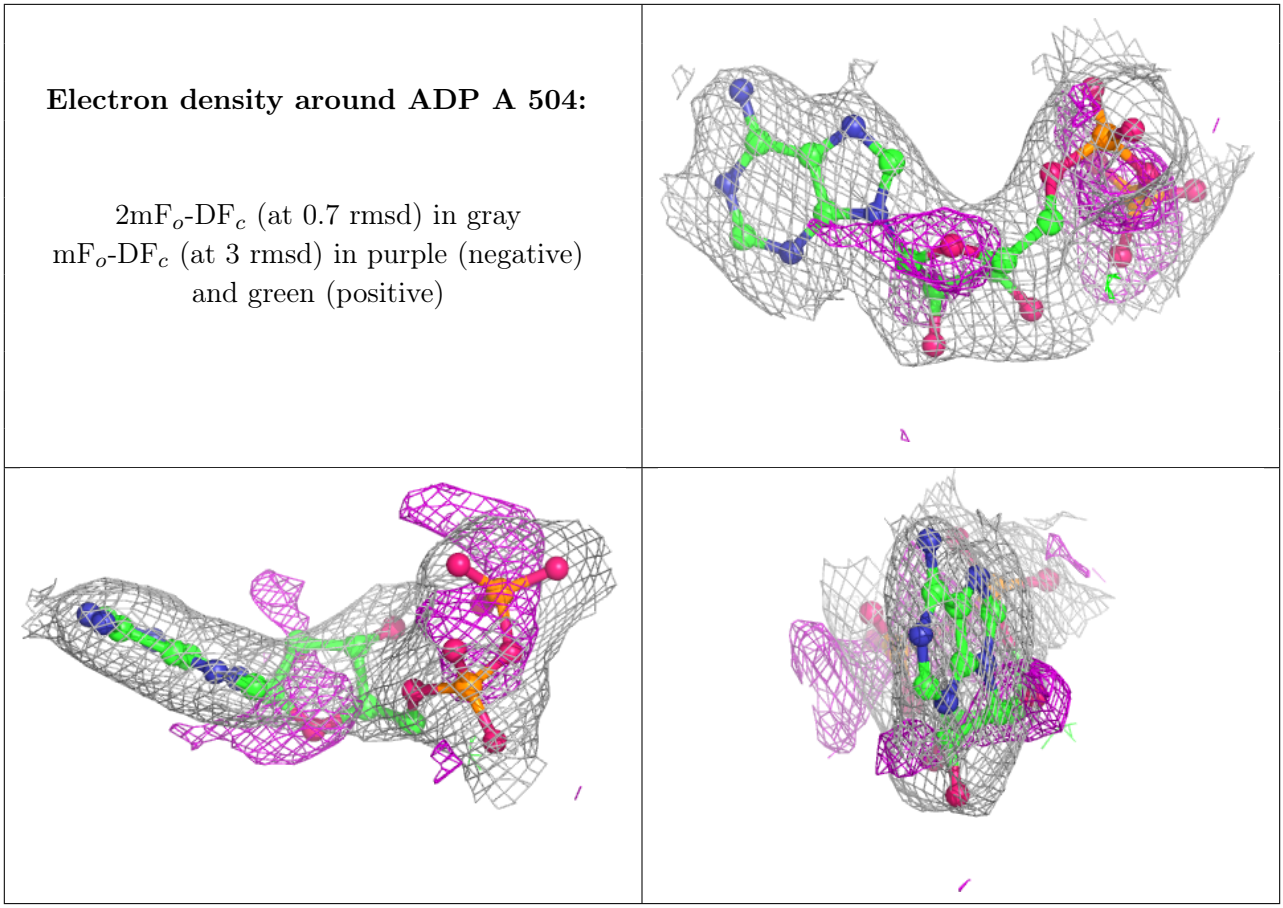
6.4 Ligands

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.

Electron density around ADP A 504:

$2mF_o$-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)

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