



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2024 – 11:14 AM EST

PDB ID : 3LC6
Title : The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli
Authors : Zheng, J.; Jia, Z.
Deposited on : 2010-01-09
Resolution : 3.10 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 : 2.36
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

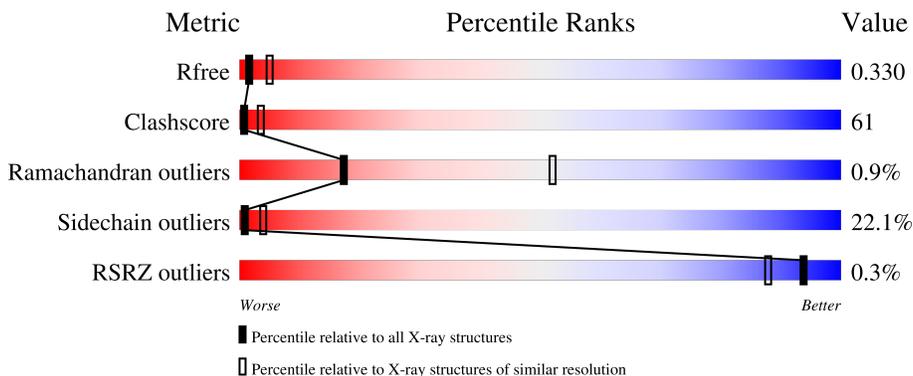
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

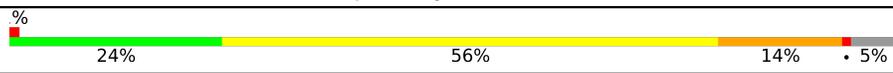
The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	578	 24% 56% 14% 5%
1	B	578	 27% 52% 14% 7%

2 Entry composition [i](#)

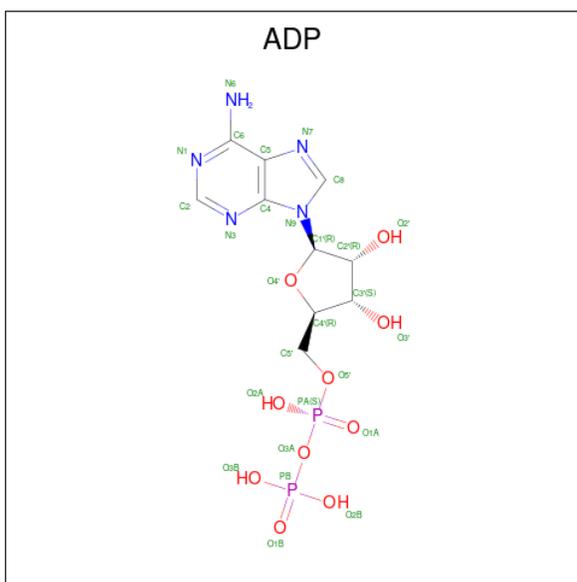
There are 5 unique types of molecules in this entry. The entry contains 9107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	Total 4526	C 2906	N 800	O 799	S 21	0	0	0
1	B	539	Total 4454	C 2861	N 785	O 788	S 20	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

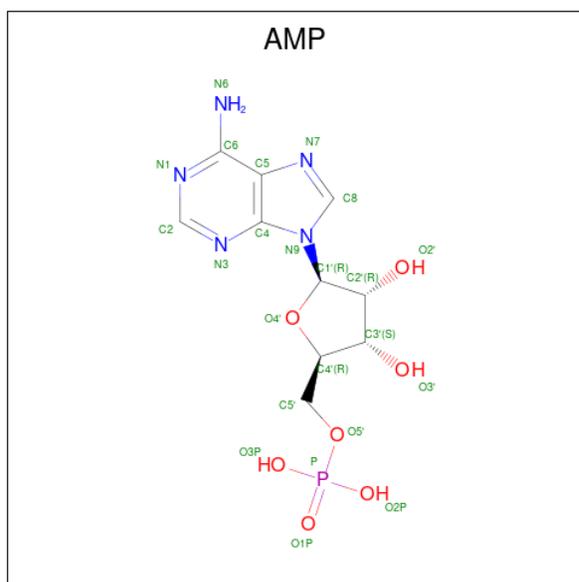


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

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

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	23	10	5	7	1	0	0

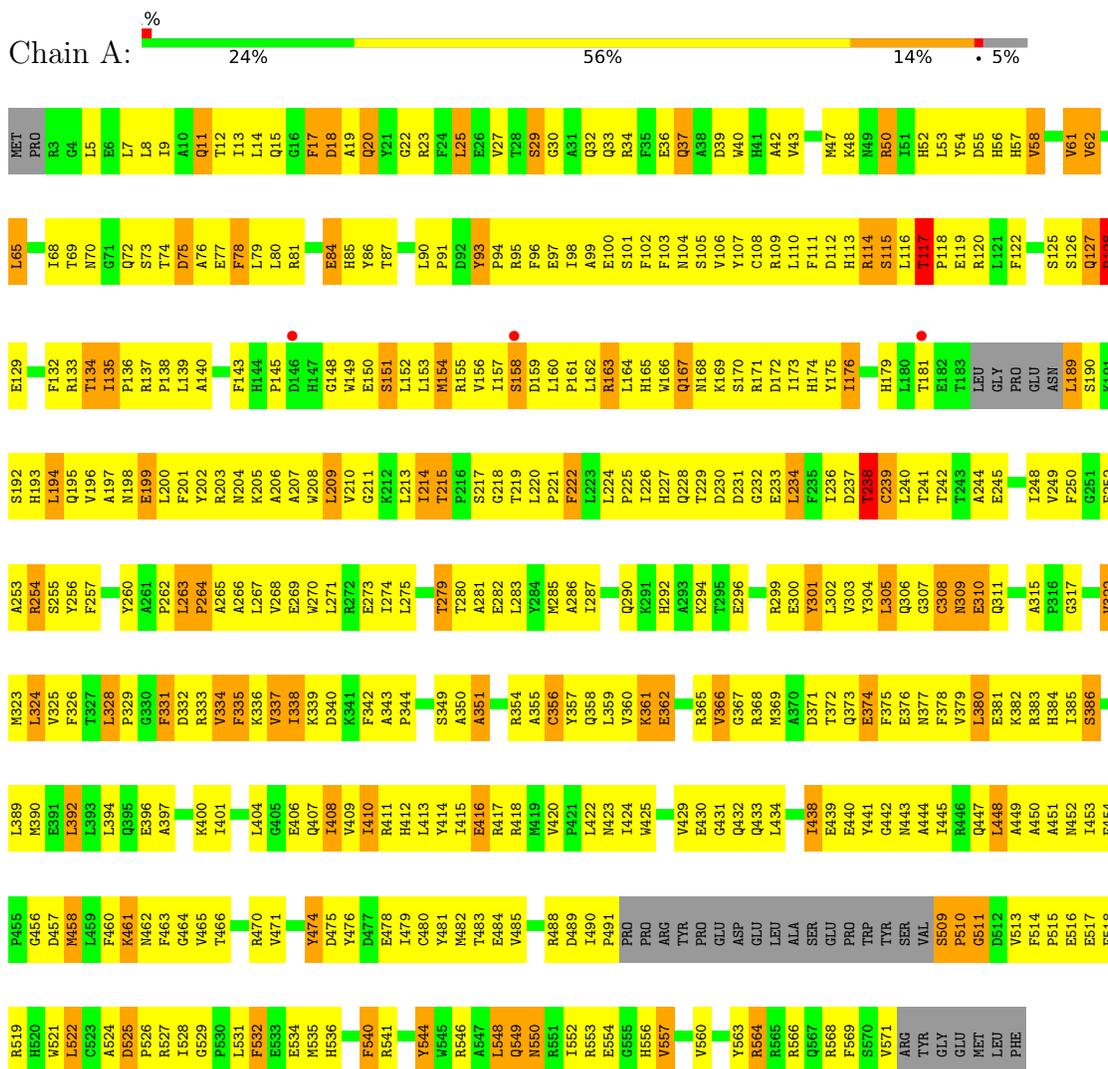
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	45	Total O 45 45	0	0

3 Residue-property plots

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: Isocitrate dehydrogenase kinase/phosphatase



- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



F518	F519	H520	L522	D525	T528	G529	P530	L531	F532	M535	H536	A537	D538	L539	F540	R541	A542	D543	Y544	W545	R546	A547	L548	Q549	N550	R551	L552	R553	E554	G555	H556	Y557	E558	D559	V560	Y561	A562	Y563	R564	R565	R566	R567	R568	F569	S570	V571	H572	Y573	G574	GLU	MET	LEU	PHE							
I453	F454	P455	M456	F459	F460	K461	K462	F463	G464	V465	T466	R467	R470	V471	V472	F473	V474	D475	Y476	D477	E478	I479	G480	Y481	M482	Q483	E484	V485	D486	L487	P488	PRO	PRO	PRO	PRO	PRO	ARG	TYR	PRO	GLU	ASP	GLU	LEU	ALA	SER	GLU	TRP	TYR	SER	VAL	SER	PRO	G511	F514	P515	E516	E517			
L392	L393	L394	Q395	E396	A397	A398	E399	K400	I401	T402	D403	L404	Q407	I408	V409	I410	R411	H412	L413	Y414	I415	E416	R417	R418	M419	V420	P421	L422	M423	I424	W425	L426	E427	Q428	V429	E430	G431	Q432	Q433	L434	R435	D436	A437	I438	E439	E440	Y441	G442	M443	A444	T445	R446	Q447	L448	A449	A450	A451	N452		
F331	D332	R333	V334	F335	K336	V337	I338	K339	D340	K341	F342	ALA	PRO	GLN	LYS	GLU	MET	SER	ALA	A351	H352	V353	R354	A355	C356	Y357	Q358	L359	V360	Y298	K361	E362	H363	D364	R365	L366	G367	R368	M369	A370	D371	T372	L373	I374	E375	F376	N377	F378	V379	L380	E381	K382	R383	H384	V385	T387	A388	L389	M390	E391
V288	E289	W270	L271	I274	L275	F276	G277	K278	T279	T280	A281	E282	L283	Y284	M285	A286	I287	C288	G289	Q290	K291	H292	D293	A293	K294	T295	E296	S297	Y298	R299	E300	Y301	Y304	L305	Q306	M309	E310	Q311	F312	I313	E314	A315	P316	G317	I318	R319	G320	M321	V322	M323	L324	V325	F326	T327	L328	P329	G330			
N204	W208	L209	K212	L213	I214	T215	P216	S217	G218	T219	L220	P221	F222	L223	I226	H227	Q228	T229	D230	D231	G232	E233	L234	F235	I236	D237	T238	C239	L240	T241	T242	T243	A244	E245	A246	S247	I248	V249	P250	G251	F252	A253	R254	S255	Y256	F257	M258	V259	Y260	A261	N198	E199	L200	P201	Y202	A266	L267			
T134	I135	P136	R137	L138	P139	A140	K141	D142	F143	H144	P145	W149	L152	L153	M154	R155	V156	I157	S158	D159	P161	L162	R163	L164	M168	K169	S170	D172	I173	H174	Y175	I176	I177	R178	H179	L180	T181	P186	L189	S192	H193	L194	Q195	V196	A197	N198	E199	L200	P201	Y202	A266	L267								
MET	P2	R3	G4	L5	L7	L8	R81	I9	Q11	G16	A19	Q20	Y21	F24	L25	E26	V27	T28	F96	E97	I98	A99	E100	S101	F102	E36	Q37	A38	D39	W40	V43	Q44	M47	K48	N49	R50	I51	H52	L53	Y54	H57	V58	G59	L60	V61	V62	S126	E63	Q64	L65	R66	O67	I68	T69						
Q72	D75	F76	L79	L80	R81	V82	H85	Y86	T87	R88	L89	L90	P91	D92	Y93	P94	R95	F96	E97	I98	A99	E100	S101	F102	E36	Q37	A38	D39	W40	V43	Q44	M47	K48	N49	R50	I51	H52	L53	Y54	H57	V58	G59	L60	V61	V62	S126	E63	Q64	L65	R66	O67	I68	T69							

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 133.76Å 187.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (10.00-3.10) 83.7 (10.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.46 (at 3.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.287 , 0.332 0.292 , 0.330	Depositor DCC
R_{free} test set	1191 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9107	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: ADP, MG, AMP

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	0.62	2/4643 (0.0%)	0.80	7/6283 (0.1%)
1	B	0.57	1/4567 (0.0%)	0.77	1/6179 (0.0%)
All	All	0.60	3/9210 (0.0%)	0.79	8/12462 (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	1	5
1	B	0	2
All	All	1	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	CYS	CB-SG	-6.93	1.70	1.82
1	A	511	GLY	N-CA	6.30	1.55	1.46
1	A	356	CYS	CB-SG	-5.39	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	N-CA-C	-8.62	89.69	112.10
1	A	239	CYS	N-CA-C	7.35	130.85	111.00
1	A	509	SER	N-CA-CB	-6.98	100.02	110.50
1	A	238	THR	N-CA-C	6.78	129.31	111.00
1	B	240	LEU	CA-CB-CG	6.74	130.80	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	CYS	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	128	PRO	Peptide
1	A	230	ASP	Peptide
1	A	350	ALA	Peptide
1	A	510	PRO	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	4526	0	4449	592	7
1	B	4454	0	4376	518	7
2	A	27	0	12	5	0
3	A	1	0	0	0	0
4	B	23	0	12	2	0
5	A	31	0	0	12	0
5	B	45	0	0	11	0
All	All	9107	0	8849	1095	7

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 61.

The worst 5 of 1095 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:279:THR:OG1	1:A:282:GLU:HG3	1.16	1.29
1:A:128:PRO:HB2	1:A:129:GLU:CA	1.56	1.29
1:A:200:LEU:HD23	1:A:201:PHE:N	1.48	1.29
1:B:550:ASN:O	1:B:554:GLU:HG3	1.31	1.29
1:A:23:ARG:O	1:A:27:VAL:HG23	1.37	1.25

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASN:ND2	1:B:427:GLU:CD[2_455]	1.48	0.72
1:A:423:ASN:CG	1:B:427:GLU:OE2[2_455]	1.55	0.65
1:A:423:ASN:ND2	1:B:427:GLU:OE1[2_455]	1.74	0.46
1:A:423:ASN:ND2	1:B:427:GLU:OE2[2_455]	1.98	0.22
1:A:423:ASN:CG	1:B:427:GLU:CD[2_455]	2.01	0.19

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	541/578 (94%)	470 (87%)	65 (12%)	6 (1%)	14	46
1	B	529/578 (92%)	457 (86%)	68 (13%)	4 (1%)	19	54
All	All	1070/1156 (93%)	927 (87%)	133 (12%)	10 (1%)	17	52

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	GLY
1	A	366	VAL
1	A	511	GLY
1	B	118	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	480/508 (94%)	382 (80%)	98 (20%)	1	5
1	B	472/508 (93%)	360 (76%)	112 (24%)	1	2
All	All	952/1016 (94%)	742 (78%)	210 (22%)	1	4

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	PHE
1	B	247	SER
1	B	478	GLU
1	B	116	LEU
1	B	171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	536	HIS
1	B	407	GLN
1	B	64	GLN
1	B	292	HIS
1	B	32	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 3 ligands modelled in this entry, 1 is 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
2	ADP	A	1762	3	24,29,29	0.86	1 (4%)	29,45,45	1.61	4 (13%)
4	AMP	B	1604	-	22,25,25	1.04	1 (4%)	25,38,38	1.48	2 (8%)

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
2	ADP	A	1762	3	-	5/12/32/32	0/3/3/3
4	AMP	B	1604	-	-	5/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1604	AMP	C5-C4	2.45	1.47	1.40
2	A	1762	ADP	C5-C4	2.02	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1762	ADP	PA-O3A-PB	-4.21	118.39	132.83
2	A	1762	ADP	N3-C2-N1	-4.13	122.23	128.68
4	B	1604	AMP	N3-C2-N1	-3.83	122.69	128.68
4	B	1604	AMP	C4-C5-N7	-3.38	105.88	109.40
2	A	1762	ADP	C3'-C2'-C1'	2.82	105.22	100.98

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1762	ADP	C5'-O5'-PA-O3A
2	A	1762	ADP	O4'-C4'-C5'-O5'

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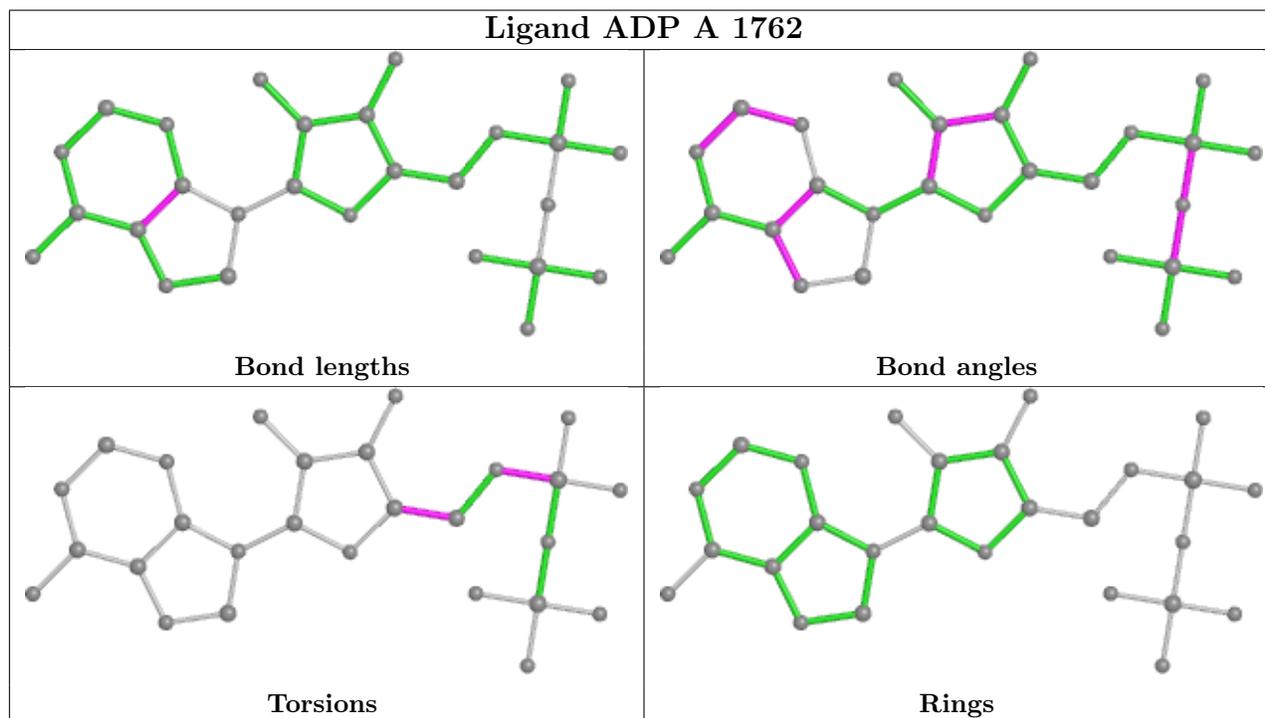
Mol	Chain	Res	Type	Atoms
4	B	1604	AMP	C5'-O5'-P-O2P
4	B	1604	AMP	C5'-O5'-P-O3P
2	A	1762	ADP	C3'-C4'-C5'-O5'

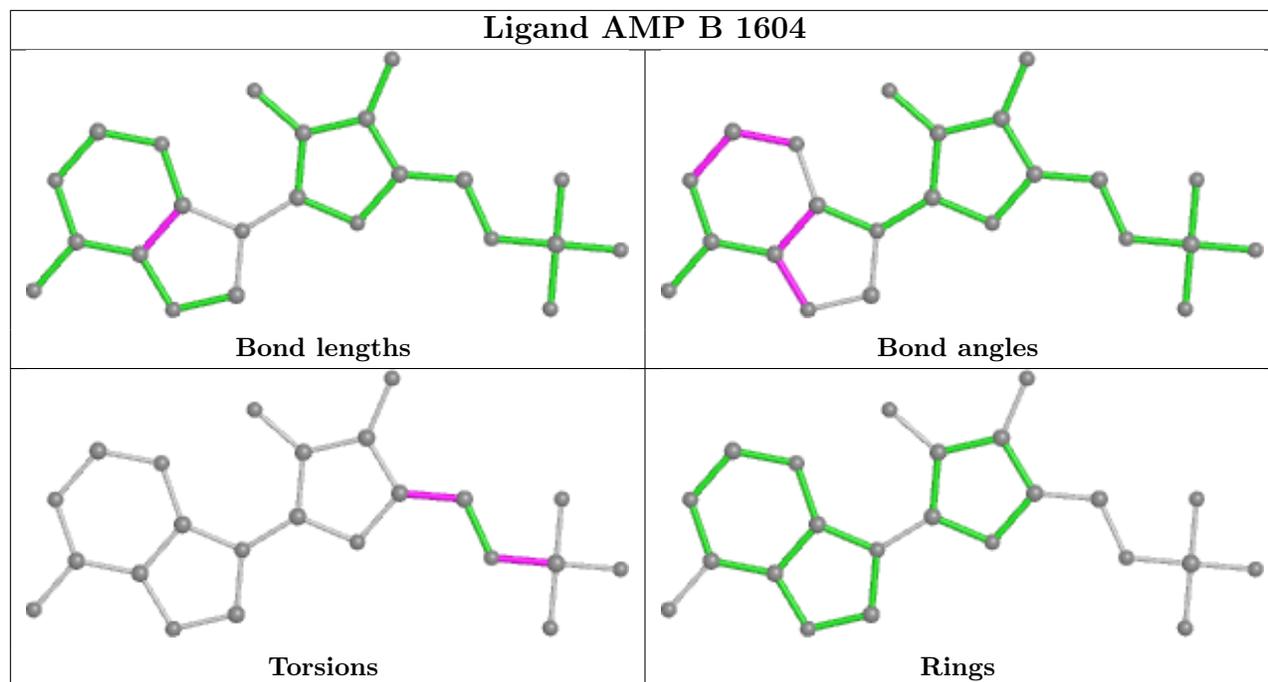
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1762	ADP	5	0
4	B	1604	AMP	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 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](#)

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	547/578 (94%)	-0.25	3 (0%) 91 81	2, 15, 29, 37	0
1	B	539/578 (93%)	-0.18	0 100 100	4, 18, 28, 34	0
All	All	1086/1156 (93%)	-0.22	3 (0%) 94 88	2, 17, 29, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	3.2
1	A	158	SER	2.3
1	A	146	ASP	2.3

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.

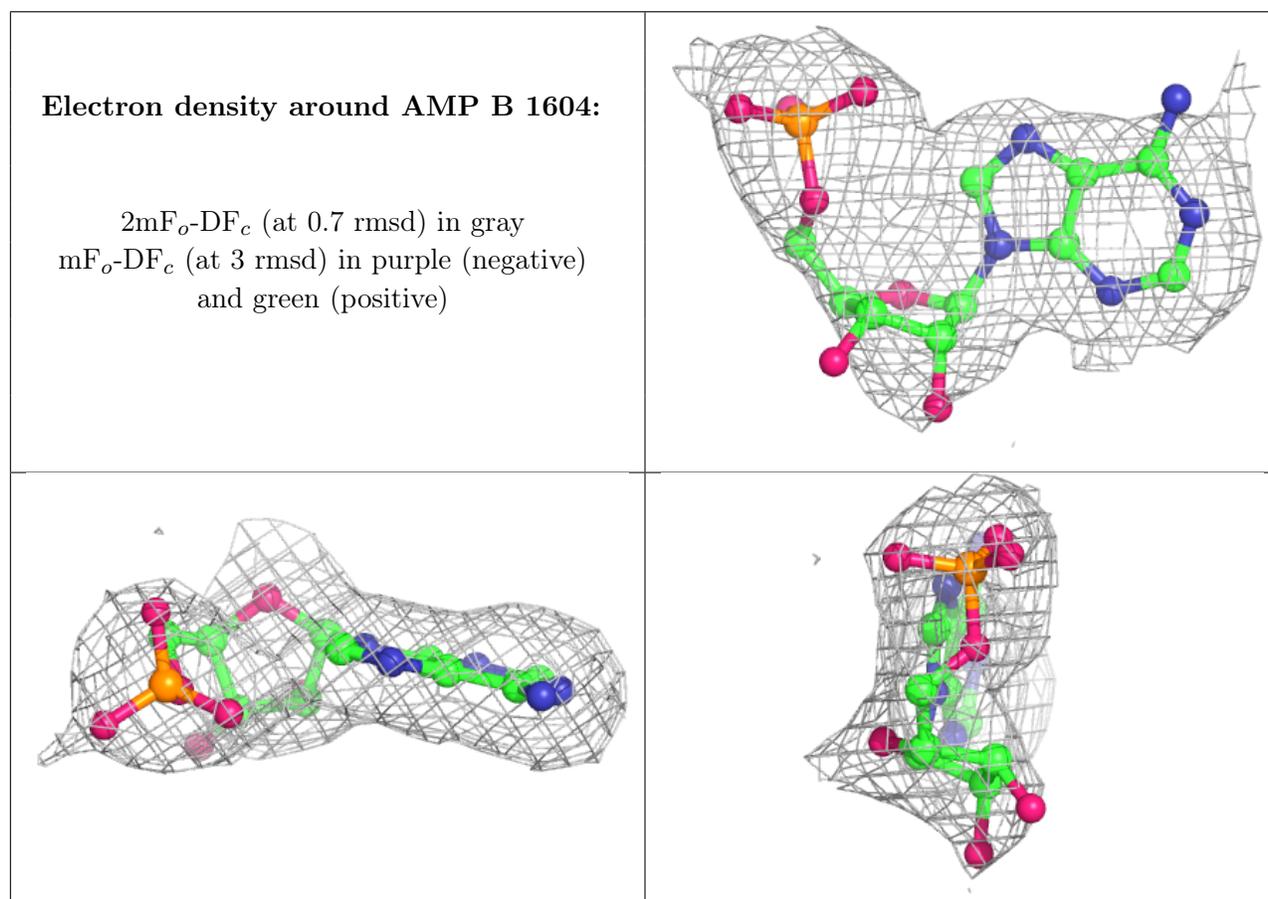
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AMP	B	1604	23/23	0.93	0.18	23,25,31,34	0
2	ADP	A	1762	27/27	0.95	0.15	6,10,11,12	0

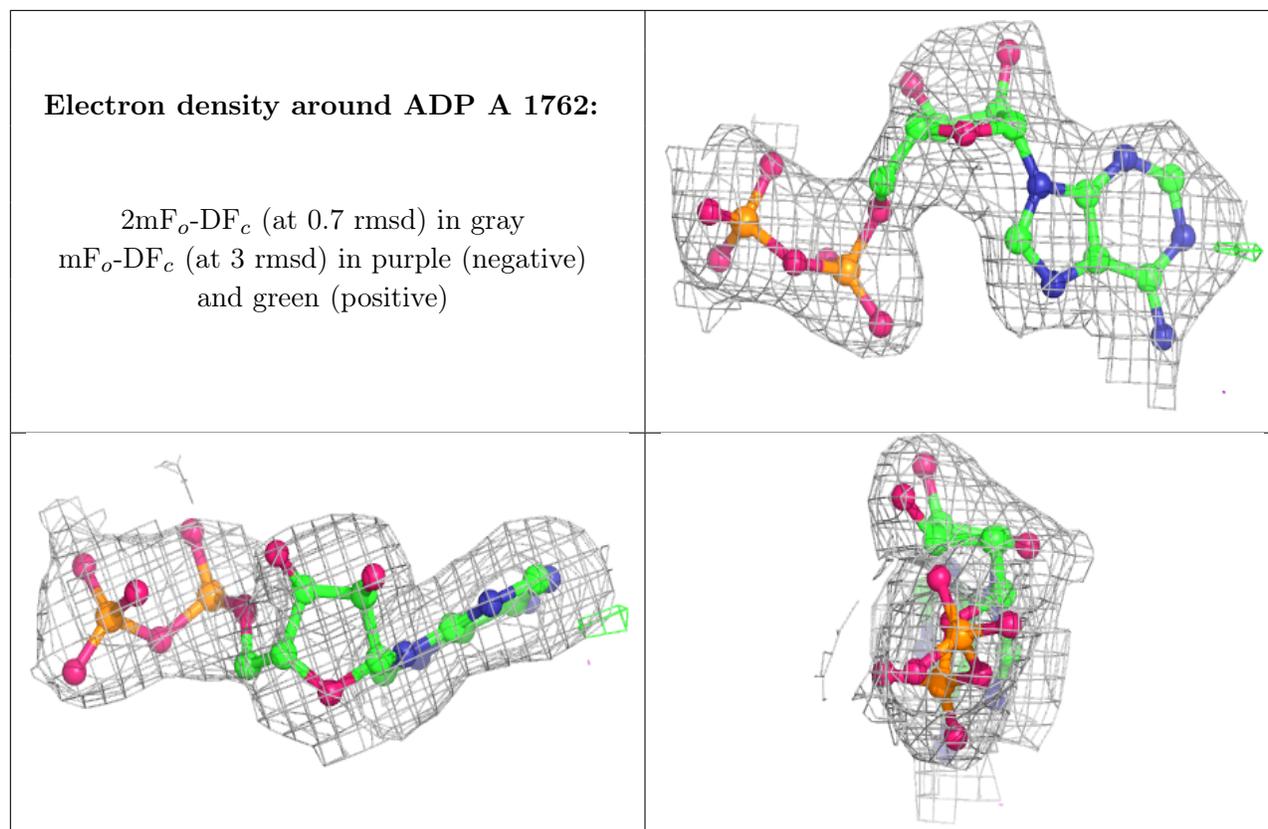
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	579	1/1	0.98	0.20	15,15,15,15	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.