



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2019 – 05:02 PM EDT

PDB ID : 1PHP
Title : STRUCTURE OF THE ADP COMPLEX OF THE 3-PHOSPHOGLYCERATE KINASE FROM BACILLUS STEAROTHERMOPHILUS AT 1.65 ANGSTROMS
Authors : Davies, G.J.; Watson, H.C.
Deposited on : 1994-04-12
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

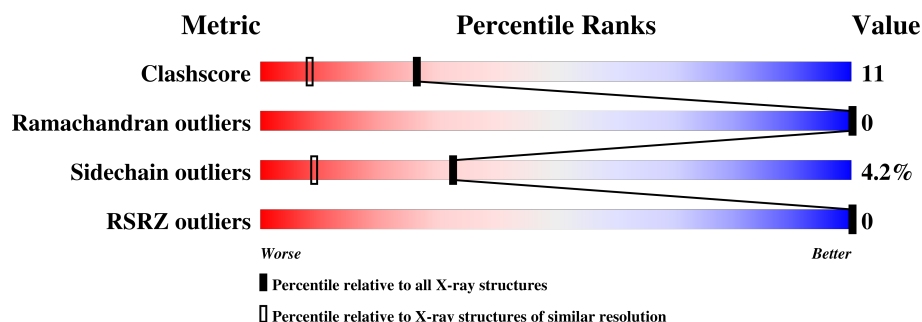
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	122126	1616 (1.66-1.66)
Ramachandran outliers	120053	1584 (1.66-1.66)
Sidechain outliers	120020	1584 (1.66-1.66)
RSRZ outliers	108989	1487 (1.66-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	394	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3670 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.

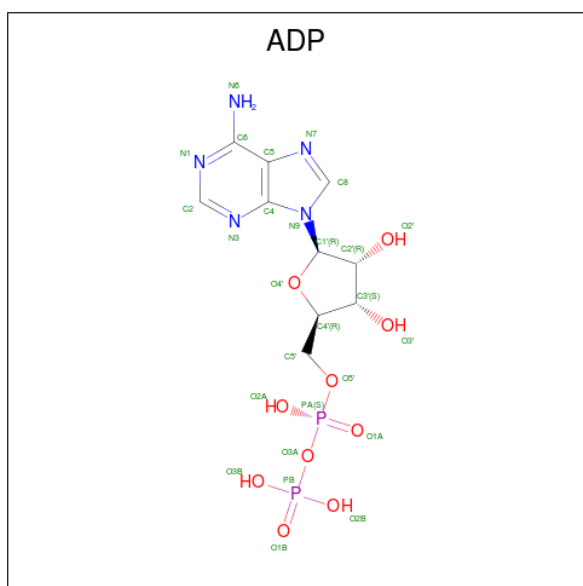
- Molecule 1 is a protein called 3-PHOSPHOGLYCERATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3008	1909	519	570	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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		

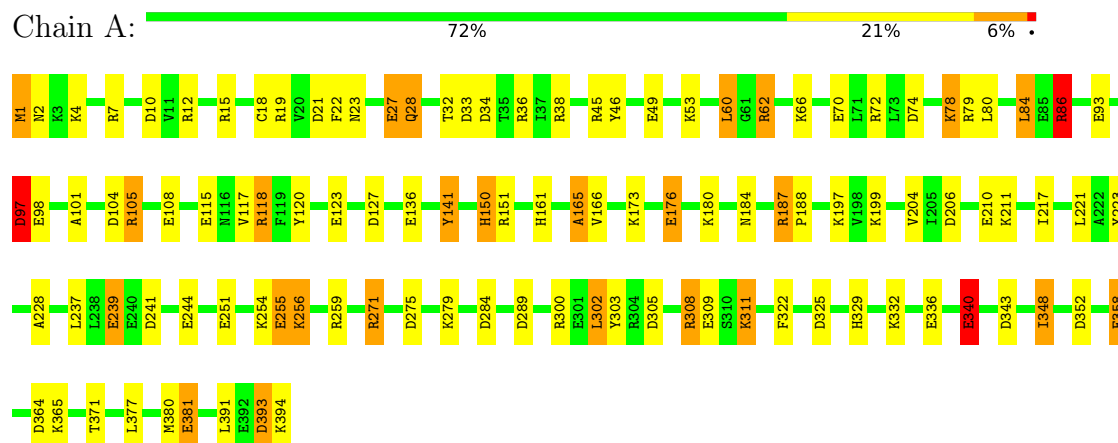
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	634	Total 634	O 634	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: 3-PHOSPHOGLYCERATE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.41 Å 73.93 Å 68.57 Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.65 9.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.65) 50.6 (9.98-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.156 , (Not available) 0.147 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 78.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3670	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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

5.1 Standard geometry

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	1.10	3/3057 (0.1%)	2.16	114/4126 (2.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE1	-7.05	1.17	1.25
1	A	381	GLU	CD-OE2	-6.17	1.18	1.25
1	A	123	GLU	CD-OE2	-5.49	1.19	1.25

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH1	28.01	134.31	120.30
1	A	7	ARG	CD-NE-CZ	20.69	152.56	123.60
1	A	7	ARG	NE-CZ-NH1	17.61	129.10	120.30
1	A	45	ARG	NE-CZ-NH2	-16.79	111.91	120.30
1	A	38	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	A	151	ARG	NE-CZ-NH1	15.90	128.25	120.30
1	A	105	ARG	CD-NE-CZ	15.39	145.14	123.60
1	A	308	ARG	NE-CZ-NH2	14.52	127.56	120.30
1	A	340	GLU	CB-CG-CD	12.26	147.31	114.20
1	A	7	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	45	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	A	289	ASP	CB-CG-OD1	10.65	127.89	118.30
1	A	15	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	A	33	ASP	CB-CG-OD1	10.31	127.58	118.30
1	A	62	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	303	TYR	CB-CG-CD2	-10.10	114.94	121.00
1	A	255	GLU	CA-CB-CG	10.08	135.57	113.40
1	A	38	ARG	CD-NE-CZ	9.99	137.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ASP	CB-CG-OD1	9.92	127.23	118.30
1	A	97	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	A	97	ASP	CB-CG-OD1	-9.81	109.47	118.30
1	A	34	ASP	CB-CG-OD1	9.63	126.97	118.30
1	A	38	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	10	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	97	ASP	OD1-CG-OD2	9.24	140.86	123.30
1	A	352	ASP	CB-CG-OD2	9.18	126.56	118.30
1	A	27	GLU	N-CA-CB	9.06	126.91	110.60
1	A	104	ASP	CB-CG-OD1	-8.94	110.25	118.30
1	A	325	ASP	CB-CG-OD2	-8.61	110.56	118.30
1	A	303	TYR	CB-CG-CD1	8.59	126.15	121.00
1	A	49	GLU	OE1-CD-OE2	8.37	133.35	123.30
1	A	62	ARG	CD-NE-CZ	8.24	135.14	123.60
1	A	62	ARG	NH1-CZ-NH2	-8.12	110.46	119.40
1	A	10	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	105	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	A	34	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	A	86	ARG	CD-NE-CZ	-7.90	112.55	123.60
1	A	364	ASP	CB-CG-OD1	7.87	125.38	118.30
1	A	60	LEU	CB-CG-CD2	7.82	124.29	111.00
1	A	105	ARG	N-CA-CB	-7.69	96.76	110.60
1	A	86	ARG	N-CA-CB	7.67	124.41	110.60
1	A	12	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	A	22	PHE	CB-CG-CD2	-7.53	115.53	120.80
1	A	151	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	165	ALA	N-CA-CB	-7.36	99.80	110.10
1	A	108	GLU	CG-CD-OE1	7.35	132.99	118.30
1	A	271	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	19	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	187	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	136	GLU	CG-CD-OE2	-6.93	104.45	118.30
1	A	352	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	A	289	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	120	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	A	343	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	A	127	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	136	GLU	CG-CD-OE1	6.54	131.38	118.30
1	A	118	ARG	CD-NE-CZ	-6.34	114.73	123.60
1	A	12	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	12	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	A	18	CYS	O-C-N	6.23	132.67	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLU	CB-CA-C	-6.22	97.96	110.40
1	A	211	LYS	CB-CG-CD	6.18	127.67	111.60
1	A	305	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	A	115	GLU	CG-CD-OE1	6.04	130.39	118.30
1	A	300	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	A	358	GLU	CA-CB-CG	6.03	126.67	113.40
1	A	244	GLU	OE1-CD-OE2	6.02	130.53	123.30
1	A	275	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	123	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	A	108	GLU	CG-CD-OE2	-5.93	106.44	118.30
1	A	105	ARG	CB-CA-C	5.91	122.23	110.40
1	A	79	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	241	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	275	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	259	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	A	1	MET	CB-CA-C	5.84	122.07	110.40
1	A	271	ARG	CA-CB-CG	5.82	126.19	113.40
1	A	27	GLU	CG-CD-OE2	5.76	129.83	118.30
1	A	380	MET	CG-SD-CE	5.71	109.34	100.20
1	A	393	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	322	PHE	CB-CG-CD2	-5.69	116.81	120.80
1	A	358	GLU	CB-CG-CD	5.69	129.55	114.20
1	A	223	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	46	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	256	LYS	CA-C-N	5.62	127.43	116.20
1	A	136	GLU	CB-CA-C	-5.61	99.19	110.40
1	A	70	GLU	CG-CD-OE1	5.56	129.42	118.30
1	A	228	ALA	N-CA-CB	5.55	117.87	110.10
1	A	308	ARG	CA-CB-CG	-5.55	101.20	113.40
1	A	72	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	34	ASP	CA-C-N	5.52	129.35	117.20
1	A	27	GLU	CG-CD-OE1	-5.52	107.26	118.30
1	A	74	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	176	GLU	CA-CB-CG	5.48	125.46	113.40
1	A	239	GLU	CG-CD-OE1	5.41	129.12	118.30
1	A	348	ILE	CA-CB-CG1	5.40	121.26	111.00
1	A	279	LYS	O-C-N	5.39	131.33	122.70
1	A	340	GLU	CG-CD-OE2	5.38	129.07	118.30
1	A	210	GLU	CB-CA-C	-5.31	99.78	110.40
1	A	206	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	244	GLU	CG-CD-OE2	-5.29	107.72	118.30
1	A	28	GLN	N-CA-CB	-5.28	101.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	VAL	CA-CB-CG2	5.24	118.76	110.90
1	A	302	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	223	TYR	CA-CB-CG	-5.17	103.57	113.40
1	A	255	GLU	CB-CA-C	-5.17	100.06	110.40
1	A	206	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	141	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	A	53	LYS	N-CA-C	-5.14	97.12	111.00
1	A	141	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	97	ASP	N-CA-CB	5.12	119.83	110.60
1	A	311	LYS	CD-CE-NZ	5.12	123.49	111.70
1	A	101	ALA	CB-CA-C	5.06	117.68	110.10
1	A	161	HIS	CA-CB-CG	-5.05	105.02	113.60

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	3008	0	3055	68	0
2	A	1	0	0	0	0
3	A	27	0	12	1	0
4	A	634	0	0	48	2
All	All	3670	0	3067	68	2

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 11.

All (68) 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:93:GLU:HG2	4:A:782:HOH:O	1.80	0.82
1:A:365:LYS:HD3	4:A:629:HOH:O	1.80	0.82
1:A:377:LEU:HD22	4:A:498:HOH:O	1.82	0.79
1:A:21:ASP:OD2	4:A:563:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HD13	4:A:498:HOH:O	1.83	0.77
1:A:197:LYS:HG3	4:A:909:HOH:O	1.87	0.73
1:A:239:GLU:OE1	4:A:700:HOH:O	2.07	0.72
1:A:66:LYS:HE3	4:A:561:HOH:O	1.90	0.71
1:A:62:ARG:NH2	4:A:409:HOH:O	2.24	0.70
1:A:78:LYS:HE2	4:A:741:HOH:O	1.92	0.69
1:A:60:LEU:HG	4:A:981:HOH:O	1.91	0.69
1:A:60:LEU:CG	4:A:981:HOH:O	2.41	0.69
1:A:62:ARG:HG2	4:A:835:HOH:O	1.92	0.69
1:A:329:HIS:ND1	4:A:842:HOH:O	2.28	0.67
1:A:118:ARG:NH2	4:A:672:HOH:O	2.30	0.64
1:A:60:LEU:CD1	4:A:981:HOH:O	2.47	0.63
1:A:309:GLU:HG2	4:A:1001:HOH:O	2.01	0.61
1:A:165:ALA:HB1	4:A:947:HOH:O	2.00	0.60
1:A:84:LEU:HB3	1:A:86:ARG:HG3	1.85	0.59
1:A:204:VAL:HG21	4:A:498:HOH:O	2.03	0.58
1:A:377:LEU:CG	4:A:498:HOH:O	2.52	0.58
1:A:377:LEU:HB3	4:A:498:HOH:O	2.04	0.57
1:A:150:HIS:CD2	1:A:150:HIS:H	2.24	0.56
1:A:141:TYR:CD2	4:A:947:HOH:O	2.59	0.55
1:A:180:LYS:HE2	4:A:457:HOH:O	2.06	0.55
1:A:237:LEU:HD22	3:A:396:ADP:C2	2.42	0.55
1:A:308:ARG:HD2	1:A:340:GLU:OE2	2.07	0.54
1:A:377:LEU:CB	4:A:498:HOH:O	2.54	0.54
1:A:204:VAL:HG23	4:A:497:HOH:O	2.07	0.54
1:A:377:LEU:CD1	4:A:498:HOH:O	2.50	0.53
1:A:80:LEU:HG	1:A:84:LEU:HD22	1.91	0.52
1:A:377:LEU:O	1:A:381:GLU:HG3	2.10	0.51
1:A:150:HIS:H	1:A:150:HIS:HD2	1.57	0.51
1:A:309:GLU:CG	4:A:1001:HOH:O	2.57	0.51
1:A:187:ARG:HA	1:A:188:PRO:C	2.30	0.50
1:A:97:ASP:OD1	4:A:603:HOH:O	2.19	0.49
1:A:176:GLU:HG3	4:A:931:HOH:O	2.12	0.48
1:A:394:LYS:HE2	4:A:541:HOH:O	2.14	0.48
1:A:173:LYS:HE2	4:A:773:HOH:O	2.14	0.47
1:A:391:LEU:HD23	4:A:947:HOH:O	2.13	0.47
1:A:199:LYS:HB2	1:A:239:GLU:OE1	2.14	0.47
1:A:332:LYS:O	1:A:336:GLU:HG3	2.15	0.47
1:A:150:HIS:HE1	4:A:636:HOH:O	1.99	0.46
1:A:1:MET:HG2	1:A:176:GLU:HA	1.98	0.46
1:A:251:GLU:HG2	4:A:623:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:HB3	4:A:1001:HOH:O	2.16	0.44
1:A:21:ASP:HA	4:A:913:HOH:O	2.19	0.43
1:A:254:LYS:HB3	1:A:254:LYS:HE2	1.72	0.43
1:A:2:ASN:O	1:A:393:ASP:HA	2.19	0.43
1:A:271:ARG:HD3	4:A:590:HOH:O	2.19	0.43
1:A:4:LYS:HA	1:A:394:LYS:HE3	2.00	0.42
1:A:180:LYS:HE3	1:A:184:ASN:O	2.19	0.42
1:A:377:LEU:CD2	4:A:498:HOH:O	2.50	0.42
1:A:105:ARG:HD3	4:A:619:HOH:O	2.18	0.42
1:A:117:VAL:HG12	4:A:922:HOH:O	2.19	0.42
1:A:150:HIS:CD2	1:A:150:HIS:N	2.87	0.42
1:A:27:GLU:OE1	1:A:32:THR:HG21	2.20	0.42
1:A:371:THR:HG23	4:A:726:HOH:O	2.19	0.42
1:A:141:TYR:CE2	4:A:947:HOH:O	2.55	0.41
1:A:60:LEU:HD12	4:A:981:HOH:O	2.18	0.41
1:A:117:VAL:CG1	4:A:922:HOH:O	2.68	0.41
1:A:255:GLU:HG3	4:A:623:HOH:O	2.20	0.41
1:A:86:ARG:HH11	1:A:86:ARG:HD3	1.52	0.41
1:A:199:LYS:NZ	4:A:746:HOH:O	2.54	0.41
1:A:309:GLU:CB	4:A:1001:HOH:O	2.68	0.41
1:A:217:ILE:HD12	1:A:221:LEU:HD21	2.02	0.40
1:A:23:ASN:O	1:A:36:ARG:NH1	2.49	0.40
1:A:365:LYS:CD	4:A:629:HOH:O	2.55	0.40

All (2) 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)
4:A:742:HOH:O	4:A:813:HOH:O[2_846]	2.07	0.13
4:A:716:HOH:O	4:A:953:HOH:O[2_856]	2.16	0.04

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	392/394 (100%)	387 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	310/310 (100%)	297 (96%)	13 (4%)	32	9

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	78	LYS
1	A	84	LEU
1	A	86	ARG
1	A	97	ASP
1	A	98	GLU
1	A	150	HIS
1	A	256	LYS
1	A	302	LEU
1	A	311	LYS
1	A	340	GLU
1	A	348	ILE
1	A	358	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	28	GLN
1	A	92	ASN
1	A	150	HIS

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	277	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	A	396	2	24,29,29	1.77	4 (16%)	25,45,45	2.11	10 (40%)

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	A	396	2	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	396	ADP	PB-O3A	6.00	1.69	1.60
3	A	396	ADP	O4'-C1'	3.45	1.46	1.41
3	A	396	ADP	C2'-C3'	3.10	1.61	1.53
3	A	396	ADP	PB-O2B	-2.18	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	396	ADP	C4'-O4'-C1'	-4.87	104.75	109.83
3	A	396	ADP	C2-N1-C6	3.41	124.68	118.77
3	A	396	ADP	O2'-C2'-C3'	3.16	122.06	111.80
3	A	396	ADP	N6-C6-N1	2.83	124.45	118.57
3	A	396	ADP	C4-C5-N7	2.67	112.19	109.40
3	A	396	ADP	N3-C2-N1	-2.67	124.38	128.68
3	A	396	ADP	C5-C6-N1	-2.41	114.63	120.31
3	A	396	ADP	O3B-PB-O2B	2.40	116.91	107.57
3	A	396	ADP	O3B-PB-O1B	2.25	119.39	110.53
3	A	396	ADP	C5'-C4'-C3'	-2.22	106.84	115.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	396	ADP	C5'-O5'-PA-O1A

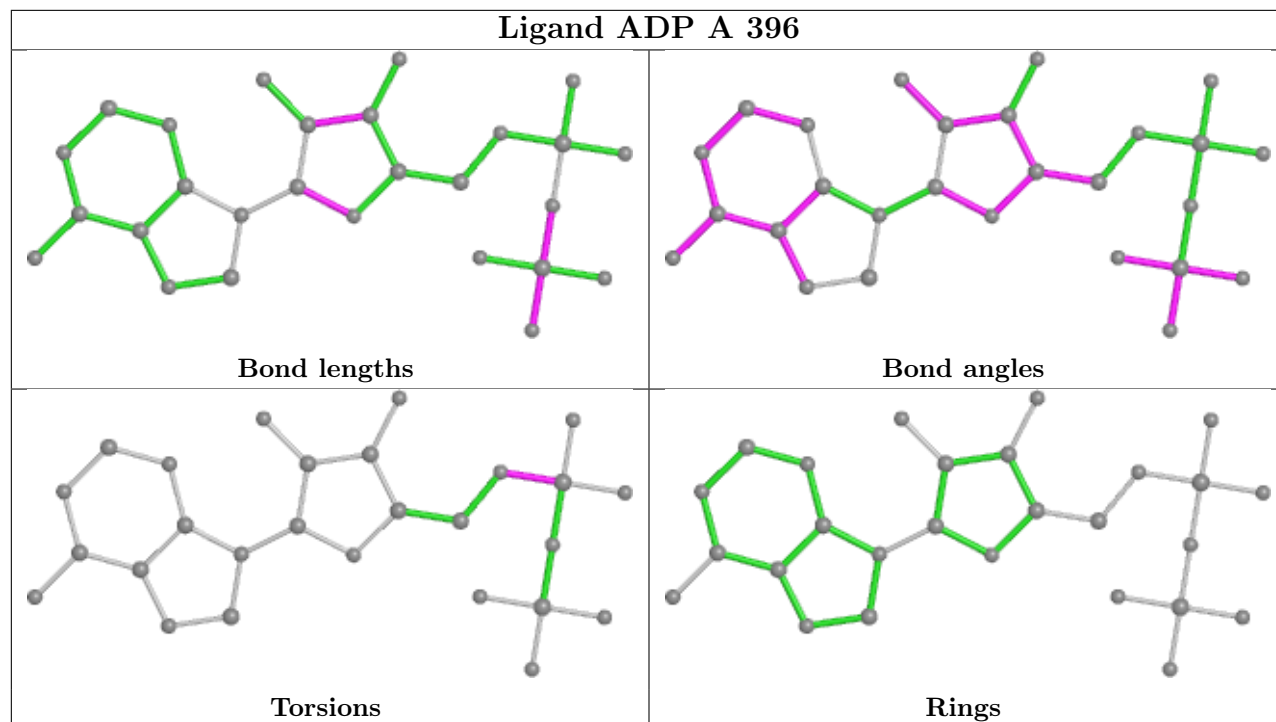
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	396	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](#)

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	394/394 (100%)	-1.20	0 100 100	10, 18, 39, 74	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](#)

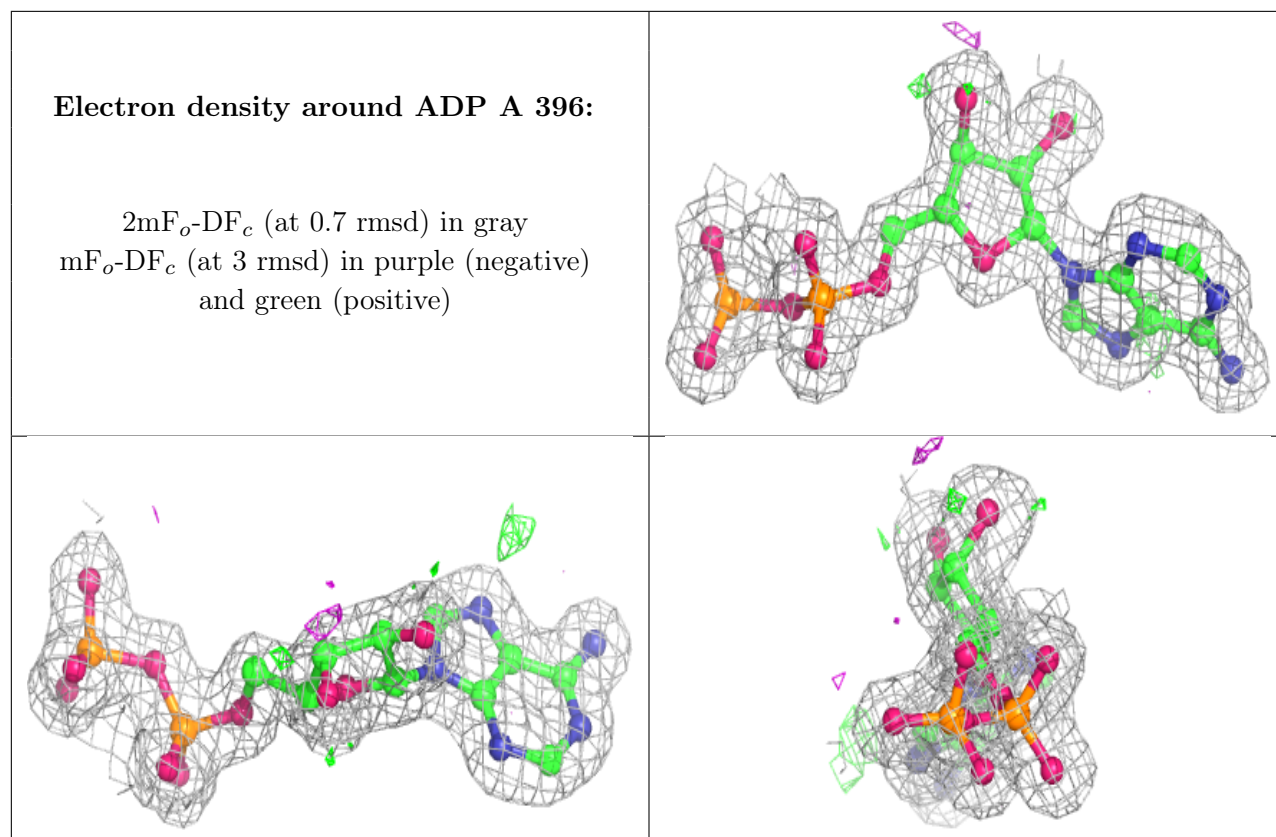
There are no carbohydrates in this entry.

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
3	ADP	A	396	27/27	0.99	0.03	13,15,19,21	0
2	MG	A	395	1/1	0.99	0.02	21,21,21,21	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.