



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:59 PM UTC

PDB ID : 1PHP / pdb_00001php
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.

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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

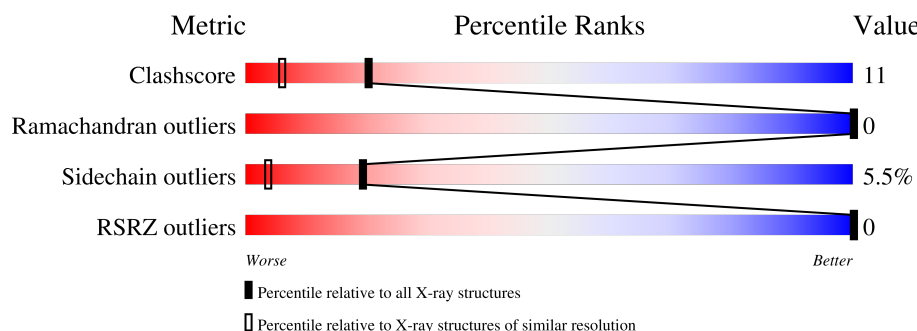
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 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	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.

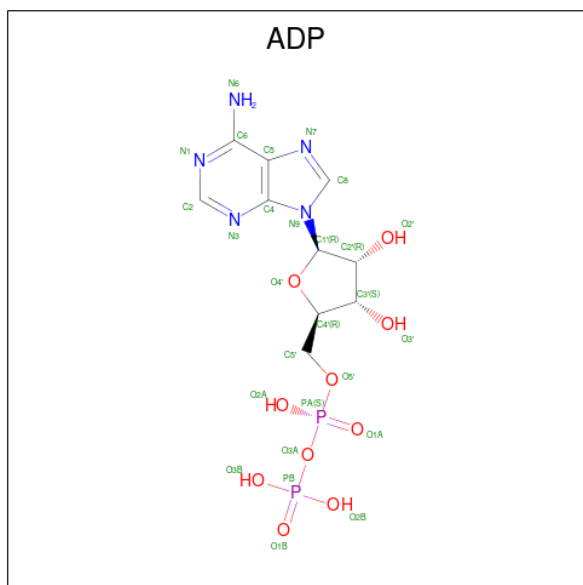
- Molecule 1 is a protein called 3-PHOSPHOGLYCERATE KINASE.

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

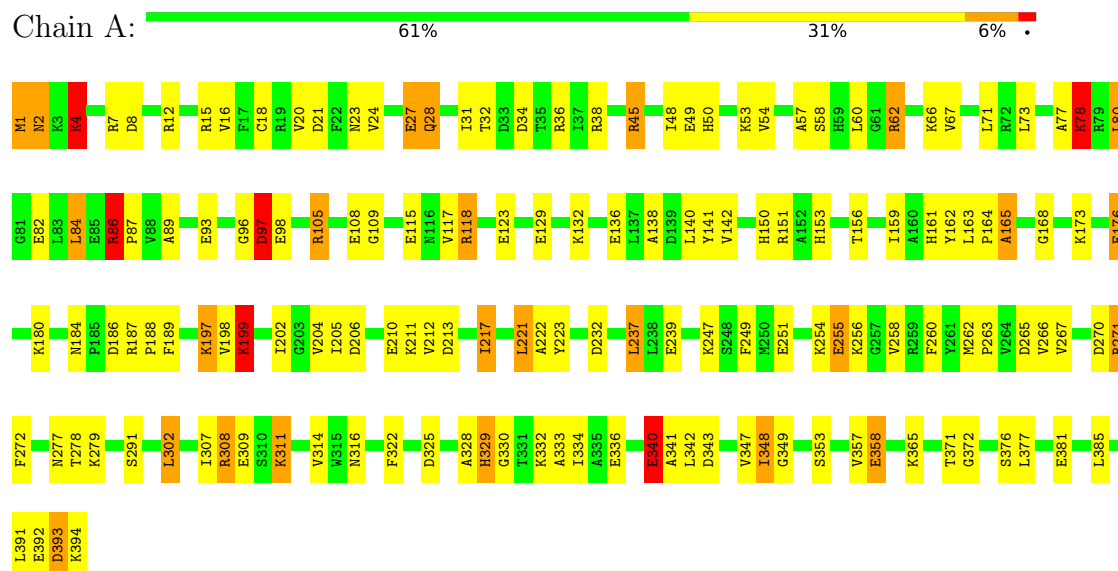
- Molecule 4 is water.

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

3 Residue-property plots

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: 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 10.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.65) 50.4 (10.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
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)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 83.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: ADP, MG

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	1.42	5/3057 (0.2%)	2.38	166/4126 (4.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	ASN	CA-C	5.84	1.59	1.52
1	A	31	ILE	CA-CB	5.57	1.60	1.54
1	A	164	PRO	CA-C	5.50	1.59	1.52
1	A	57	ALA	CA-C	5.32	1.58	1.52
1	A	277	ASN	CA-C	5.02	1.59	1.52

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLU	CB-CG-CD	20.42	147.31	112.60
1	A	7	ARG	CD-NE-CZ	20.12	152.56	124.40
1	A	105	ARG	CD-NE-CZ	14.82	145.14	124.40
1	A	62	ARG	NE-CZ-NH1	12.80	134.31	121.50
1	A	255	GLU	CA-CB-CG	10.74	135.57	114.10
1	A	358	GLU	CB-CG-CD	9.97	129.55	112.60
1	A	272	PHE	CA-CB-CG	-9.90	103.90	113.80
1	A	27	GLU	N-CA-CB	9.90	126.91	110.77
1	A	232	ASP	CA-CB-CG	9.77	122.37	112.60
1	A	38	ARG	CD-NE-CZ	9.42	137.59	124.40
1	A	308	ARG	NE-CZ-NH2	9.29	127.56	119.20
1	A	222	ALA	CA-C-O	-9.01	109.92	120.10
1	A	277	ASN	OD1-CG-ND2	8.96	131.56	122.60
1	A	161	HIS	CA-CB-CG	-8.78	105.02	113.80
1	A	329	HIS	CA-CB-CG	-8.56	105.24	113.80
1	A	86	ARG	CD-NE-CZ	-8.47	112.55	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LEU	CA-C-O	8.40	129.70	120.63
1	A	105	ARG	N-CA-CB	-8.13	96.76	110.41
1	A	45	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	A	2	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	A	27	GLU	CB-CA-C	-7.91	97.96	110.14
1	A	62	ARG	CD-NE-CZ	7.67	135.14	124.40
1	A	392	GLU	CA-C-O	7.66	129.79	121.05
1	A	7	ARG	NE-CZ-NH1	7.61	129.10	121.50
1	A	206	ASP	CA-CB-CG	-7.54	105.06	112.60
1	A	97	ASP	OD1-CG-OD2	7.48	140.86	122.90
1	A	279	LYS	O-C-N	7.39	131.33	123.42
1	A	28	GLN	N-CA-CB	-7.37	101.10	112.30
1	A	18	CYS	O-C-N	7.23	132.67	123.12
1	A	247	LYS	CA-C-O	-7.16	112.96	120.55
1	A	34	ASP	CA-C-O	-7.15	111.28	119.78
1	A	38	ARG	NE-CZ-NH1	7.12	128.62	121.50
1	A	211	LYS	CB-CG-CD	7.12	127.67	111.30
1	A	189	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	86	ARG	CA-C-O	7.10	127.02	119.50
1	A	330	GLY	O-C-N	7.09	129.06	122.19
1	A	357	VAL	O-C-N	7.08	128.74	121.87
1	A	15	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	87	PRO	CB-CA-C	7.01	120.20	111.23
1	A	165	ALA	N-CA-CB	-6.99	99.80	110.77
1	A	222	ALA	O-C-N	6.94	130.34	122.22
1	A	258	VAL	CA-C-O	-6.93	112.86	121.11
1	A	118	ARG	CD-NE-CZ	-6.91	114.73	124.40
1	A	314	VAL	CA-C-O	-6.87	113.17	120.53
1	A	62	ARG	NH1-CZ-NH2	-6.80	110.46	119.30
1	A	151	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	A	347	VAL	CA-C-O	-6.72	113.40	120.39
1	A	48	ILE	O-C-N	6.63	128.41	121.91
1	A	97	ASP	N-CA-CB	6.60	119.83	110.12
1	A	18	CYS	CA-C-O	-6.59	113.48	120.40
1	A	159	ILE	CA-C-O	-6.58	113.53	120.57
1	A	255	GLU	CB-CA-C	-6.46	100.06	110.79
1	A	308	ARG	CA-CB-CG	-6.45	101.20	114.10
1	A	199	LYS	CG-CD-CE	6.39	126.01	111.30
1	A	348	ILE	CA-CB-CG1	6.39	121.26	110.40
1	A	212	VAL	N-CA-C	6.38	117.00	110.05
1	A	349	GLY	CA-C-O	-6.37	116.03	121.57
1	A	211	LYS	N-CA-C	6.36	121.45	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	GLU	CG-CD-OE1	6.34	132.99	118.40
1	A	8	ASP	CA-C-O	-6.32	111.79	119.43
1	A	1	MET	CB-CA-C	6.30	122.07	110.10
1	A	265	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	358	GLU	CA-CB-CG	6.29	126.67	114.10
1	A	163	LEU	O-C-N	6.28	125.73	121.71
1	A	221	LEU	O-C-N	-6.25	115.49	122.12
1	A	49	GLU	CB-CA-C	-6.21	100.47	110.79
1	A	82	GLU	N-CA-CB	6.19	118.98	110.01
1	A	136	GLU	CB-CA-C	-6.18	99.19	110.63
1	A	80	LEU	CA-C-O	-6.17	114.34	120.82
1	A	328	ALA	CA-C-N	6.17	128.55	120.28
1	A	328	ALA	C-N-CA	6.17	128.55	120.28
1	A	105	ARG	CB-CA-C	6.17	122.23	109.95
1	A	97	ASP	CB-CA-C	-6.14	100.59	110.79
1	A	164	PRO	N-CA-C	-6.14	101.57	111.14
1	A	129	GLU	CA-C-O	-6.12	113.94	120.42
1	A	136	GLU	CG-CD-OE2	-6.07	104.45	118.40
1	A	271	ARG	CA-CB-CG	6.05	126.19	114.10
1	A	376	SER	O-C-N	6.04	129.04	122.15
1	A	325	ASP	CA-C-O	-6.01	114.17	120.55
1	A	162	TYR	CA-C-O	-5.96	112.50	119.05
1	A	221	LEU	N-CA-CB	-5.89	101.23	110.06
1	A	86	ARG	N-CA-CB	5.88	124.41	111.25
1	A	217	ILE	N-CA-CB	-5.88	101.17	111.39
1	A	58	SER	CA-C-O	5.87	127.73	121.45
1	A	343	ASP	CA-CB-CG	-5.86	106.74	112.60
1	A	20	VAL	O-C-N	5.86	129.12	122.97
1	A	96	GLY	CA-C-O	-5.85	118.24	122.45
1	A	49	GLU	CB-CG-CD	-5.81	102.72	112.60
1	A	142	VAL	CA-C-O	-5.80	114.30	120.39
1	A	393	ASP	O-C-N	5.79	129.85	123.01
1	A	136	GLU	CB-CG-CD	5.79	122.45	112.60
1	A	80	LEU	O-C-N	5.78	128.02	122.07
1	A	49	GLU	O-C-N	5.76	128.23	122.12
1	A	329	HIS	N-CA-C	5.75	117.55	111.28
1	A	223	TYR	CA-CB-CG	-5.74	103.57	113.90
1	A	322	PHE	O-C-N	5.74	130.38	122.46
1	A	53	LYS	N-CA-C	-5.71	97.12	107.75
1	A	307	ILE	O-C-N	5.70	127.49	121.91
1	A	89	ALA	CA-C-O	-5.69	114.92	121.47
1	A	105	ARG	NE-CZ-NH2	5.69	124.32	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	N-CA-CB	-5.68	101.99	110.17
1	A	176	GLU	CA-CB-CG	5.68	125.46	114.10
1	A	54	VAL	N-CA-CB	-5.67	104.53	111.00
1	A	291	SER	CA-C-O	-5.65	114.59	120.70
1	A	109	GLY	CA-C-O	-5.65	112.94	119.10
1	A	136	GLU	CG-CD-OE1	5.64	131.38	118.40
1	A	217	ILE	CA-CB-CG2	5.63	120.06	110.50
1	A	118	ARG	CA-C-N	5.62	130.11	120.72
1	A	118	ARG	C-N-CA	5.62	130.11	120.72
1	A	263	PRO	O-C-N	5.61	129.81	123.03
1	A	270	ASP	CA-C-N	5.59	131.75	121.85
1	A	270	ASP	C-N-CA	5.59	131.75	121.85
1	A	24	VAL	O-C-N	5.58	127.46	121.10
1	A	278	THR	CA-CB-OG1	-5.57	101.24	109.60
1	A	249	PHE	O-C-N	-5.56	116.23	122.12
1	A	279	LYS	CA-C-O	-5.55	115.29	121.23
1	A	132	LYS	CB-CG-CD	5.54	124.04	111.30
1	A	156	THR	CA-CB-OG1	-5.54	101.29	109.60
1	A	62	ARG	O-C-N	-5.53	116.39	121.37
1	A	202	ILE	N-CA-C	5.53	116.17	110.36
1	A	376	SER	CA-CB-OG	-5.52	100.06	111.10
1	A	7	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	A	372	GLY	N-CA-C	5.50	122.52	115.32
1	A	67	VAL	CA-C-O	-5.44	114.65	120.85
1	A	213	ASP	CA-CB-CG	-5.42	107.17	112.60
1	A	186	ASP	N-CA-CB	5.42	118.25	110.06
1	A	140	LEU	O-C-N	5.42	129.45	123.33
1	A	12	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	341	ALA	O-C-N	5.40	129.84	122.82
1	A	385	LEU	O-C-N	5.39	126.67	121.28
1	A	62	ARG	CA-C-N	5.37	124.99	119.56
1	A	62	ARG	C-N-CA	5.37	124.99	119.56
1	A	78	LYS	CA-C-O	5.36	126.64	120.90
1	A	302	LEU	O-C-N	5.36	127.58	122.07
1	A	12	ARG	N-CA-C	5.35	118.32	110.30
1	A	353	SER	O-C-N	5.34	127.78	122.12
1	A	123	GLU	CB-CG-CD	5.34	121.68	112.60
1	A	330	GLY	CA-C-O	-5.34	115.00	120.66
1	A	342	LEU	CA-C-O	-5.33	114.90	120.55
1	A	277	ASN	N-CA-C	-5.32	101.79	110.20
1	A	333	ALA	CA-C-O	-5.31	114.92	120.55
1	A	16	VAL	O-C-N	5.29	128.80	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ASP	CA-C-N	5.28	127.66	120.54
1	A	34	ASP	C-N-CA	5.28	127.66	120.54
1	A	138	ALA	N-CA-C	5.26	115.99	108.74
1	A	168	GLY	N-CA-C	-5.26	104.56	112.60
1	A	77	ALA	N-CA-C	-5.25	105.45	111.07
1	A	307	ILE	CA-C-O	-5.22	115.64	121.17
1	A	50	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	115	GLU	CG-CD-OE1	5.21	130.39	118.40
1	A	108	GLU	CG-CD-OE2	-5.20	106.44	118.40
1	A	266	VAL	O-C-N	5.18	128.47	122.82
1	A	186	ASP	N-CA-C	-5.15	102.06	110.20
1	A	71	LEU	O-C-N	5.15	128.59	122.26
1	A	73	LEU	N-CA-C	5.13	118.68	112.93
1	A	334	ILE	O-C-N	5.11	127.10	121.83
1	A	210	GLU	CB-CA-C	-5.11	99.78	109.95
1	A	393	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	267	VAL	N-CA-CB	5.05	117.12	111.21
1	A	205	ILE	O-C-N	5.05	126.77	121.87
1	A	311	LYS	CA-C-O	5.05	125.51	119.60
1	A	153	HIS	CA-C-O	-5.05	115.56	121.46
1	A	197	LYS	N-CA-C	5.05	117.62	109.40
1	A	277	ASN	CA-C-N	-5.04	114.05	122.21
1	A	277	ASN	C-N-CA	-5.04	114.05	122.21
1	A	277	ASN	CA-C-O	-5.02	115.33	121.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	69	0
2	A	1	0	0	0	0
3	A	27	0	12	1	0
4	A	634	0	0	47	2
All	All	3670	0	3067	69	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 (69) 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
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:260:PHE:HE1	1:A:262:MET:HE2	1.60	0.64
1:A:118:ARG:NH2	4:A:672:HOH:O	2.30	0.64
1:A:260:PHE:CE1	1:A:262:MET:HE2	2.33	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:H	1:A:150:HIS:CD2	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:187:ARG:HA	1:A:188:PRO:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:391:LEU:HD23	4:A:947:HOH:O	2.13	0.47
1:A:1:MET:HG2	1:A:176:GLU:HA	1.98	0.46
1:A:150:HIS:HE1	4:A:636:HOH:O	1.99	0.46
1:A:251:GLU:HG2	4:A:623:HOH:O	2.16	0.45
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:2:ASN:O	1:A:393:ASP:HA	2.19	0.43
1:A:254:LYS:HE2	1:A:254:LYS:HB3	1.72	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:27:GLU:OE1	1:A:32:THR:HG21	2.20	0.42
1:A:150:HIS:CD2	1:A:150:HIS:N	2.87	0.42
1:A:371:THR:HG23	4:A:726:HOH:O	2.19	0.42
1:A:60:LEU:HD12	4:A:981:HOH:O	2.18	0.41
1:A:141:TYR:CE2	4:A:947:HOH:O	2.55	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: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

5.3.1 Protein backbone

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%)	293 (94%)	17 (6%)	19	4

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	28	GLN
1	A	45	ARG
1	A	78	LYS
1	A	84	LEU
1	A	86	ARG
1	A	97	ASP
1	A	98	GLU
1	A	198	VAL
1	A	199	LYS
1	A	237	LEU
1	A	256	LYS
1	A	302	LEU

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Mol	Chain	Res	Type
1	A	311	LYS
1	A	340	GLU
1	A	348	ILE
1	A	358	GLU

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

Mol	Chain	Res	Type
1	A	28	GLN
1	A	92	ASN
1	A	150	HIS
1	A	207	ASN
1	A	277	ASN
1	A	329	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 oligosaccharides 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	28,29,29	1.05	2 (7%)	43,45,45	1.64	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	A	396	2	-	1/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	396	ADP	C2'-C3'	2.98	1.61	1.53
3	A	396	ADP	PB-O2B	-2.29	1.46	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	396	ADP	C2'-C1'-N9	3.99	123.22	113.30
3	A	396	ADP	C2-N1-C6	3.62	124.68	118.73
3	A	396	ADP	O2'-C2'-C3'	3.20	122.06	111.82
3	A	396	ADP	N3-C2-N1	-2.78	124.38	128.58
3	A	396	ADP	N6-C6-N1	2.73	124.45	118.38
3	A	396	ADP	O2A-PA-O3A	2.50	114.04	107.27
3	A	396	ADP	O3B-PB-O2B	2.43	116.91	107.80
3	A	396	ADP	C5'-C4'-C3'	-2.32	106.84	115.21
3	A	396	ADP	O3B-PB-O1B	2.20	119.39	110.83
3	A	396	ADP	C4'-O4'-C1'	-2.14	104.75	109.47
3	A	396	ADP	O3A-PB-O1B	-2.12	99.87	111.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

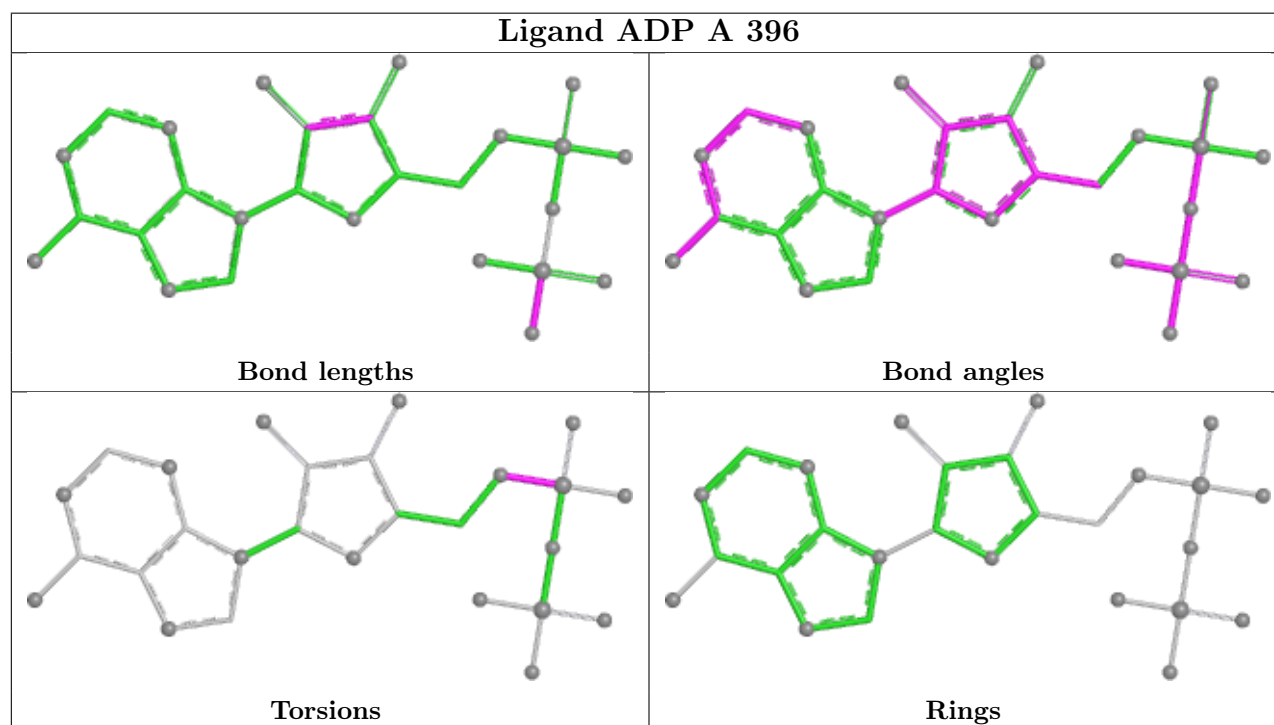
Mol	Chain	Res	Type	Atoms
3	A	396	ADP	C5'-O5'-PA-O1A

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%)	-0.73	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](#)

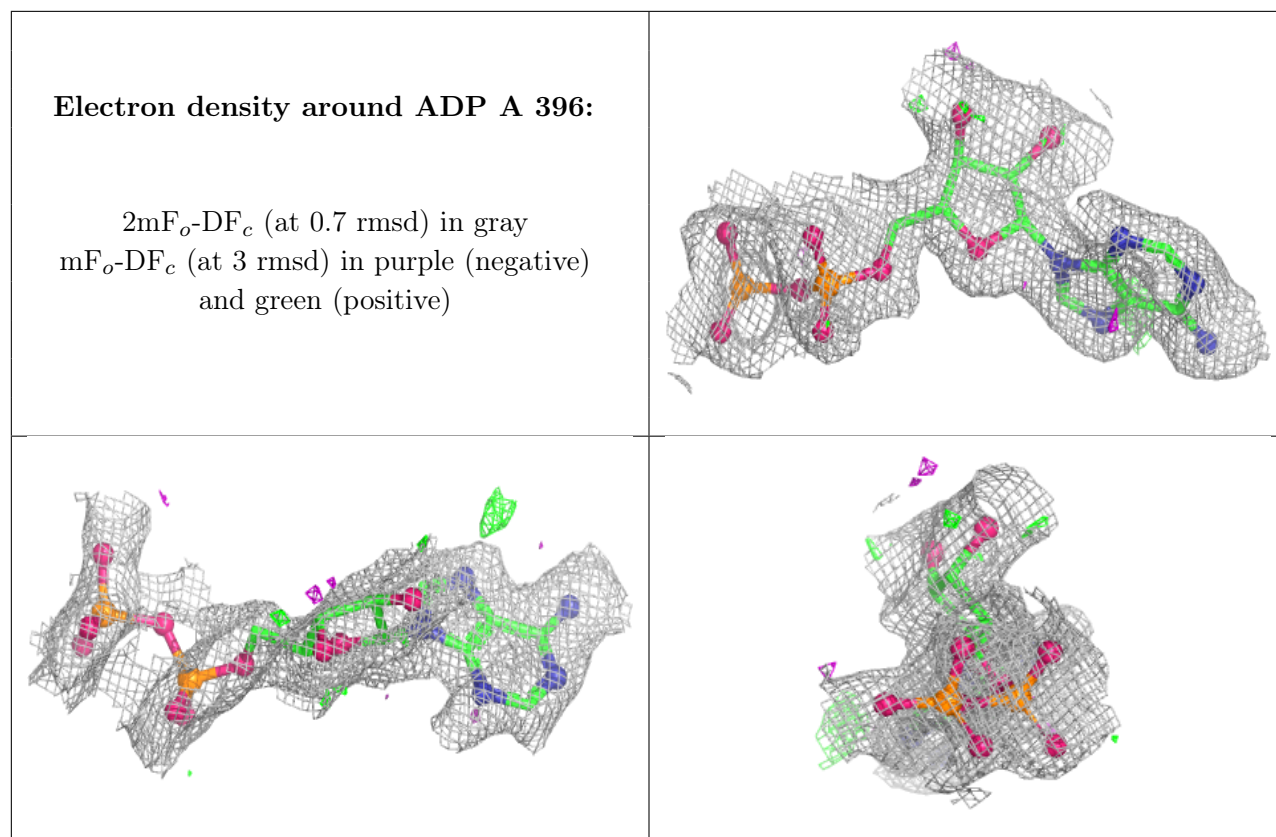
There are no oligosaccharides in this entry.

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	395	1/1	0.98	0.04	21,21,21,21	0
3	ADP	A	396	27/27	0.99	0.03	13,15,19,21	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.