



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:49 AM UTC

PDB ID : 1NDP / pdb_00001ndp
Title : ADENOSINE 5'-DIPHOSPHATE BINDING AND THE ACTIVE SITE OF
NUCLEOSIDE DIPHOSPHATE KINASE
Authors : Janin, J.; Morera, S.; Dumas, C.; Lascu, I.; Lebras, G.; Veron, M.
Deposited on : 1993-11-29
Resolution : 2.20 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

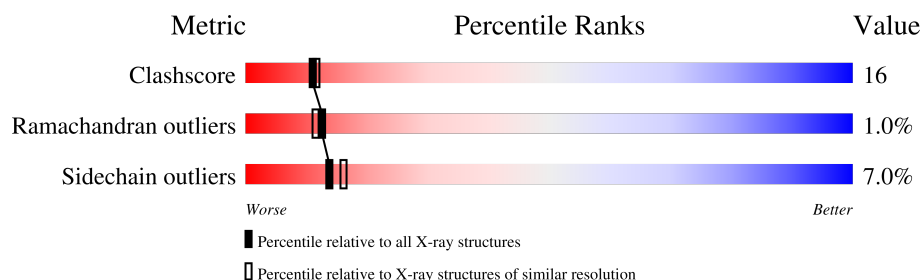
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	155	
1	B	155	

2 Entry composition [i](#)

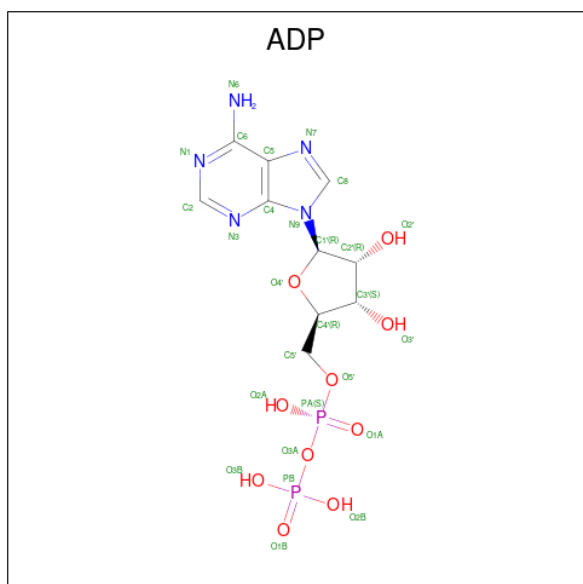
There are 4 unique types of molecules in this entry. The entry contains 2507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NUCLEOSIDE DIPHOSPHATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1147	736	198	211	2			
1	B	150	Total	C	N	O	S	0	0	0
			1147	736	198	211	2			

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

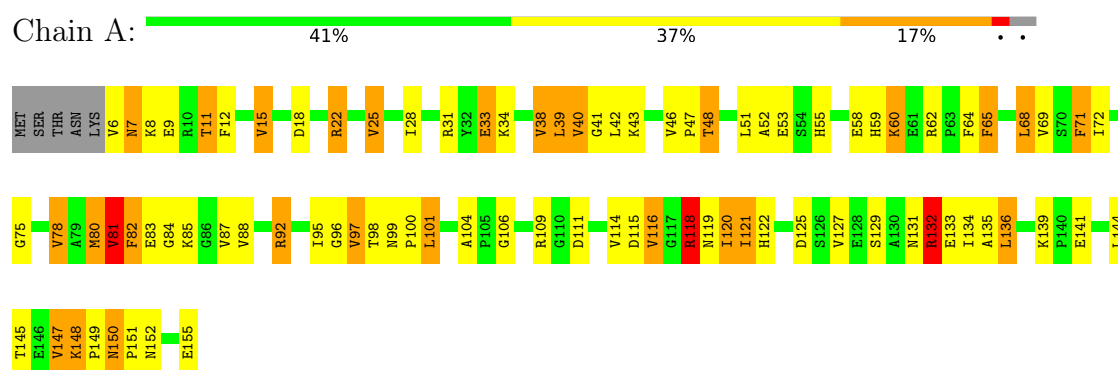
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0
4	B	85	Total 85	O 85	0	0

3 Residue-property plots

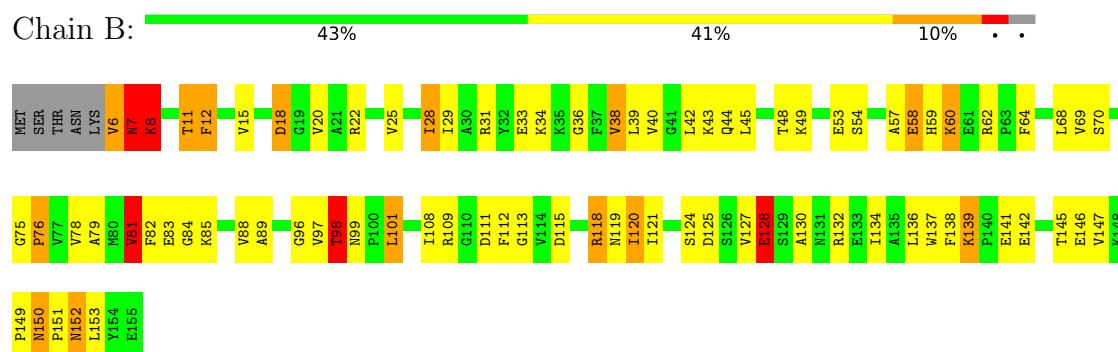
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

• Molecule 1: NUCLEOSIDE DIPHOSPHATE KINASE



• Molecule 1: NUCLEOSIDE DIPHOSPHATE KINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	73.18Å 73.18Å 158.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2507	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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	1.08	2/1171 (0.2%)	2.65	94/1583 (5.9%)
1	B	1.11	2/1171 (0.2%)	2.51	78/1583 (4.9%)
All	All	1.09	4/2342 (0.2%)	2.58	172/3166 (5.4%)

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	4
1	B	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	ILE	CA-CB	5.78	1.62	1.54
1	B	112	PHE	C-N	-5.46	1.28	1.34
1	A	120	ILE	CA-CB	5.30	1.61	1.54
1	A	131	ASN	C-N	-5.04	1.27	1.33

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	CD-NE-CZ	24.20	158.28	124.40
1	A	118	ARG	NH1-CZ-NH2	20.14	145.49	119.30
1	A	118	ARG	NE-CZ-NH2	-19.82	101.37	119.20
1	A	118	ARG	CD-NE-CZ	-13.98	104.82	124.40
1	A	47	PRO	CA-C-N	10.64	137.84	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PRO	C-N-CA	10.64	137.84	122.09
1	A	75	GLY	O-C-N	10.23	132.00	121.77
1	A	131	ASN	CA-C-O	-10.18	109.76	120.55
1	A	131	ASN	O-C-N	9.98	132.70	122.12
1	B	128	GLU	CB-CG-CD	9.79	129.24	112.60
1	A	81	VAL	CB-CA-C	9.63	124.39	110.33
1	B	81	VAL	CB-CA-C	9.40	124.05	110.33
1	A	46	VAL	N-CA-C	-9.28	97.38	107.77
1	A	7	ASN	CA-CB-CG	9.27	121.87	112.60
1	B	139	LYS	N-CA-C	-9.24	97.53	110.29
1	A	133	GLU	CA-C-O	-9.07	110.80	120.42
1	B	18	ASP	CA-CB-CG	8.74	121.34	112.60
1	B	29	ILE	O-C-N	8.58	130.32	121.91
1	A	38	VAL	O-C-N	8.57	132.02	122.93
1	B	108	ILE	O-C-N	8.54	130.28	121.91
1	B	7	ASN	CA-CB-CG	8.51	121.11	112.60
1	A	118	ARG	NE-CZ-NH1	-8.39	113.11	121.50
1	B	120	ILE	N-CA-C	8.33	126.67	109.34
1	B	18	ASP	CA-C-N	8.33	129.22	119.98
1	B	18	ASP	C-N-CA	8.33	129.22	119.98
1	A	135	ALA	CA-C-N	8.28	131.57	120.65
1	A	135	ALA	C-N-CA	8.28	131.57	120.65
1	A	151	PRO	CA-C-O	8.21	129.00	118.98
1	A	78	VAL	CB-CA-C	7.86	121.21	110.99
1	A	46	VAL	O-C-N	7.59	127.38	121.46
1	B	145	THR	N-CA-C	-7.49	104.67	113.88
1	A	120	ILE	N-CA-C	7.47	124.88	109.34
1	B	119	ASN	CA-C-N	7.38	135.26	121.97
1	B	119	ASN	C-N-CA	7.38	135.26	121.97
1	B	120	ILE	N-CA-CB	-7.34	99.12	111.23
1	A	129	SER	O-C-N	7.13	130.28	122.15
1	A	115	ASP	N-CA-CB	-7.13	98.43	110.83
1	A	129	SER	CA-C-O	-7.12	112.87	120.42
1	A	53	GLU	CB-CG-CD	7.07	124.61	112.60
1	A	151	PRO	CA-C-N	7.06	135.19	122.06
1	A	151	PRO	C-N-CA	7.06	135.19	122.06
1	A	134	ILE	CA-C-N	7.02	130.02	120.54
1	A	134	ILE	C-N-CA	7.02	130.02	120.54
1	A	25	VAL	CA-C-O	-7.01	113.05	121.18
1	A	106	GLY	N-CA-C	-7.01	105.59	113.79
1	B	118	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	A	141	GLU	CB-CG-CD	6.94	124.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	PHE	CA-CB-CG	-6.92	106.88	113.80
1	A	122	HIS	CA-CB-CG	-6.92	106.89	113.80
1	A	111	ASP	CA-CB-CG	6.91	119.51	112.60
1	B	64	PHE	CA-C-O	-6.88	111.31	119.15
1	A	34	LYS	CA-C-N	6.85	130.73	120.31
1	A	34	LYS	C-N-CA	6.85	130.73	120.31
1	A	119	ASN	OD1-CG-ND2	6.79	129.39	122.60
1	B	119	ASN	OD1-CG-ND2	6.79	129.39	122.60
1	A	131	ASN	CA-C-N	6.78	129.91	120.29
1	A	131	ASN	C-N-CA	6.78	129.91	120.29
1	B	152	ASN	O-C-N	6.67	132.27	122.39
1	B	151	PRO	CA-C-O	6.63	128.01	118.86
1	A	33	GLU	CA-C-N	6.63	129.82	120.28
1	A	33	GLU	C-N-CA	6.63	129.82	120.28
1	B	36	GLY	CA-C-O	6.54	125.49	118.95
1	A	104	ALA	N-CA-C	6.51	117.91	109.64
1	B	98	THR	O-C-N	6.50	128.76	122.07
1	B	20	VAL	O-C-N	6.49	128.51	121.83
1	A	55	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	B	76	PRO	CA-C-N	6.44	131.95	123.06
1	B	76	PRO	C-N-CA	6.44	131.95	123.06
1	A	80	MET	O-C-N	6.42	130.67	123.48
1	A	78	VAL	N-CA-CB	6.42	119.98	111.90
1	B	96	GLY	N-CA-C	-6.36	104.59	111.21
1	A	119	ASN	CA-C-N	6.36	133.42	121.97
1	A	119	ASN	C-N-CA	6.36	133.42	121.97
1	B	113	GLY	O-C-N	6.32	128.78	123.29
1	B	146	GLU	CA-C-N	-6.25	115.06	122.93
1	B	146	GLU	C-N-CA	-6.25	115.06	122.93
1	B	62	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	B	145	THR	CA-C-O	6.23	126.28	119.24
1	A	60	LYS	CA-C-O	-6.19	113.11	120.10
1	B	68	LEU	O-C-N	6.19	128.47	122.03
1	A	59	HIS	CB-CA-C	-6.18	100.12	110.56
1	A	52	ALA	O-C-N	-6.18	115.67	122.09
1	B	31	ARG	NE-CZ-NH2	-6.17	113.64	119.20
1	A	15	VAL	N-CA-CB	6.14	118.52	111.39
1	A	119	ASN	CB-CA-C	6.13	119.67	111.14
1	A	150	ASN	N-CA-C	-6.13	102.55	109.60
1	B	12	PHE	CA-C-O	6.10	127.03	120.32
1	B	44	GLN	N-CA-CB	6.10	120.14	110.57
1	B	18	ASP	CA-C-O	6.07	127.38	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	O-C-N	6.07	128.19	121.94
1	B	138	PHE	O-C-N	6.06	130.70	123.24
1	A	68	LEU	O-C-N	6.05	128.56	122.08
1	A	22	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	B	12	PHE	CA-CB-CG	-6.05	107.75	113.80
1	A	40	VAL	O-C-N	6.03	128.23	122.20
1	B	127	VAL	CB-CA-C	6.01	120.26	112.14
1	B	88	VAL	CB-CA-C	5.98	119.58	111.87
1	B	98	THR	OG1-CB-CG2	5.96	121.21	109.30
1	B	15	VAL	N-CA-C	-5.91	98.51	107.73
1	A	88	VAL	CA-C-O	-5.91	114.97	121.29
1	A	106	GLY	CA-C-O	-5.88	114.45	119.56
1	A	62	ARG	CA-C-N	5.84	125.98	119.32
1	A	62	ARG	C-N-CA	5.84	125.98	119.32
1	B	33	GLU	N-CA-C	-5.82	104.84	111.07
1	B	112	PHE	CA-C-N	-5.81	117.30	122.47
1	B	112	PHE	C-N-CA	-5.81	117.30	122.47
1	B	69	VAL	CA-C-O	-5.81	114.91	120.95
1	A	46	VAL	N-CA-CB	5.80	118.36	111.23
1	B	8	LYS	CG-CD-CE	5.74	124.50	111.30
1	B	84	GLY	O-C-N	5.73	130.20	123.61
1	A	104	ALA	N-CA-CB	-5.71	101.01	109.98
1	A	78	VAL	N-CA-C	-5.67	98.27	107.28
1	B	101	LEU	O-C-N	5.66	128.61	122.15
1	B	150	ASN	N-CA-CB	-5.66	102.16	110.14
1	A	139	LYS	N-CA-C	-5.65	102.94	110.07
1	A	116	VAL	CA-C-O	-5.62	115.42	121.27
1	A	18	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	155	GLU	CA-CB-CG	5.59	125.28	114.10
1	B	152	ASN	CA-C-O	-5.59	111.80	119.12
1	A	59	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	115	ASP	N-CA-C	5.56	118.46	109.40
1	A	31	ARG	CD-NE-CZ	-5.55	116.64	124.40
1	B	48	THR	N-CA-CB	5.52	119.29	110.46
1	B	141	GLU	CA-CB-CG	5.50	125.09	114.10
1	A	127	VAL	CB-CA-C	5.50	119.00	111.97
1	B	78	VAL	N-CA-CB	5.48	118.58	111.67
1	B	97	VAL	CB-CA-C	5.47	120.27	111.29
1	B	141	GLU	CA-C-O	5.46	125.68	119.18
1	A	81	VAL	CA-C-O	5.45	126.14	120.36
1	B	38	VAL	O-C-N	5.44	128.90	123.18
1	A	121	ILE	N-CA-CB	-5.39	101.84	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	GLU	CB-CG-CD	-5.38	103.46	112.60
1	A	71	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	54	SER	N-CA-C	-5.34	105.53	111.36
1	A	60	LYS	O-C-N	5.34	128.47	122.22
1	A	83	GLU	CB-CA-C	-5.34	99.17	109.37
1	A	96	GLY	N-CA-C	-5.34	106.16	111.56
1	A	31	ARG	CA-C-N	5.33	127.85	120.29
1	A	31	ARG	C-N-CA	5.33	127.85	120.29
1	B	125	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	141	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	82	PHE	O-C-N	5.30	130.08	123.19
1	B	59	HIS	CA-CB-CG	-5.28	108.52	113.80
1	B	76	PRO	N-CA-CB	5.28	108.01	103.31
1	A	132	ARG	CA-CB-CG	5.25	124.59	114.10
1	A	40	VAL	CA-C-O	-5.24	113.64	119.20
1	A	75	GLY	CA-C-O	-5.24	114.03	121.52
1	B	98	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	65	PHE	CA-C-N	5.23	125.90	119.99
1	A	65	PHE	C-N-CA	5.23	125.90	119.99
1	A	101	LEU	O-C-N	5.22	128.69	122.27
1	A	7	ASN	CB-CA-C	5.20	120.77	110.42
1	B	58	GLU	CA-C-O	5.19	125.78	119.49
1	B	111	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	97	VAL	CB-CA-C	5.17	118.73	111.70
1	B	48	THR	N-CA-C	-5.15	102.90	110.52
1	A	99	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	111	ASP	O-C-N	5.12	129.63	122.36
1	B	75	GLY	O-C-N	5.10	126.87	121.77
1	B	6	VAL	CA-C-N	5.10	131.27	121.54
1	B	6	VAL	C-N-CA	5.10	131.27	121.54
1	A	95	ILE	O-C-N	5.10	128.53	121.90
1	B	70	SER	CB-CA-C	-5.09	102.34	110.79
1	A	39	LEU	O-C-N	5.08	129.38	122.57
1	B	89	ALA	CB-CA-C	5.07	119.21	110.79
1	B	137	TRP	N-CA-C	5.07	119.52	113.23
1	A	7	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	115	ASP	N-CA-C	5.02	117.99	109.76
1	B	28	ILE	CA-C-N	5.01	126.87	120.56
1	B	28	ILE	C-N-CA	5.01	126.87	120.56
1	B	138	PHE	CA-C-O	-5.00	115.25	121.11
1	B	112	PHE	N-CA-C	5.00	121.08	114.12

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	132	ARG	Sidechain
1	A	22	ARG	Sidechain
1	A	92	ARG	Sidechain
1	B	118	ARG	Sidechain

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	1147	0	1167	42	0
1	B	1147	0	1167	37	0
2	A	27	0	12	2	0
2	B	27	0	12	0	0
3	B	1	0	0	0	0
4	A	73	0	0	1	0
4	B	85	0	0	4	0
All	All	2507	0	2358	77	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 16.

All (77) 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:B:6:VAL:HG13	1:B:8:LYS:H	1.23	1.04
1:A:48:THR:HG22	1:A:51:LEU:H	1.23	1.03
1:A:92:ARG:HD2	1:A:125:ASP:HA	1.66	0.78
1:B:7:ASN:O	1:B:8:LYS:HE2	1.85	0.76
1:B:6:VAL:HG13	1:B:7:ASN:H	1.52	0.74
1:A:58:GLU:HG2	4:A:186:HOH:O	1.89	0.71
1:B:8:LYS:HD3	1:B:83:GLU:OE2	1.91	0.70
1:A:9:GLU:HG2	1:A:87:VAL:HG12	1.77	0.67
1:B:49:LYS:O	1:B:53:GLU:HG3	1.94	0.66
1:B:6:VAL:HG13	1:B:8:LYS:N	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:O	1:B:22:ARG:HG3	1.97	0.64
1:B:12:PHE:HE1	1:B:79:ALA:HB1	1.61	0.63
1:B:98:THR:HA	1:B:109:ARG:NH1	2.14	0.62
1:A:15:VAL:HB	1:A:78:VAL:HG22	1.84	0.60
1:B:40:VAL:CG2	1:B:81:VAL:HG22	2.32	0.60
1:A:8:LYS:HZ1	1:A:147:VAL:HG23	1.67	0.59
1:B:130:ALA:O	1:B:134:ILE:HG13	2.04	0.58
1:A:144:LEU:HD11	1:B:76:PRO:HG3	1.85	0.57
1:A:150:ASN:OD1	1:A:152:ASN:ND2	2.38	0.56
1:B:12:PHE:CE1	1:B:79:ALA:HB1	2.41	0.55
1:A:40:VAL:CG2	1:A:81:VAL:HG22	2.36	0.55
1:A:8:LYS:NZ	1:A:147:VAL:HG23	2.22	0.54
1:B:99:ASN:ND2	1:B:101:LEU:H	2.06	0.54
1:A:60:LYS:HA	1:A:65:PHE:CD1	2.42	0.54
1:B:150:ASN:H	1:B:153:LEU:HD12	1.73	0.54
1:B:150:ASN:OD1	1:B:152:ASN:ND2	2.37	0.53
1:A:48:THR:HG22	1:A:51:LEU:N	2.07	0.53
1:A:51:LEU:CD1	1:A:136:LEU:HD22	2.39	0.53
1:A:149:PRO:O	1:A:150:ASN:C	2.52	0.53
2:A:160:ADP:H8	2:A:160:ADP:H5'1	1.74	0.52
1:A:41:GLY:O	1:A:80:MET:HA	2.10	0.52
1:A:98:THR:HA	1:A:109:ARG:NH1	2.24	0.52
1:A:43:LYS:HA	1:B:42:LEU:O	2.09	0.51
1:B:38:VAL:O	1:B:82:PHE:HA	2.11	0.51
1:A:11:THR:O	1:A:81:VAL:HA	2.10	0.50
1:B:83:GLU:OE2	1:B:147:VAL:HG11	2.12	0.50
1:A:40:VAL:HG23	1:A:81:VAL:HG22	1.93	0.49
1:A:97:VAL:O	1:A:109:ARG:HD2	2.12	0.49
1:A:28:ILE:HG21	1:A:121:ILE:HD12	1.94	0.49
1:A:38:VAL:HG11	1:A:147:VAL:HG12	1.93	0.49
1:B:139:LYS:O	1:B:142:GLU:HB2	2.13	0.49
1:B:58:GLU:HG2	4:B:179:HOH:O	2.13	0.49
1:A:69:VAL:HA	1:A:72:ILE:HG22	1.96	0.48
1:A:150:ASN:OD1	1:A:152:ASN:HB2	2.13	0.47
1:B:99:ASN:ND2	4:B:188:HOH:O	2.47	0.47
1:A:60:LYS:HA	1:A:65:PHE:CG	2.49	0.47
1:A:25:VAL:HG13	1:A:78:VAL:HG21	1.97	0.47
1:A:71:PHE:CE1	1:A:118:ARG:NH2	2.83	0.47
1:B:28:ILE:HG21	1:B:121:ILE:HD12	1.95	0.47
1:A:33:GLU:OE2	1:B:25:VAL:HB	2.16	0.46
1:A:6:VAL:C	1:A:8:LYS:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PRO:HA	1:A:109:ARG:HB3	1.99	0.45
1:B:34:LYS:HE3	4:B:246:HOH:O	2.15	0.45
2:A:160:ADP:H5'1	2:A:160:ADP:C8	2.51	0.45
1:B:39:LEU:HD13	1:B:82:PHE:CZ	2.51	0.45
1:A:42:LEU:O	1:B:43:LYS:HA	2.17	0.45
1:B:128:GLU:H	1:B:128:GLU:CD	2.24	0.45
1:A:132:ARG:HH12	1:A:136:LEU:HD12	1.81	0.45
1:B:40:VAL:HG23	1:B:81:VAL:HG22	1.99	0.45
1:A:7:ASN:H	1:A:85:LYS:HA	1.81	0.45
1:B:132:ARG:NH1	1:B:136:LEU:HD22	2.32	0.44
1:A:64:PHE:CD1	1:A:68:LEU:HD22	2.53	0.44
1:A:64:PHE:HD1	1:A:68:LEU:HD22	1.83	0.43
1:B:38:VAL:CG2	1:B:149:PRO:HB3	2.49	0.43
1:B:57:ALA:O	1:B:60:LYS:HD2	2.18	0.43
1:B:38:VAL:HG23	1:B:149:PRO:HB3	2.00	0.43
1:B:83:GLU:OE1	1:B:147:VAL:HG21	2.19	0.42
1:A:132:ARG:O	1:A:136:LEU:HB2	2.19	0.42
1:B:7:ASN:OD1	1:B:85:LYS:HB2	2.19	0.42
1:A:39:LEU:HD21	1:A:42:LEU:HD22	2.01	0.42
1:A:101:LEU:HG	1:A:114:VAL:O	2.21	0.41
1:A:9:GLU:HB3	1:A:84:GLY:O	2.20	0.41
1:B:34:LYS:CE	4:B:246:HOH:O	2.68	0.41
1:A:148:LYS:HB2	1:A:148:LYS:HE3	1.95	0.41
1:A:39:LEU:HD13	1:A:82:PHE:CZ	2.55	0.41
1:B:11:THR:O	1:B:81:VAL:HA	2.21	0.40
1:A:98:THR:O	1:A:100:PRO:HD3	2.22	0.40

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	148/155 (96%)	142 (96%)	5 (3%)	1 (1%)	18	19
1	B	148/155 (96%)	140 (95%)	6 (4%)	2 (1%)	9	7
All	All	296/310 (96%)	282 (95%)	11 (4%)	3 (1%)	12	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	ASN
1	B	120	ILE
1	A	120	ILE

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	122/127 (96%)	113 (93%)	9 (7%)	13	14
1	B	122/127 (96%)	114 (93%)	8 (7%)	15	18
All	All	244/254 (96%)	227 (93%)	17 (7%)	14	16

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

Mol	Chain	Res	Type
1	A	11	THR
1	A	48	THR
1	A	81	VAL
1	A	116	VAL
1	A	132	ARG
1	A	136	LEU
1	A	145	THR
1	A	147	VAL
1	A	148	LYS
1	B	8	LYS
1	B	11	THR
1	B	45	LEU
1	B	60	LYS

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Mol	Chain	Res	Type
1	B	81	VAL
1	B	98	THR
1	B	124	SER
1	B	128	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	B	59	HIS
1	B	99	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 oligosaccharides 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	160	-	28,29,29	1.27	3 (10%)	43,45,45	1.51	9 (20%)
2	ADP	B	160	3	28,29,29	1.04	4 (14%)	43,45,45	1.35	5 (11%)

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	160	-	-	4/16/32/32	0/3/3/3
2	ADP	B	160	3	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	160	ADP	PA-O3A	3.95	1.63	1.59
2	B	160	ADP	C2-N1	2.48	1.38	1.33
2	A	160	ADP	PB-O3B	-2.40	1.45	1.54
2	B	160	ADP	PB-O1B	-2.14	1.43	1.50
2	B	160	ADP	PA-O2A	-2.10	1.45	1.55
2	A	160	ADP	PA-O2A	-2.07	1.45	1.55
2	B	160	ADP	PB-O3B	-2.01	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	160	ADP	O4'-C1'-N9	-4.06	100.29	108.09
2	A	160	ADP	O5'-C5'-C4'	3.87	122.18	108.99
2	A	160	ADP	C1'-N9-C8	3.45	134.75	127.09
2	A	160	ADP	C4-N9-C1'	-3.25	119.03	126.63
2	A	160	ADP	O4'-C4'-C5'	-3.13	99.30	109.33
2	A	160	ADP	N6-C6-N1	2.90	124.83	118.38
2	B	160	ADP	O2A-PA-O3A	2.46	113.91	107.27
2	B	160	ADP	O4'-C4'-C5'	-2.40	101.66	109.33
2	A	160	ADP	O2A-PA-O5'	2.39	118.40	107.57
2	A	160	ADP	O2'-C2'-C3'	2.17	118.79	111.82
2	A	160	ADP	C4-C5-N7	2.14	113.03	110.58
2	B	160	ADP	O3B-PB-O1B	2.04	118.80	110.83
2	A	160	ADP	C3'-C2'-C1'	-2.03	97.62	101.46
2	B	160	ADP	O2A-PA-O1A	-2.01	103.10	112.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	160	ADP	C5'-O5'-PA-O2A

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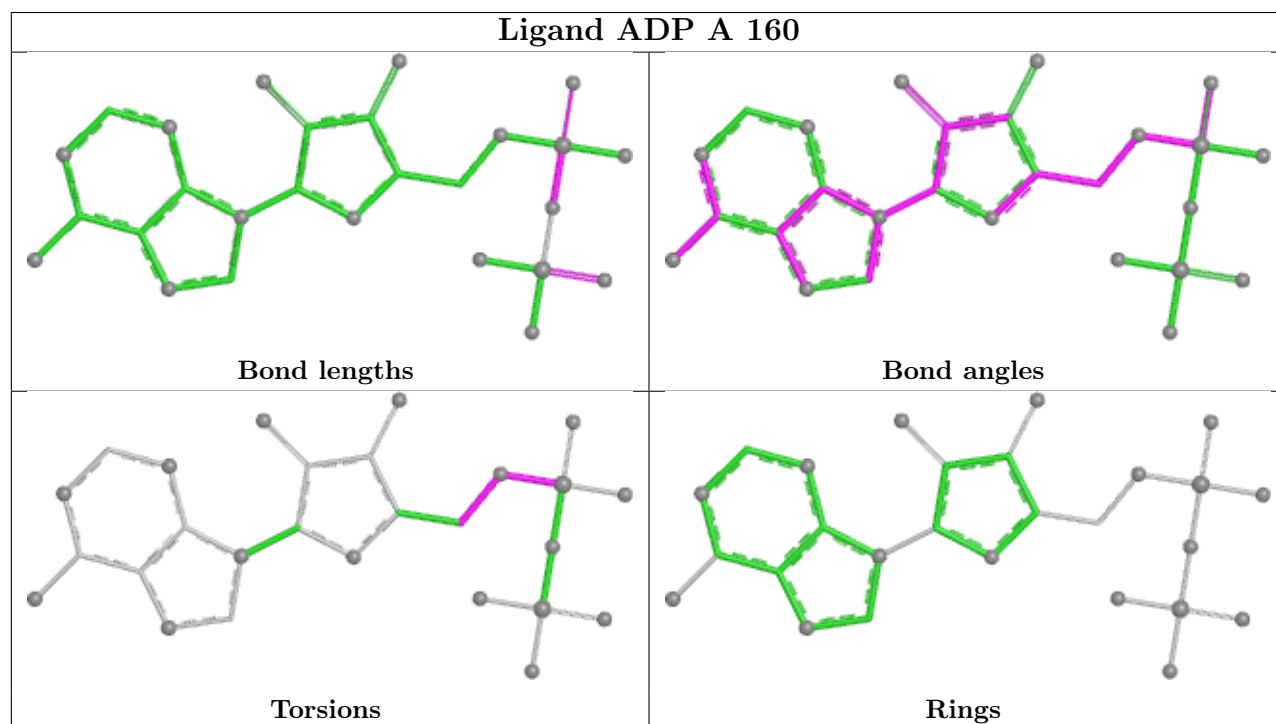
Mol	Chain	Res	Type	Atoms
2	B	160	ADP	PA-O3A-PB-O2B
2	B	160	ADP	PB-O3A-PA-O1A
2	A	160	ADP	C5'-O5'-PA-O1A
2	A	160	ADP	C5'-O5'-PA-O3A
2	A	160	ADP	C4'-C5'-O5'-PA

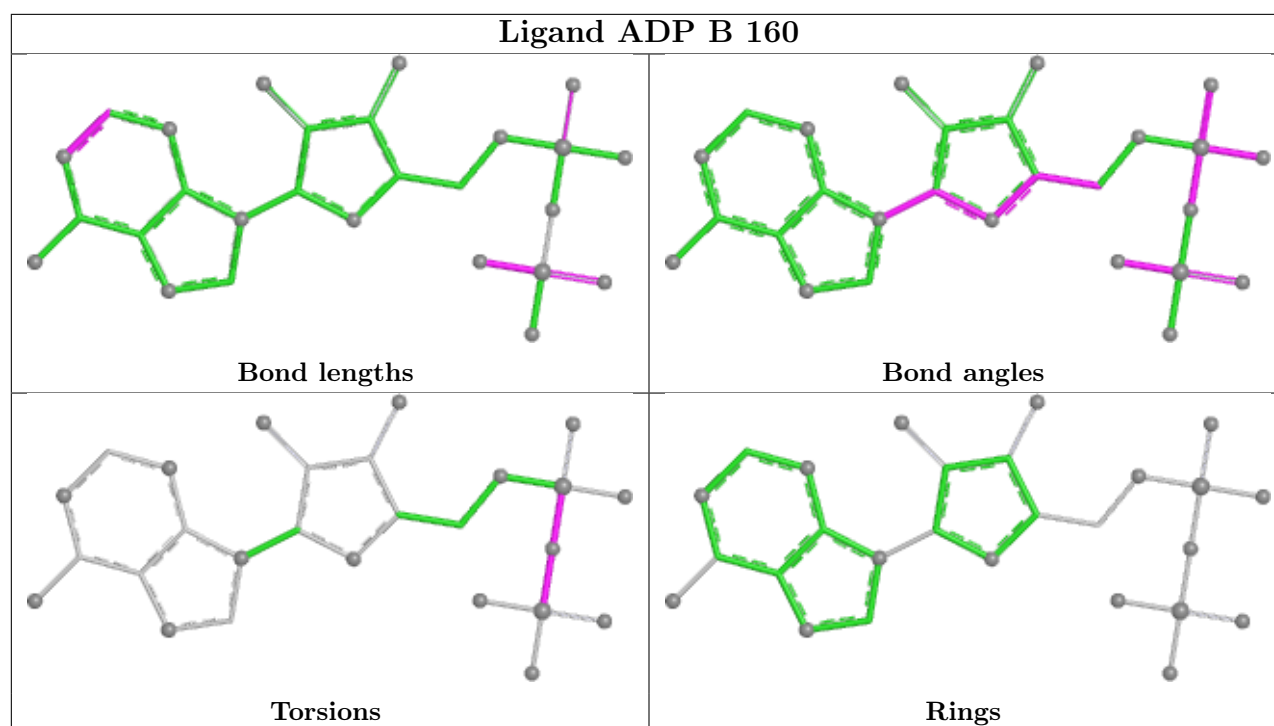
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	160	ADP	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.