

Full wwPDB X-ray Structure Validation Report (i)

May 30, 2020 – 02:21 pm BST

PDB ID	:	1NSQ
Title	:	MECHANISM OF PHOSPHATE TRANSFER BY NUCLEOSIDE DIPHOS-
		PHATE KINASE: X-RAY STRUCTURES OF A PHOSPHO-HISTIDINE
		INTERMEDIATE OF THE ENZYMES FROM DROSOPHILA AND DIC-
		TYOSTELIUM
Authors	:	Janin, J.; Chiadmi, M.; Morera, S.; Lebras, G.; Lascu, I.
Deposited on	:	1995-04-24
$\operatorname{Resolution}$:	2.18 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

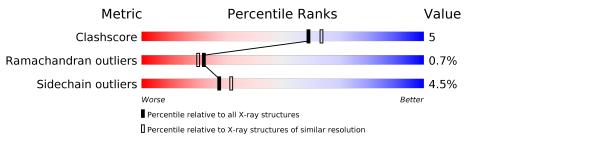
$\operatorname{MolProbity}$:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	7689(2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	153	90%	8%	••
1	В	153	80%	18%	••
1	С	153	87%	12%	••



1NSQ

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3878 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Λ	152	Total	С	Ν	Ο	Р	\mathbf{S}	0	0	0
	A	152	1207	777	205	219	1	5	0		U
1	В	152	Total	С	Ν	Ο	Р	S	0	0	0
	D	152	1207	777	205	219	1	5			
1	C	152	Total	С	Ν	Ο	Р	S	0	0	0
		152	1207	777	205	219	1	5	U	0	0

• Molecule 1 is a protein called NUCLEOSIDE DIPHOSPHATE KINASE.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	100	Total O 100 100	0	0
2	В	88	Total O 88 88	0	0
2	С	69	Total O 69 69	0	0

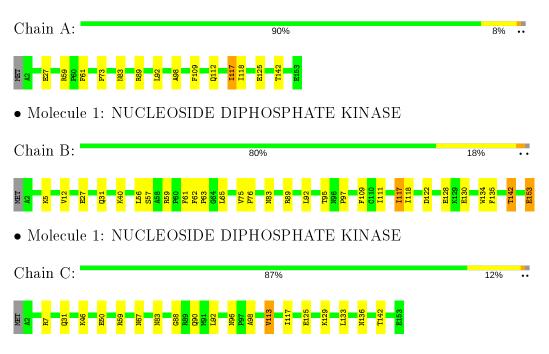


3 Residue-property plots (i)

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. Residues are colorcoded 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





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	115.75Å 115.75 Å 98.52 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 - 2.18	Depositor
% Data completeness	(Not available) (8.00-2.18)	Depositor
(in resolution range)	(100 available) (0.00 2.10)	Depositor
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3878	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP



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: HIP

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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.57	0/1221	0.75	2/1650~(0.1%)	
1	В	0.56	0/1221	0.76	2/1650~(0.1%)	
1	С	0.57	0/1221	0.77	0/1650	
All	All	0.57	0/3663	0.76	$4/4950 \ (0.1\%)$	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	117	ILE	N-CA-C	5.42	125.64	111.00
1	В	117	ILE	N-CA-C	5.38	125.52	111.00
1	А	109	PHE	N-CA-C	5.37	125.50	111.00
1	В	109	PHE	N-CA-C	5.21	125.07	111.00

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	А	1207	0	1206	7	0
1	В	1207	0	1206	16	0
1	С	1207	0	1206	12	0
2	А	100	0	0	2	0

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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 5.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:112:GLN:OE1	1:B:153:GLU:HG3	1.88	0.73
1:B:40:LYS:O	1:B:76:PRO:HD2	1.91	0.70
1:C:96:ASN:HA	1:C:113:VAL:HG13	1.74	0.70
1:C:46:LYS:O	1:C:50:GLU:HG3	1.94	0.67
1:A:98:ALA:HB2	2:A:228:HOH:O	1.98	0.64
1:B:27:GLU:O	1:B:31:GLN:HB2	2.03	0.57
1:A:73:PRO:HD2	2:A:197:HOH:O	2.05	0.57
1:A:59:ARG:HG3	1:A:61:PHE:CZ	2.41	0.55
1:B:89:ARG:CD	1:B:122:ASP:HA	2.38	0.53
1:B:89:ARG:HD2	1:B:122:ASP:HA	1.89	0.53
1:C:98:ALA:HB2	2:C:216:HOH:O	2.10	0.51
1:B:62:PHE:N	1:B:63:PRO:CD	2.75	0.49
1:A:125:GLU:CD	1:A:125:GLU:H	2.17	0.48
1:B:12:VAL:HB	1:B:75:VAL:HB	1.96	0.47
1:C:88:GLY:O	1:C:92:LEU:HD13	2.15	0.46
1:B:142:THR:HA	2:B:181:HOH:O	2.17	0.44
1:C:125:GLU:H	1:C:125:GLU:CD	2.21	0.44
1:C:7:ARG:NH1	2:C:179:HOH:O	2.50	0.44
1:A:92:LEU:HD22	1:A:118:ILE:HD13	2.00	0.44
1:B:62:PHE:HB3	1:B:63:PRO:HD3	2.00	0.44
1:C:59:ARG:HD3	1:C:59:ARG:HA	1.76	0.43
1:C:113:VAL:HG22	2:C:177:HOH:O	2.19	0.43
1:C:125:GLU:O	1:C:129:LYS:HG3	2.19	0.42
1:C:31:GLN:NE2	2:C:221:HOH:O	2.50	0.42
1:B:59:ARG:HD3	1:B:59:ARG:HA	1.79	0.42
1:C:136:ASN:HD22	1:C:136:ASN:HA	1.73	0.41
1:C:50:GLU:HB2	2:C:202:HOH:O	2.20	0.41
1:B:56:LEU:HD12	1:B:65:LEU:HD21	2.01	0.41
1:B:97:PRO:HB2	1:B:111:ILE:O	2.21	0.41
1:A:59:ARG:HG3	1:A:61:PHE:CE2	2.56	0.41
1:B:95:THR:O	1:B:97:PRO:HD3	2.20	0.41
			-

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Chain Non-H H(added) Clashes Symm-Clashes Mol H(model) В 288 0 0 0 1 2 С 69 0 0 50 All All 0 38780361834

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:O	1:B:134:TRP:HD1	2.04	0.41
1:B:40:LYS:HE2	1:B:135:PHE:CE1	2.56	0.41
1:B:92:LEU:HD22	1:B:118:ILE:HD13	2.02	0.40

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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	А	149/153~(97%)	146~(98%)	2(1%)	1 (1%)	22 20
1	В	149/153~(97%)	145~(97%)	3~(2%)	1 (1%)	22 20
1	С	149/153~(97%)	146 (98%)	2(1%)	1 (1%)	22 20
All	All	447/459 (97%)	437 (98%)	7(2%)	3 (1%)	22 20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	117	ILE
1	В	117	ILE
1	С	117	ILE

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	А	125/126~(99%)	121~(97%)	4(3%)	39 47
1	В	125/126~(99%)	118 (94%)	7~(6%)	21 23
1	С	125/126~(99%)	119~(95%)	6~(5%)	25 29
All	All	375/378~(99%)	358~(96%)	17~(4%)	27 32

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

Mol	Chain	Res	Type
1	А	27	GLU
1	А	83	ASN
1	А	89	ARG
1	А	142	THR
1	В	5	LYS
1	В	57	SER
1	В	61	PHE
1	В	83	ASN
1	В	128	GLU
1	В	142	THR
1	В	153	GLU
1	С	67	ASN
1	С	83	ASN
1	С	90	GLN
1	С	113	VAL
1	С	133	LEU
1	С	142	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	4	ASN
1	А	136	ASN
1	В	4	ASN
1	В	31	GLN
1	С	4	ASN
1	С	31	GLN
1	С	83	ASN
1	С	136	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	Tune	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	E	Bond ang	gles
	Type	Cham	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	HIP	С	119	1	10, 14, 15	1.97	2 (20%)	6,20,22	1.54	1(16%)
1	HIP	В	119	1	10, 14, 15	1.69	1 (10%)	6,20,22	1.43	1(16%)
1	HIP	А	119	1	10,14,15	2.27	2 (20%)	6,20,22	1.51	1(16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIP	С	119	1	-	1/5/12/14	0/1/1/1
1	HIP	В	119	1	-	1/5/12/14	0/1/1/1
1	HIP	А	119	1	-	1/5/12/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	119	HIP	P-O1P	6.22	1.52	1.47
1	С	119	HIP	P-O1P	5.14	1.51	1.47
1	В	119	HIP	P-O1P	4.47	1.51	1.47
1	С	119	HIP	P-O2P	-2.43	1.49	1.54
1	А	119	HIP	P-O2P	-2.38	1.49	1.54

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	119	HIP	CD2-NE2-CE1	2.28	109.34	105.78
1	В	119	HIP	O3P-P-O2P	2.27	115.49	106.57
1	А	119	HIP	CD2-NE2-CE1	2.25	109.29	105.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	С	119	HIP	C-CA-CB-CG
1	В	119	HIP	C-CA-CB-CG
1	А	119	HIP	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

