



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 1F8Y / pdb_00001f8y
Title : CRYSTAL STRUCTURE ANALYSIS OF NUCLEOSIDE 2-DEOXYRIBOSYLTRANSFERASE COMPLEXED WITH 5-METHYL-2'-DEOXYPSEUDOURIDINE
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Deposited on : 2000-07-05
Resolution : 2.40 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
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

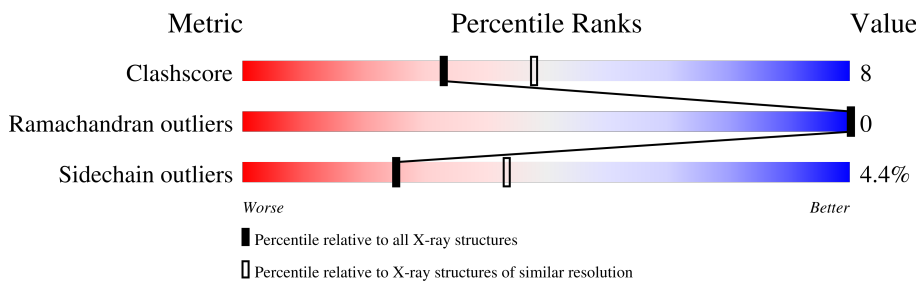
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	157	 79% 18% ...
1	B	157	 80% 17% ..

2 Entry composition [i](#)

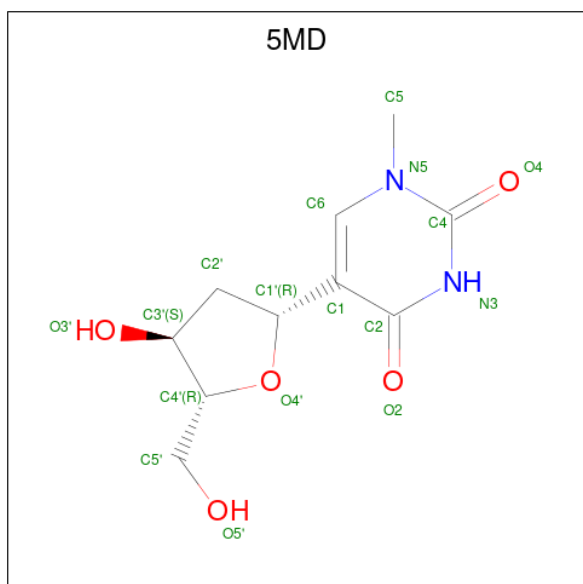
There are 3 unique types of molecules in this entry. The entry contains 2646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-DEOXYRIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1268	816	201	246	5			
1	B	156	Total	C	N	O	S	0	0	0
			1268	816	201	246	5			

- Molecule 2 is 2'-deoxy-1-methyl-pseudouridine (CCD ID: 5MD) (formula: C₁₀H₁₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	29	Total 29	O 29	0	0

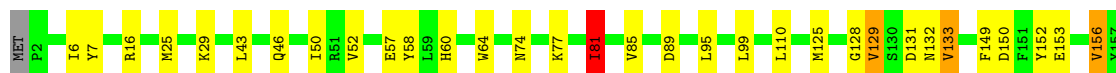
3 Residue-property plots [i](#)

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.

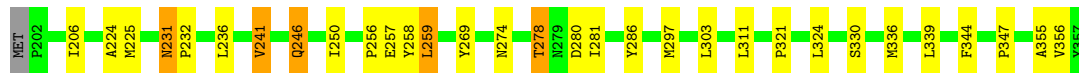
• Molecule 1: NUCLEOSIDE 2-DEOXYRIBOSYLTRANSFERASE

Chain A:  79% 18% ...



• Molecule 1: NUCLEOSIDE 2-DEOXYRIBOSYLTRANSFERASE

Chain B:  80% 17% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	149.60 Å 149.60 Å 149.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2646	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: 5MD

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	0.48	0/1301	0.95	4/1762 (0.2%)
1	B	0.46	0/1301	0.94	7/1762 (0.4%)
All	All	0.47	0/2602	0.95	11/3524 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ASP	N-CA-C	6.42	118.16	111.03
1	B	286	TYR	N-CA-C	6.17	118.58	108.52
1	B	231	ASN	CA-C-N	6.04	125.93	119.28
1	B	231	ASN	C-N-CA	6.04	125.93	119.28
1	A	81	ILE	N-CA-C	5.71	116.81	108.53
1	A	85	VAL	N-CA-C	-5.48	101.61	108.84
1	A	7	TYR	N-CA-C	-5.47	99.61	108.52
1	A	153	GLU	N-CA-C	-5.33	101.63	109.62
1	B	241	VAL	CA-C-N	5.24	126.39	119.84
1	B	241	VAL	C-N-CA	5.24	126.39	119.84
1	B	339	LEU	N-CA-C	5.08	116.50	111.07

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	1268	0	1216	23	0
1	B	1268	0	1216	21	0
2	A	17	0	14	1	0
2	B	17	0	14	3	0
3	A	47	0	0	0	0
3	B	29	0	0	2	0
All	All	2646	0	2460	39	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 8.

All (39) 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:224:ALA:HB2	1:B:336:MET:HE1	1.43	1.01
1:B:246:GLN:NE2	2:B:2:5MD:HN3	1.75	0.81
1:B:225:MET:HE3	1:B:236:LEU:HD21	1.65	0.78
1:B:206:ILE:HG22	1:B:281:ILE:HB	1.65	0.76
1:B:246:GLN:HE22	2:B:2:5MD:HN3	1.38	0.72
1:A:46:GLN:HE22	2:A:158:5MD:HN3	1.39	0.68
1:B:274:ASN:O	1:B:278:THR:HB	1.95	0.66
1:A:129:VAL:HG13	1:B:297:MET:HE3	1.87	0.56
1:A:25:MET:O	1:A:29:LYS:HG3	2.08	0.54
1:B:321:PRO:HA	1:B:355:ALA:O	2.09	0.53
1:A:156:VAL:HG13	3:B:861:HOH:O	2.08	0.52
1:A:128:GLY:HA3	1:B:269:TYR:CE1	2.45	0.52
1:A:6:ILE:HG22	1:A:81:ILE:HB	1.91	0.51
1:A:129:VAL:CG1	1:B:297:MET:HE3	2.42	0.50
1:A:60:HIS:CE1	1:B:355:ALA:HB2	2.46	0.50
1:A:50:ILE:C	1:A:50:ILE:HD12	2.38	0.48
1:A:95:LEU:O	1:A:99:LEU:HG	2.13	0.47
1:B:250:ILE:HD13	1:B:258:TYR:CZ	2.50	0.46
1:B:311:LEU:HG	1:B:330:SER:OG	2.14	0.46
1:A:57:GLU:HG2	1:A:58:TYR:CD2	2.51	0.46
1:B:257:GLU:H	1:B:257:GLU:CD	2.24	0.45
1:A:133:VAL:HG11	1:A:152:TYR:HB2	1.97	0.45
1:B:256:PRO:O	1:B:259:LEU:HB2	2.17	0.45
1:A:132:ASN:ND2	1:A:150:ASP:HB3	2.32	0.45
1:A:74:ASN:HD22	1:A:77:LYS:HE2	1.82	0.44
1:B:231:ASN:HA	1:B:232:PRO:HD3	1.81	0.44
1:B:246:GLN:NE2	2:B:2:5MD:N3	2.51	0.44
1:A:125:MET:O	1:A:129:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:MET:CE	1:B:236:LEU:HD21	2.44	0.43
1:A:131:ASP:O	1:A:149:PHE:HA	2.20	0.42
1:A:132:ASN:HD22	1:A:133:VAL:H	1.68	0.42
1:A:16:ARG:HH12	1:A:89:ASP:HB2	1.86	0.41
1:A:132:ASN:ND2	1:A:133:VAL:H	2.18	0.41
1:A:128:GLY:HA3	1:B:269:TYR:CD1	2.56	0.41
1:B:344:PHE:O	1:B:347:PRO:HD3	2.21	0.41
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.93	0.40
1:B:250:ILE:HA	3:B:872:HOH:O	2.21	0.40
1:A:50:ILE:HD11	1:A:58:TYR:CG	2.56	0.40
1:A:52:VAL:HG13	1:A:64:TRP:CZ2	2.56	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	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
1	B	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
All	All	308/314 (98%)	299 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	136/137 (99%)	131 (96%)	5 (4%)	30	51
1	B	136/137 (99%)	129 (95%)	7 (5%)	21	37
All	All	272/274 (99%)	260 (96%)	12 (4%)	25	43

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	110	LEU
1	A	129	VAL
1	A	133	VAL
1	A	156	VAL
1	B	241	VAL
1	B	246	GLN
1	B	259	LEU
1	B	278	THR
1	B	303	LEU
1	B	324	LEU
1	B	356	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	45	ASN
1	A	46	GLN
1	A	60	HIS
1	A	71	ASN
1	A	74	ASN
1	A	132	ASN
1	B	238	ASN
1	B	246	GLN
1	B	255	HIS
1	B	260	HIS
1	B	345	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	5MD	B	2	-	18,18,18	0.62	0	20,26,26	1.19	1 (5%)
2	5MD	A	158	-	18,18,18	1.03	1 (5%)	20,26,26	1.59	5 (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
2	5MD	B	2	-	-	0/5/18/18	0/2/2/2
2	5MD	A	158	-	-	0/5/18/18	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	158	5MD	C1'-C1	2.27	1.54	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	158	5MD	C5-N5-C4	2.91	121.11	117.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	5MD	C5-N5-C4	2.79	120.97	117.83
2	A	158	5MD	O4'-C1'-C1	2.75	116.88	108.91
2	A	158	5MD	O2-C2-C1	2.41	130.00	124.01
2	A	158	5MD	O4-C4-N3	-2.18	117.47	121.49
2	A	158	5MD	O4-C4-N5	2.04	124.84	122.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	5MD	3	0
2	A	158	5MD	1	0

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.