



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:56 PM UTC

PDB ID : 1DJ0 / pdb_00001dj0
Title : THE CRYSTAL STRUCTURE OF E. COLI PSEUDOURIDINE SYNTHASE
I AT 1.5 ANGSTROM RESOLUTION
Authors : Foster, P.G.; Huang, L.; Santi, D.V.; Stroud, R.M.
Deposited on : 1999-11-30
Resolution : 1.50 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
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

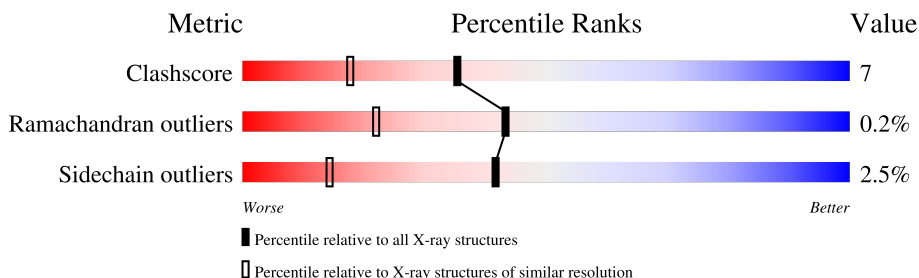
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)

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	264	 81% 15% . .
1	B	264	 81% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4663 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 PSEUDOURIDINE SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2097	1333	382	374	8			
1	B	264	Total	C	N	O	S	0	0	0
			2097	1333	382	374	8			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	255	Total	O	0	0
			255	255		
3	B	212	Total	O	0	0
			212	212		

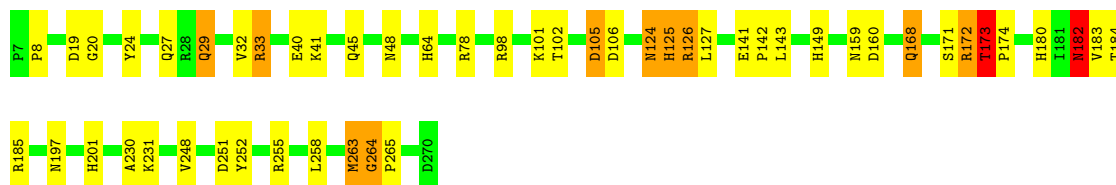
3 Residue-property plots

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.

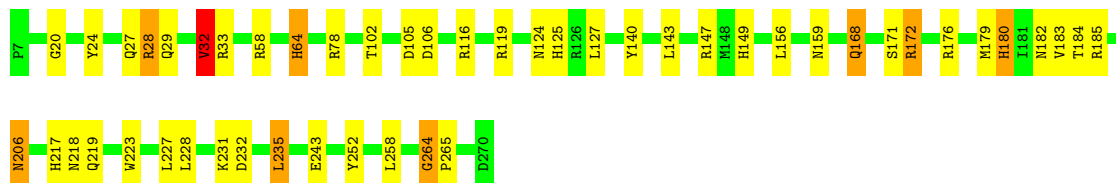
• Molecule 1: PSEUDOURIDINE SYNTHASE I

Chain A: 



• Molecule 1: PSEUDOURIDINE SYNTHASE I

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.08 Å 37.40 Å 103.48 Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	38.00 – 1.50	Depositor
% Data completeness (in resolution range)	95.2 (38.00-1.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4663	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:
CL

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	0.82	0/2153	1.65	28/2929 (1.0%)
1	B	0.75	0/2153	1.68	35/2929 (1.2%)
All	All	0.78	0/4306	1.66	63/5858 (1.1%)

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	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASN	CA-CB-CG	14.96	127.56	112.60
1	A	173	THR	CA-C-O	11.08	135.34	120.16
1	A	105	ASP	CA-CB-CG	-10.47	102.13	112.60
1	A	263	MET	CA-CB-CG	10.00	134.11	114.10
1	B	58	ARG	CD-NE-CZ	9.49	137.69	124.40
1	A	264	GLY	CA-C-O	-8.73	109.03	121.52
1	A	33	ARG	CD-NE-CZ	8.50	136.30	124.40
1	B	231	LYS	N-CA-C	8.22	122.48	111.30
1	B	159	ASN	CA-CB-CG	8.21	120.81	112.60
1	B	206	ASN	CA-C-O	8.07	128.97	120.42
1	B	140	TYR	N-CA-C	7.47	119.21	111.14
1	B	64	HIS	CB-CG-CD2	-7.29	121.72	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	LEU	O-C-N	7.29	129.58	122.07
1	B	172	ARG	N-CA-CB	7.25	121.54	110.44
1	B	217	HIS	CA-CB-CG	7.13	120.93	113.80
1	B	206	ASN	O-C-N	-7.10	114.05	122.15
1	A	255	ARG	CD-NE-CZ	6.91	134.08	124.40
1	A	265	PRO	N-CA-CB	6.83	110.11	102.60
1	A	172	ARG	N-CA-C	-6.82	96.27	110.80
1	B	176	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	A	201	HIS	CA-CB-CG	-6.64	107.16	113.80
1	B	32	VAL	CA-CB-CG2	6.53	121.50	110.40
1	B	119	ARG	NE-CZ-NH2	-6.53	113.32	119.20
1	A	29	GLN	CB-CG-CD	6.23	123.20	112.60
1	B	264	GLY	CA-C-O	-6.22	112.63	121.52
1	B	78	ARG	CD-NE-CZ	-6.12	115.83	124.40
1	B	140	TYR	CA-CB-CG	6.12	124.92	113.90
1	A	142	PRO	N-CA-CB	6.11	108.77	103.27
1	B	28	ARG	CD-NE-CZ	6.06	132.88	124.40
1	B	171	SER	CA-C-O	-5.99	114.92	121.87
1	A	252	TYR	O-C-N	5.98	126.22	121.55
1	A	180	HIS	CA-CB-CG	5.91	119.71	113.80
1	A	125	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	B	265	PRO	N-CA-CB	5.89	109.08	102.60
1	B	265	PRO	CA-N-CD	-5.71	103.51	111.50
1	A	33	ARG	N-CA-CB	-5.68	101.60	110.87
1	B	116	ARG	NH1-CZ-NH2	5.61	126.60	119.30
1	B	171	SER	CA-C-N	-5.61	112.22	122.38
1	B	171	SER	C-N-CA	-5.61	112.22	122.38
1	B	27	GLN	N-CA-C	5.55	118.28	109.96
1	B	78	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	251	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	228	LEU	CA-C-O	-5.45	115.10	120.82
1	B	32	VAL	CA-C-N	5.44	128.50	120.82
1	B	32	VAL	C-N-CA	5.44	128.50	120.82
1	A	197	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	218	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	A	106	ASP	CA-CB-CG	-5.38	107.22	112.60
1	B	32	VAL	CA-CB-CG1	-5.37	101.26	110.40
1	B	180	HIS	O-C-N	5.36	128.76	123.46
1	A	8	PRO	CA-C-O	5.33	128.72	122.12
1	A	197	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	141	GLU	CA-C-N	5.29	125.55	119.83
1	A	141	GLU	C-N-CA	5.29	125.55	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASP	CA-CB-CG	-5.28	107.32	112.60
1	B	116	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	159	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	98	ARG	CD-NE-CZ	-5.21	117.10	124.40
1	A	19	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	227	LEU	CA-C-O	5.18	126.04	120.55
1	A	230	ALA	N-CA-C	5.12	117.76	111.82
1	A	40	GLU	CA-C-O	-5.05	114.16	119.97
1	B	28	ARG	CB-CG-CD	-5.04	99.71	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ASN	Mainchain
1	A	264	GLY	Peptide,Mainchain
1	B	264	GLY	Peptide,Mainchain

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	2097	0	2066	33	0
1	B	2097	0	2066	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	255	0	0	8	0
3	B	212	0	0	3	0
All	All	4663	0	4132	62	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 7.

All (62) 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:182:ASN:HD21	1:B:184:THR:HG23	1.11	1.06
1:B:125:HIS:HD2	1:B:127:LEU:H	1.21	0.88
1:B:182:ASN:ND2	1:B:184:THR:HG23	1.90	0.87
1:A:124:ASN:HD21	1:A:143:LEU:H	1.27	0.82
1:A:125:HIS:HD2	1:A:127:LEU:H	1.27	0.82
1:B:20:GLY:H	1:B:64:HIS:HD2	1.28	0.79
1:A:182:ASN:HD21	1:A:184:THR:HG23	1.47	0.78
1:A:20:GLY:H	1:A:64:HIS:HD2	1.31	0.78
1:B:124:ASN:HD22	1:B:185:ARG:HH22	1.30	0.78
1:A:124:ASN:HD22	1:A:185:ARG:HH22	1.31	0.77
1:B:149:HIS:HD2	1:B:183:VAL:H	1.32	0.75
1:B:182:ASN:HD21	1:B:184:THR:CG2	1.96	0.75
1:B:20:GLY:H	1:B:64:HIS:CD2	2.04	0.74
1:A:20:GLY:H	1:A:64:HIS:CD2	2.05	0.73
1:B:125:HIS:CD2	1:B:127:LEU:H	2.09	0.69
1:A:182:ASN:ND2	1:A:184:THR:HG23	2.09	0.67
1:B:124:ASN:HD21	1:B:143:LEU:H	1.43	0.66
1:A:41:LYS:O	1:A:45:GLN:HG3	1.98	0.64
1:A:149:HIS:HD2	1:A:183:VAL:H	1.45	0.63
1:B:24:TYR:CD1	1:B:32:VAL:HG11	2.34	0.63
1:A:125:HIS:CD2	1:A:127:LEU:H	2.13	0.60
1:A:182:ASN:HD21	1:A:184:THR:CG2	2.17	0.57
1:B:32:VAL:HG12	1:B:33:ARG:N	2.22	0.54
1:A:126:ARG:HG3	3:A:761:HOH:O	2.06	0.54
1:B:149:HIS:CD2	1:B:183:VAL:H	2.19	0.53
1:B:232:ASP:HB3	1:B:235:LEU:CD2	2.39	0.53
1:B:32:VAL:HG12	1:B:33:ARG:H	1.74	0.52
1:A:171:SER:C	1:A:172:ARG:O	2.45	0.52
1:A:172:ARG:O	1:A:173:THR:C	2.53	0.51
1:A:168:GLN:HB2	3:A:780:HOH:O	2.09	0.51
1:A:182:ASN:ND2	3:A:616:HOH:O	2.44	0.50
1:B:102:THR:HG23	3:B:791:HOH:O	2.12	0.49
1:B:156:LEU:HD21	1:B:180:HIS:HA	1.94	0.49
1:B:168:GLN:HB2	3:B:792:HOH:O	2.12	0.49
1:B:179:MET:O	1:B:180:HIS:HB3	2.14	0.48
1:A:172:ARG:O	1:A:173:THR:O	2.31	0.48
1:A:126:ARG:HD2	3:A:623:HOH:O	2.13	0.48
1:B:20:GLY:N	1:B:64:HIS:HD2	2.05	0.47
1:B:147:ARG:HH11	1:B:147:ARG:HD2	1.55	0.47
1:A:48:ASN:HD22	1:A:78:ARG:HH21	1.63	0.46
1:B:219:GLN:HG3	1:B:223:TRP:CE3	2.51	0.46
1:A:24:TYR:HE1	1:A:33:ARG:HH11	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:HIS:HE1	1:B:243:GLU:O	1.99	0.46
1:A:173:THR:HA	1:A:174:PRO:HD3	1.80	0.45
1:B:232:ASP:HB3	1:B:235:LEU:HD23	1.98	0.45
1:A:149:HIS:CD2	1:A:183:VAL:H	2.31	0.45
1:A:124:ASN:ND2	1:A:143:LEU:H	2.06	0.45
1:A:248:VAL:HB	1:A:263:MET:HB2	1.99	0.45
1:B:206:ASN:HB3	3:B:703:HOH:O	2.17	0.44
1:A:27:GLN:HE21	1:A:29:GLN:HB2	1.82	0.43
1:A:101:LYS:HD3	1:A:258:LEU:HD23	2.00	0.43
1:A:160:ASP:OD2	1:A:231:LYS:HE3	2.18	0.42
1:A:102:THR:HB	3:A:807:HOH:O	2.20	0.42
1:B:180:HIS:CD2	1:B:180:HIS:C	2.97	0.42
1:A:149:HIS:HE1	3:A:746:HOH:O	2.01	0.42
1:A:149:HIS:CD2	1:A:182:ASN:HA	2.55	0.42
1:B:252:TYR:CD2	1:B:258:LEU:HD12	2.55	0.41
1:B:64:HIS:CE1	1:B:243:GLU:O	2.73	0.41
1:A:32:VAL:HG23	3:A:676:HOH:O	2.21	0.41
1:B:24:TYR:CD1	1:B:32:VAL:CG1	3.03	0.41
1:A:124:ASN:ND2	1:A:185:ARG:HH22	2.10	0.40
1:A:126:ARG:NE	3:A:735:HOH:O	2.55	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	262/264 (99%)	252 (96%)	9 (3%)	1 (0%)	30	12
1	B	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
All	All	524/528 (99%)	509 (97%)	14 (3%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	THR

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	217/217 (100%)	213 (98%)	4 (2%)	51	24
1	B	217/217 (100%)	210 (97%)	7 (3%)	34	8
All	All	434/434 (100%)	423 (98%)	11 (2%)	42	14

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	A	126	ARG
1	A	168	GLN
1	A	182	ASN
1	B	28	ARG
1	B	29	GLN
1	B	32	VAL
1	B	105	ASP
1	B	168	GLN
1	B	172	ARG
1	B	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	48	ASN
1	A	64	HIS
1	A	124	ASN
1	A	125	HIS
1	A	149	HIS
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	186	HIS
1	A	218	ASN
1	B	64	HIS
1	B	124	ASN
1	B	125	HIS
1	B	149	HIS
1	B	182	ASN
1	B	186	HIS
1	B	202	HIS
1	B	218	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.