



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7YQP / pdb_00007yqp
Title : Xcc Nicotinamide Phosphoribosyltransferase
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Deposited on : 2022-08-08
Resolution : 2.09 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)	:	2.0
EDS	:	3.0
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

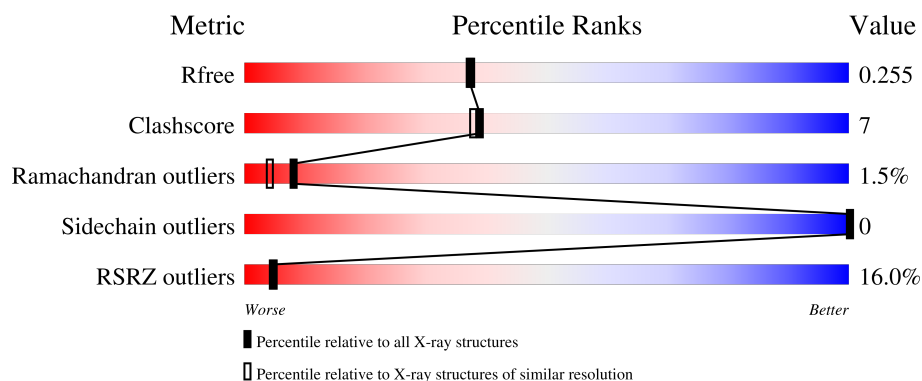
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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))
R_{free}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	482	14% 75% 12% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3330 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 Pre-B cell enhancing factor related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3259	2070	575	607	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A0H2X5R2
A	-12	GLY	-	expression tag	UNP A0A0H2X5R2
A	-11	SER	-	expression tag	UNP A0A0H2X5R2
A	-10	SER	-	expression tag	UNP A0A0H2X5R2
A	-9	HIS	-	expression tag	UNP A0A0H2X5R2
A	-8	HIS	-	expression tag	UNP A0A0H2X5R2
A	-7	HIS	-	expression tag	UNP A0A0H2X5R2
A	-6	HIS	-	expression tag	UNP A0A0H2X5R2
A	-5	HIS	-	expression tag	UNP A0A0H2X5R2
A	-4	HIS	-	expression tag	UNP A0A0H2X5R2
A	-3	SER	-	expression tag	UNP A0A0H2X5R2
A	-2	GLN	-	expression tag	UNP A0A0H2X5R2
A	-1	GLY	-	expression tag	UNP A0A0H2X5R2
A	0	SER	-	expression tag	UNP A0A0H2X5R2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.90Å 115.90Å 160.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.49 – 2.09 54.49 – 2.09	Depositor EDS
% Data completeness (in resolution range)	67.4 (54.49-2.09) 67.3 (54.49-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.218 , 0.253 0.222 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3330	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/3327	0.41	1/4528 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	TYR	CB-CA-C	5.56	120.87	110.70

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	A	3259	0	3219	44	0
2	A	71	0	0	10	0
All	All	3330	0	3219	44	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 (44) 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:265:TYR:HB3	1:A:269:ARG:NH1	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:NH2	1:A:313:ALA:HA	1.95	0.81
1:A:265:TYR:HB3	1:A:269:ARG:HH12	1.46	0.80
1:A:1:MET:HE3	1:A:2:HIS:H	1.47	0.77
1:A:9:LEU:O	2:A:501:HOH:O	2.02	0.77
1:A:280:ARG:HH22	1:A:313:ALA:HA	1.49	0.73
1:A:433:HIS:O	2:A:502:HOH:O	2.07	0.71
1:A:27:ASP:HB3	1:A:386:ARG:HH21	1.57	0.69
1:A:280:ARG:CZ	1:A:313:ALA:O	2.43	0.67
1:A:464:ASP:OD1	2:A:503:HOH:O	2.13	0.66
1:A:19:TRP:N	2:A:508:HOH:O	2.24	0.63
1:A:280:ARG:NH2	1:A:313:ALA:CA	2.61	0.62
1:A:17:SER:HB3	1:A:78:PRO:HD2	1.83	0.60
1:A:393:ASP:HB3	1:A:408:ARG:HB3	1.85	0.59
1:A:387:VAL:O	1:A:390:ALA:N	2.26	0.58
1:A:216:HIS:NE2	1:A:453:GLU:OE2	2.34	0.57
1:A:387:VAL:O	1:A:389:GLY:N	2.38	0.56
1:A:265:TYR:O	1:A:269:ARG:HD3	2.04	0.56
1:A:410:ARG:C	1:A:427:LEU:HD12	2.31	0.56
1:A:279:LEU:O	1:A:281:GLU:N	2.40	0.54
1:A:283:ILE:HD11	1:A:290:VAL:HG21	1.92	0.52
1:A:182:VAL:HG11	1:A:188:ALA:HB2	1.91	0.52
1:A:343:ARG:NE	2:A:504:HOH:O	2.14	0.51
1:A:294:PRO:O	2:A:505:HOH:O	2.20	0.51
1:A:410:ARG:HB3	1:A:427:LEU:HD13	1.93	0.50
1:A:53:LYS:NZ	2:A:509:HOH:O	2.24	0.49
1:A:136:LEU:HD13	1:A:380:LEU:HB2	1.94	0.48
1:A:280:ARG:NH2	1:A:313:ALA:C	2.72	0.48
1:A:291:VAL:HG12	1:A:332:ILE:HG22	1.96	0.47
1:A:343:ARG:NH2	2:A:504:HOH:O	2.45	0.47
1:A:316:HIS:CE1	1:A:324:LYS:HE2	2.48	0.47
1:A:150:GLN:O	2:A:506:HOH:O	2.20	0.47
1:A:31:PHE:CE2	1:A:382:CYS:HB2	2.51	0.46
1:A:333:GLN:HE21	1:A:335:ASP:H	1.62	0.46
1:A:142:VAL:HG11	1:A:378:PHE:HZ	1.81	0.46
1:A:300:VAL:HA	1:A:345:ILE:HG12	1.97	0.45
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.16	0.45
1:A:415:ARG:NH1	1:A:420:GLY:O	2.51	0.44
1:A:293:ARG:HG2	2:A:505:HOH:O	2.18	0.43
1:A:264:SER:HB3	1:A:302:VAL:HG23	2.01	0.42
1:A:415:ARG:HD2	1:A:422:TYR:CZ	2.54	0.42
1:A:333:GLN:HG3	1:A:337:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASP:HB2	1:A:386:ARG:HE	1.86	0.41
1:A:349:ILE:HG13	1:A:350:THR:N	2.36	0.41

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	410/482 (85%)	384 (94%)	20 (5%)	6 (2%)	8 4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ARG
1	A	433	HIS
1	A	163	SER
1	A	430	VAL
1	A	388	ASP
1	A	264	SER

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	339/391 (87%)	339 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	GLN

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](#)

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

6.1 Protein, DNA and RNA chains

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	420/482 (87%)	0.96	67 (15%) 5 5	33, 52, 94, 141	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	THR	8.5
1	A	265	TYR	7.7
1	A	283	ILE	7.6
1	A	271	ILE	7.5
1	A	395	TYR	7.1
1	A	394	VAL	5.9
1	A	387	VAL	5.5
1	A	270	ALA	5.3
1	A	290	VAL	5.0
1	A	280	ARG	4.8
1	A	431	ALA	4.6
1	A	256	ALA	4.4
1	A	278	THR	4.4
1	A	279	LEU	4.1
1	A	258	VAL	3.9
1	A	388	ASP	3.9
1	A	257	ILE	3.8
1	A	430	VAL	3.8
1	A	293	ARG	3.8
1	A	277	THR	3.7
1	A	284	ILE	3.6
1	A	406	SER	3.5
1	A	285	ALA	3.5
1	A	292	ILE	3.4
1	A	267	ILE	3.4
1	A	294	PRO	3.4
1	A	434	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	433	HIS	3.3
1	A	295	ASP	3.2
1	A	1	MET	3.2
1	A	226	ALA	3.2
1	A	435	GLY	3.2
1	A	23	PRO	3.1
1	A	296	SER	3.1
1	A	36	ARG	3.0
1	A	291	VAL	3.0
1	A	428	ASP	3.0
1	A	259	ALA	2.9
1	A	335	ASP	2.8
1	A	390	ALA	2.7
1	A	263	ASP	2.7
1	A	22	TYR	2.7
1	A	260	VAL	2.7
1	A	281	GLU	2.6
1	A	328	HIS	2.6
1	A	219	VAL	2.6
1	A	329	VAL	2.6
1	A	342	LEU	2.5
1	A	389	GLY	2.4
1	A	393	ASP	2.4
1	A	314	PHE	2.4
1	A	27	ASP	2.4
1	A	269	ARG	2.4
1	A	261	VAL	2.3
1	A	180	ARG	2.3
1	A	162	THR	2.3
1	A	2	HIS	2.2
1	A	449	GLN	2.2
1	A	408	ARG	2.2
1	A	85	ARG	2.2
1	A	348	ARG	2.1
1	A	429	GLU	2.1
1	A	17	SER	2.1
1	A	374	ASP	2.1
1	A	468	LEU	2.1
1	A	313	ALA	2.0
1	A	418	ALA	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.