



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:42 PM UTC

PDB ID : 1PGS / pdb_00001pgs
Title : THE THREE-DIMENSIONAL STRUCTURE OF PNGASE F, A GLYCOSYLASPARAGINASE FROM FLAVOBACTERIUM MENINGOSEPTICUM
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Deposited on : 1994-10-06
Resolution : 1.80 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

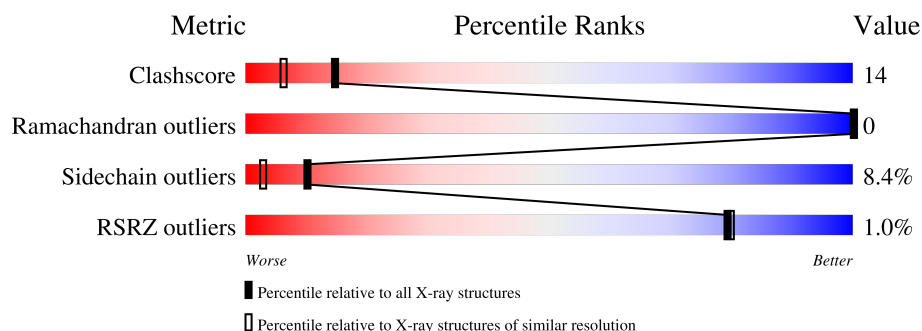
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	314	77% 17% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2667 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 PEPTIDE-N(4)-(N-ACETYL-BETA-D-GLUCOSAMINYL) ASPARAGINE AMIDASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	4	0	0
			2437	1553	408	468	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	THR	ALA	conflict	UNP P21163

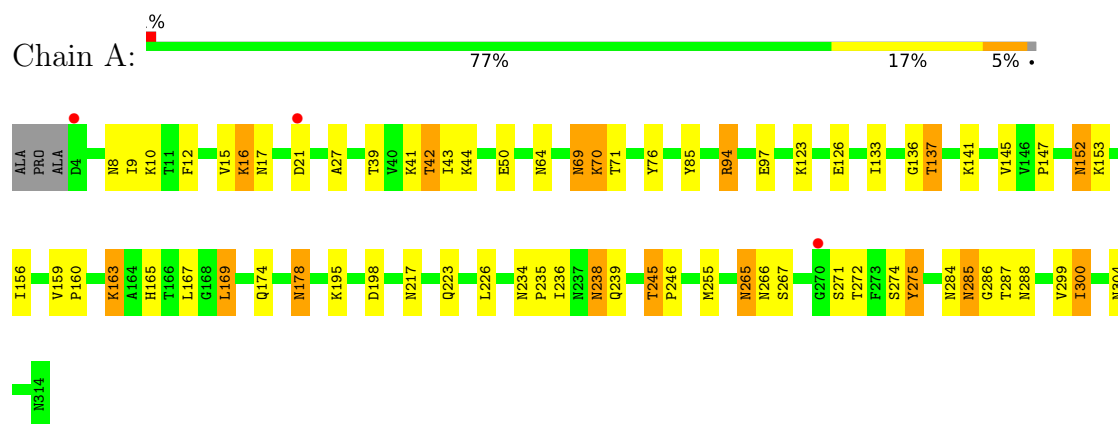
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: PEPTIDE-N(4)-(N-ACETYL-BETA-D-GLUCOSAMINYL)ASPARAGINE AMIDASE F



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.07Å 85.14Å 48.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.80) 83.7 (20.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.79Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.168 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2667	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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	1.31	5/2504 (0.2%)	1.22	4/3413 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	PHE	CA-C	-6.16	1.44	1.52
1	A	223	GLN	CA-C	-6.13	1.45	1.52
1	A	126	GLU	CD-OE1	6.04	1.36	1.25
1	A	245	THR	C-N	-6.00	1.25	1.33
1	A	42	THR	CA-C	-5.15	1.46	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	THR	O-C-N	-9.23	110.70	121.32
1	A	21	ASP	N-CA-CB	5.49	121.00	111.40
1	A	198	ASP	N-CA-C	-5.42	103.54	110.53
1	A	159	VAL	CB-CA-C	-5.02	106.27	110.94

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	2437	0	2342	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	230	0	0	4	0
All	All	2667	0	2342	66	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 14.

All (66) 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:ASN:HD22	1:A:267:SER:H	1.11	0.98
1:A:85:TYR:H	1:A:239:GLN:HE21	1.15	0.94
1:A:238:ASN:HD22	1:A:238:ASN:H	1.05	0.93
1:A:284:ASN:ND2	1:A:286:GLY:H	1.71	0.88
1:A:178:ASN:HD22	1:A:178:ASN:H	1.16	0.87
1:A:265:ASN:ND2	1:A:267:SER:H	1.72	0.87
1:A:85:TYR:H	1:A:239:GLN:NE2	1.79	0.81
1:A:238:ASN:HD22	1:A:238:ASN:N	1.79	0.78
1:A:165:HIS:HD2	1:A:167:LEU:H	1.33	0.76
1:A:284:ASN:HD22	1:A:286:GLY:H	1.33	0.76
1:A:69:ASN:HD22	1:A:71:THR:H	1.38	0.71
1:A:238:ASN:H	1:A:238:ASN:ND2	1.85	0.70
1:A:69:ASN:ND2	1:A:71:THR:H	1.88	0.69
1:A:265:ASN:HD22	1:A:267:SER:N	1.88	0.66
1:A:44:LYS:HE3	1:A:97:GLU:OE2	1.95	0.65
1:A:178:ASN:HD22	1:A:178:ASN:N	1.91	0.65
1:A:300:ILE:HD13	1:A:300:ILE:N	2.13	0.64
1:A:69:ASN:HD22	1:A:69:ASN:C	2.05	0.64
1:A:285:ASN:ND2	1:A:287:THR:H	1.99	0.60
1:A:285:ASN:HD22	1:A:285:ASN:C	2.09	0.60
1:A:299:VAL:C	1:A:300:ILE:HD13	2.26	0.59
1:A:141:LYS:H	1:A:304:ASN:ND2	2.00	0.59
1:A:284:ASN:HD22	1:A:285:ASN:N	2.01	0.59
1:A:284:ASN:HD22	1:A:284:ASN:C	2.10	0.58
1:A:285:ASN:HD22	1:A:287:THR:H	1.51	0.58
1:A:145:VAL:HG23	1:A:300:ILE:HD12	1.86	0.57
1:A:169:LEU:HD23	2:A:496:HOH:O	2.04	0.57
1:A:152:ASN:HD22	1:A:152:ASN:H	1.54	0.56
1:A:234:ASN:ND2	1:A:236:ILE:H	2.05	0.55
1:A:15:VAL:HG21	1:A:27:ALA:CB	2.39	0.53
1:A:41:LYS:HE3	1:A:136:GLY:HA3	1.89	0.53
1:A:152:ASN:HD22	1:A:152:ASN:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HD12	1:A:133:ILE:CD1	2.41	0.51
1:A:76:TYR:CZ	1:A:147:PRO:HD3	2.45	0.51
1:A:163:LYS:HE2	2:A:454:HOH:O	2.10	0.50
1:A:178:ASN:H	1:A:178:ASN:ND2	1.95	0.50
1:A:195:LYS:HD2	1:A:288:ASN:HB2	1.95	0.48
1:A:15:VAL:HG21	1:A:27:ALA:HB1	1.95	0.48
1:A:284:ASN:ND2	1:A:286:GLY:N	2.52	0.48
1:A:9:ILE:HD12	1:A:133:ILE:HD11	1.96	0.46
1:A:69:ASN:HD22	1:A:70:LYS:N	2.14	0.46
1:A:9:ILE:CD1	1:A:133:ILE:HD12	2.46	0.46
1:A:41:LYS:HE2	1:A:137:THR:H	1.80	0.46
1:A:165:HIS:HD2	1:A:167:LEU:N	2.09	0.46
1:A:300:ILE:N	1:A:300:ILE:CD1	2.79	0.45
1:A:69:ASN:HD21	1:A:71:THR:HB	1.82	0.45
1:A:42:THR:HG22	1:A:43:ILE:N	2.31	0.44
1:A:174:GLN:HG3	1:A:272:THR:OG1	2.18	0.44
1:A:234:ASN:HD22	1:A:235:PRO:HD2	1.82	0.44
1:A:8:ASN:OD1	1:A:10:LYS:HE2	2.18	0.43
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.80	0.43
1:A:94:ARG:HD3	2:A:660:HOH:O	2.18	0.43
1:A:234:ASN:HD22	1:A:236:ILE:H	1.67	0.43
1:A:266:ASN:HD22	1:A:266:ASN:HA	1.65	0.43
1:A:178:ASN:N	1:A:178:ASN:ND2	2.60	0.43
1:A:160:PRO:HG2	1:A:165:HIS:HB3	2.01	0.42
1:A:275:TYR:CD1	1:A:275:TYR:C	2.97	0.42
1:A:69:ASN:HD22	1:A:71:THR:N	2.12	0.42
1:A:245:THR:N	1:A:246:PRO:CD	2.82	0.42
1:A:265:ASN:HD22	1:A:265:ASN:C	2.28	0.42
1:A:226:LEU:N	1:A:226:LEU:HD12	2.35	0.41
1:A:16:LYS:HG3	1:A:17:ASN:N	2.34	0.41
1:A:285:ASN:ND2	1:A:285:ASN:C	2.78	0.41
1:A:165:HIS:HE1	2:A:494:HOH:O	2.04	0.40
1:A:217:ASN:ND2	1:A:274:SER:H	2.20	0.40
1:A:285:ASN:HD22	1:A:286:GLY:N	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	309/314 (98%)	298 (96%)	11 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	263/266 (99%)	241 (92%)	22 (8%)	10	3

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	39	THR
1	A	50	GLU
1	A	64	ASN
1	A	69	ASN
1	A	70	LYS
1	A	94	ARG
1	A	123	LYS
1	A	137	THR
1	A	152	ASN
1	A	153	LYS
1	A	156	ILE
1	A	163	LYS

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Mol	Chain	Res	Type
1	A	169	LEU
1	A	178	ASN
1	A	238	ASN
1	A	255	MET
1	A	265	ASN
1	A	271	SER
1	A	275	TYR
1	A	285	ASN
1	A	300	ILE

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	17	ASN
1	A	25	GLN
1	A	69	ASN
1	A	152	ASN
1	A	165	HIS
1	A	172	ASN
1	A	178	ASN
1	A	217	ASN
1	A	220	ASN
1	A	234	ASN
1	A	238	ASN
1	A	239	GLN
1	A	265	ASN
1	A	266	ASN
1	A	284	ASN
1	A	285	ASN
1	A	304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	311/314 (99%)	-0.52	3 (0%) 79 80	7, 17, 39, 76	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASP	2.6
1	A	21	ASP	2.4
1	A	270	GLY	2.4

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.