



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:16 AM UTC

PDB ID : 8BRY / pdb_00008bry
Title : Room-temperature structure of Pedobacter heparinus N-acetylglucosamine 2-epimerase at atmospheric pressure
Authors : Lieske, J.; Saouane, S.; Assmann, M.; Zaun, H.; Kuballa, J.; Meents, A.
Deposited on : 2022-11-24
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
Mogul	:	2022.3.0, CSD as543be (2022)
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

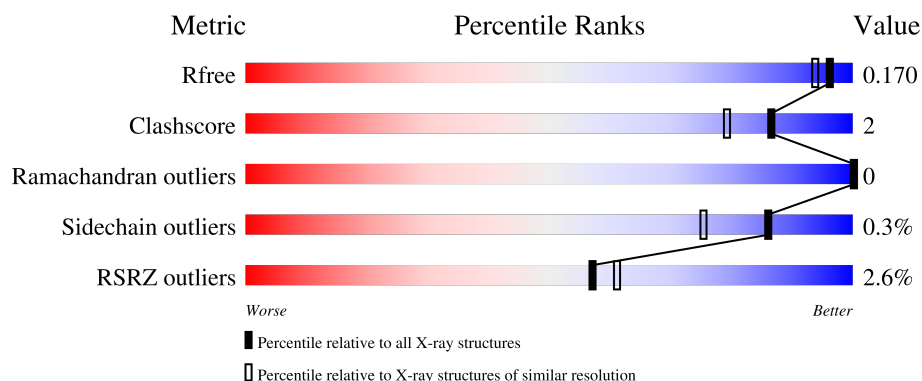
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

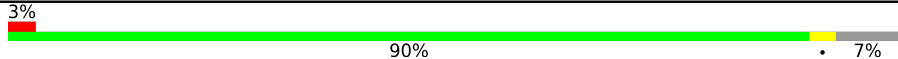
The reported resolution of this entry is 1.50 Å.

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))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 $\leq 5\%$. 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	418	
1	B	418	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13517 atoms, of which 6356 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 N-acetylglucosamine 2-epimerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	22	0
			6645	2178	3241	583	627	16			
1	B	386	Total	C	H	N	O	S	0	9	0
			6388	2101	3115	557	599	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP C6Y403
A	-13	GLY	-	expression tag	UNP C6Y403
A	-12	SER	-	expression tag	UNP C6Y403
A	-11	SER	-	expression tag	UNP C6Y403
A	-10	HIS	-	expression tag	UNP C6Y403
A	-9	HIS	-	expression tag	UNP C6Y403
A	-8	HIS	-	expression tag	UNP C6Y403
A	-7	HIS	-	expression tag	UNP C6Y403
A	-6	HIS	-	expression tag	UNP C6Y403
A	-5	HIS	-	expression tag	UNP C6Y403
A	-4	SER	-	expression tag	UNP C6Y403
A	-3	GLN	-	expression tag	UNP C6Y403
A	-2	ASP	-	expression tag	UNP C6Y403
A	-1	PRO	-	expression tag	UNP C6Y403
A	0	ASN	-	expression tag	UNP C6Y403
A	1	SER	-	expression tag	UNP C6Y403
B	-14	MET	-	initiating methionine	UNP C6Y403
B	-13	GLY	-	expression tag	UNP C6Y403
B	-12	SER	-	expression tag	UNP C6Y403
B	-11	SER	-	expression tag	UNP C6Y403
B	-10	HIS	-	expression tag	UNP C6Y403
B	-9	HIS	-	expression tag	UNP C6Y403
B	-8	HIS	-	expression tag	UNP C6Y403
B	-7	HIS	-	expression tag	UNP C6Y403
B	-6	HIS	-	expression tag	UNP C6Y403

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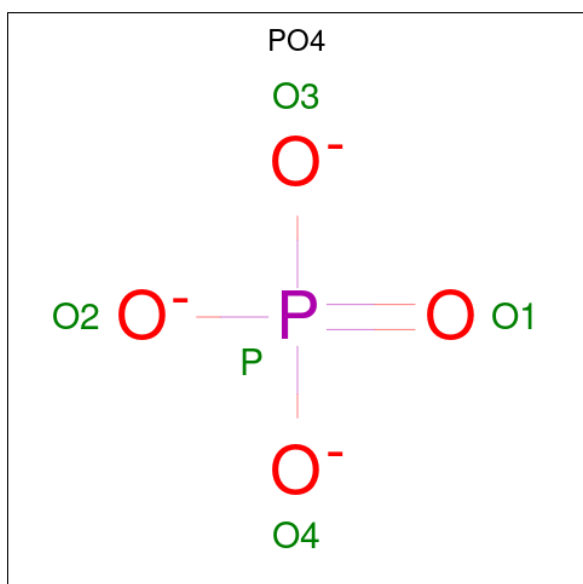
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP C6Y403
B	-4	SER	-	expression tag	UNP C6Y403
B	-3	GLN	-	expression tag	UNP C6Y403
B	-2	ASP	-	expression tag	UNP C6Y403
B	-1	PRO	-	expression tag	UNP C6Y403
B	0	ASN	-	expression tag	UNP C6Y403
B	1	SER	-	expression tag	UNP C6Y403

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

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

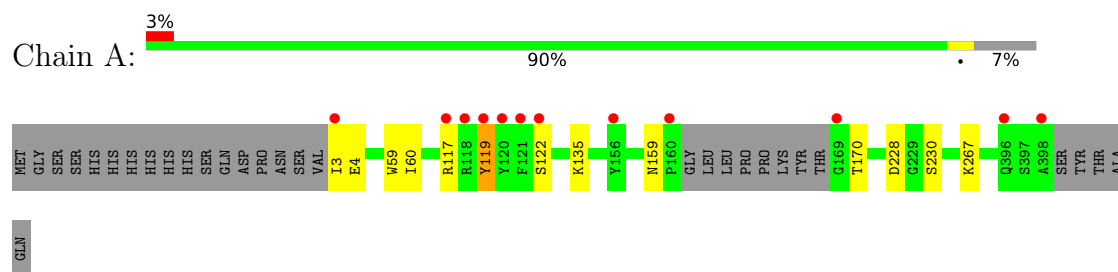
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	262	Total 262	O 262	0	0
4	B	210	Total 210	O 210	0	0

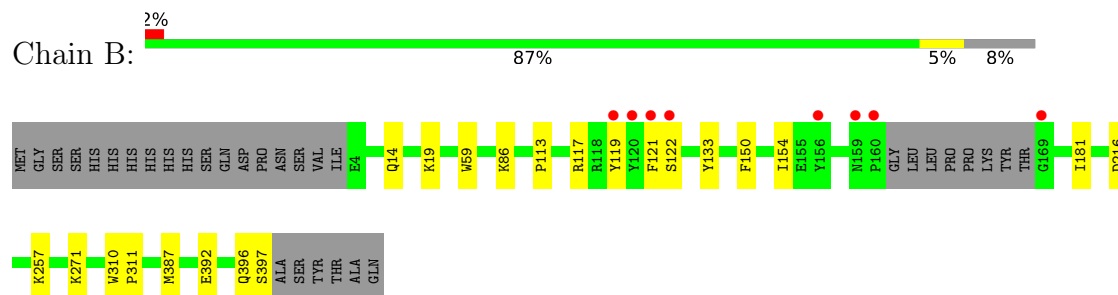
3 Residue-property plots [i](#)

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 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: N-acetylglucosamine 2-epimerase



- Molecule 1: N-acetylglucosamine 2-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.95Å 94.63Å 82.47Å 90.00° 102.53° 90.00°	Depositor
Resolution (Å)	17.62 – 1.50 17.62 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (17.62-1.50) 87.1 (17.62-1.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.06 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.18-3855_9999	Depositor
R, R_{free}	0.154 , 0.164 0.159 , 0.170	Depositor DCC
R_{free} test set	1306 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13517	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.40	0/3500	0.61	0/4739
1	B	0.37	0/3369	0.61	0/4563
All	All	0.39	0/6869	0.61	0/9302

There are no bond length outliers.

There are no bond angle outliers.

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	3404	3241	3220	15	0
1	B	3273	3115	3103	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	262	0	0	3	0
4	B	210	0	0	0	0
All	All	7161	6356	6323	28	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 2.

All (28) 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:59:TRP:CD1	1:A:122:SER:HG	1.89	0.90
1:A:59:TRP:HD1	1:A:122:SER:HG	1.33	0.77
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.51	0.75
1:B:59:TRP:CD1	1:B:122:SER:HG	2.10	0.69
1:A:117:ARG:HD3	1:A:119:TYR:CZ	2.31	0.64
1:A:170:THR:HG23	1:B:113:PRO:O	1.99	0.63
1:B:121:PHE:HE1	1:B:181:ILE:HG21	1.66	0.59
1:B:121:PHE:CE1	1:B:181:ILE:HG21	2.38	0.58
1:A:60[B]:ILE:HD12	4:A:691:HOH:O	2.05	0.56
1:A:117:ARG:HD3	1:A:119:TYR:CE1	2.42	0.54
1:B:86:LYS:HD2	1:B:133:TYR:OH	2.10	0.52
1:B:216:ASP:OD1	1:B:271[A]:LYS:HE2	2.11	0.50
1:A:117:ARG:HH11	1:A:117:ARG:CG	2.22	0.47
1:B:396:GLN:HA	1:B:396:GLN:OE1	2.14	0.47
1:A:119:TYR:N	1:A:119:TYR:CD2	2.82	0.47
1:B:19:LYS:HE2	1:B:19:LYS:HB3	1.85	0.46
1:A:159:ASN:ND2	1:A:159:ASN:O	2.51	0.44
1:A:135[B]:LYS:CE	4:A:738:HOH:O	2.66	0.44
1:B:14:GLN:NE2	1:B:387:MET:HG3	2.34	0.43
1:B:310:TRP:CG	1:B:311:PRO:HD3	2.54	0.42
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.78	0.42
1:A:228:ASP:OD1	1:A:230:SER:OG	2.30	0.42
1:B:257:LYS:NZ	1:B:392:GLU:OE2	2.45	0.42
1:A:135[B]:LYS:HE3	4:A:738:HOH:O	2.21	0.41
1:A:3:ILE:CG2	1:A:4:GLU:N	2.83	0.41
1:B:117:ARG:NE	1:B:119:TYR:CE2	2.89	0.41
1:B:59:TRP:NE1	1:B:122:SER:HG	2.17	0.40
1:B:150:PHE:CE2	1:B:154:ILE:HD11	2.56	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	406/418 (97%)	397 (98%)	9 (2%)	0	100	100
1	B	391/418 (94%)	382 (98%)	9 (2%)	0	100	100
All	All	797/836 (95%)	779 (98%)	18 (2%)	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	352/357 (99%)	351 (100%)	1 (0%)	86	75
1	B	338/357 (95%)	337 (100%)	1 (0%)	86	75
All	All	690/714 (97%)	688 (100%)	2 (0%)	86	75

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	TYR
1	B	397	SER

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

Mol	Chain	Res	Type
1	A	159	ASN
1	A	296	ASN
1	B	14	GLN
1	B	79	GLN
1	B	102	GLN
1	B	261	ASN
1	B	285	HIS
1	B	296	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	PO4	B	502	-	4,4,4	0.88	0	6,6,6	0.45	0
3	PO4	A	502	-	4,4,4	0.85	0	6,6,6	0.74	0

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

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	388/418 (92%)	-0.28	12 (3%) 51 55	10, 23, 54, 112	22 (5%)
1	B	386/418 (92%)	-0.11	8 (2%) 63 67	13, 29, 63, 105	9 (2%)
All	All	774/836 (92%)	-0.20	20 (2%) 57 61	10, 25, 62, 112	31 (4%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	TYR	6.5
1	B	119	TYR	5.2
1	A	119	TYR	4.7
1	B	121	PHE	4.7
1	A	160	PRO	4.5
1	A	121	PHE	4.1
1	B	159	ASN	4.0
1	A	3	ILE	3.7
1	B	160	PRO	3.6
1	A	169	GLY	3.6
1	B	120	TYR	3.4
1	A	398	ALA	3.3
1	B	169	GLY	2.6
1	A	156	TYR	2.5
1	A	396	GLN	2.4
1	B	122	SER	2.3
1	A	118	ARG	2.2
1	B	156	TYR	2.2
1	A	122	SER	2.1
1	A	117	ARG	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	502	5/5	0.84	0.20	31,37,52,52	5
3	PO4	A	502	5/5	0.89	0.12	34,47,69,81	0
2	CL	B	501	1/1	0.99	0.05	17,17,17,17	0
2	CL	A	501	1/1	1.00	0.02	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.