

wwPDB X-ray Structure Validation Summary Report (i)

Aug 19, 2023 – 10:22 PM EDT

PDB ID : 2HLH

Title : Crystal structure of fucosyltransferase NodZ from Bradyrhizobium Authors : Brzezinski, K.; Stepkowski, T.; Panjikar, S.; Bujacz, G.; Jaskolski, M.

Deposited on : 2006-07-07

Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

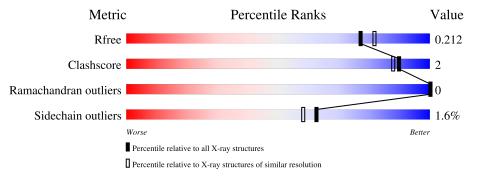
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 <=5%

\mathbf{M}	ol	Chain	Length	Quality of chain		
1		A	330	80%	6% •	13%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2644 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.

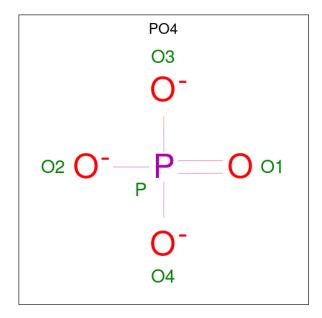
• Molecule 1 is a protein called Nodulation fucosyltransferase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	286	Total	С	N	О	S	80	10	0
1	Λ	200	2344	1490	417	421	16	00	10	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	HIS	-	expression tag	UNP Q9AQ17
A	326	HIS	-	expression tag	UNP Q9AQ17
A	327	HIS	-	expression tag	UNP Q9AQ17
A	328	HIS	-	expression tag	UNP Q9AQ17
A	329	HIS	-	expression tag	UNP Q9AQ17
A	330	HIS	-	expression tag	UNP Q9AQ17

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	Δ	1	Total O P	0	0	
	A	1	5 4 1	0		
2	Λ	1	Total O P	0	0	
	A	1	5 4 1	0		
2	Λ	1	Total O P	0	0	
	Α	1	5 4 1	0	0	
2	Λ	1	Total O P	0	0	
2	A	1	5 4 1		0	

• Molecule 3 is water.

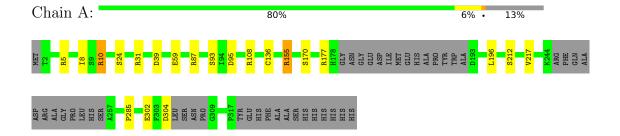
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	274	Total O 280 280	0	6



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.

• Molecule 1: Nodulation fucosyltransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	130.10Å 130.10Å 83.30Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 - 1.95	Depositor
Resolution (A)	14.92 - 1.95	EDS
% Data completeness	99.9 (15.00-1.95)	Depositor
(in resolution range)	99.9 (14.92-1.95)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	8.76 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.161 , 0.206	Depositor
R, R_{free}	0.174 , 0.212	DCC
R_{free} test set	1085 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 46.3	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2644	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	Boı	nd lengths	Bo	nd angles
Moi Chain RM		RMSZ	$2MSZ \mid \# Z > 5$		# Z > 5
1	A	0.86	1/2446 (0.0%)	0.89	8/3309 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	93	SER	CB-OG	-5.45	1.35	1.42

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	5	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	155	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	95	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	108	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	31	ARG	NE-CZ-NH2	-5.55	117.52	120.30

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	2344	0	2296	8	0
2	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	280	0	0	1	0
All	All	2644	0	2296	8	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.

The worst 5 of 8 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:10[B]:ARG:NH2	3:A:433:HOH:O	2.04	0.78
1:A:10[B]:ARG:HD2	1:A:39:ASP:OD2	2.04	0.57
1:A:177:ARG:NH2	2:A:334:PO4:O3	2.38	0.55
1:A:59:GLU:OE2	1:A:155:ARG:NH2	2.48	0.46
1:A:24:SER:HA	1:A:136:CYS:HB3	1.99	0.44

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	288/330 (87%)	284 (99%)	4 (1%)	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	Analysed Rotameric		Percentiles	
1	A	258/283 (91%)	253 (98%)	5 (2%)	57 50	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10[A]	ARG
1	A	10[B]	ARG
1	A	196	LEU
1	A	212	SER
1	A	304	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	169	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	В	ond leng	gths	В	ond ang	gles
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	PO4	A	333	-	4,4,4	0.67	0	6,6,6	1.07	1 (16%)
2	PO4	A	334	-	4,4,4	1.15	0	6,6,6	1.10	0
2	PO4	A	331	-	4,4,4	1.38	1 (25%)	6,6,6	1.25	1 (16%)
2	PO4	A	332	-	4,4,4	1.24	1 (25%)	6,6,6	1.05	0

All (2) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	A	331	PO4	P-O2	2.10	1.60	1.54
2	A	332	PO4	P-O4	-2.02	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	A	331	PO4	O3-P-O1	-2.44	101.96	110.89
2	A	333	PO4	O3-P-O1	-2.02	103.49	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	334	PO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

