WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 07:55 PM EST

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PDB ID	:	2OCX
Title	:	Crystal structure of Se-Met fucosyltransferase NodZ from Bradyrhizobium
Authors	:	Brzezinski, K.; Stepkowski, T.; Panjikar, S.; Bujacz, G.; Jaskolski, M.
Deposited on	:	2006-12-21
Resolution	:	2.20 Å(reported)

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 2.20 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.
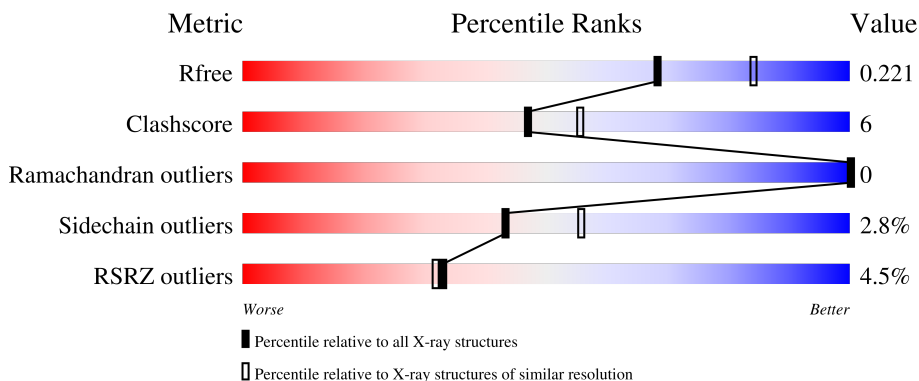
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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	330	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRS	A	334	-	X	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 2614 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 NodZ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	292	Total 2410	C 1533	N 430	O 429	S 10	Se 8	63	12	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9AQ17
A	133	MSE	MET	modified residue	UNP Q9AQ17
A	185	MSE	MET	modified residue	UNP Q9AQ17
A	203	MSE	MET	modified residue	UNP Q9AQ17
A	259	MSE	MET	modified residue	UNP Q9AQ17
A	271	MSE	MET	modified residue	UNP Q9AQ17
A	313	MSE	MET	modified residue	UNP Q9AQ17
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: O_4P).

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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	4	1	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	180	181	181	0	1

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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 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: Nodulation fucosyltransferase NodZ
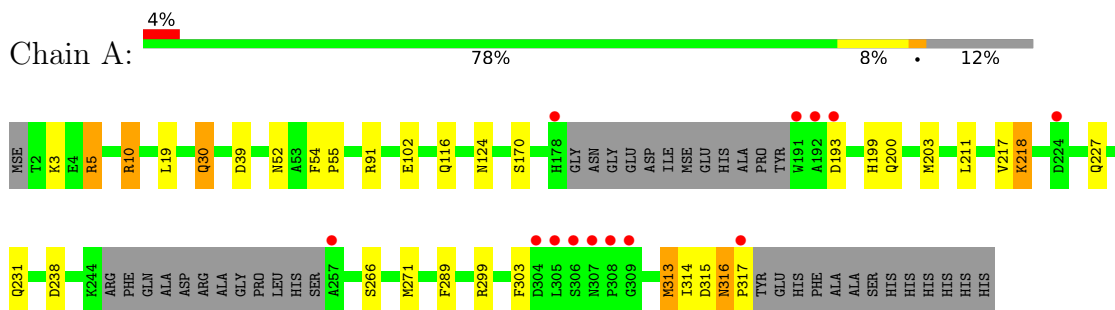
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.20Å　124.20Å　96.20Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	19.96　–　2.20 14.92　–　2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.96-2.20) 99.7 (14.92-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184　,　0.217 0.194　,　0.221	Depositor DCC
R_{free} test set	1062 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.7	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2614	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, 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	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.77	0/2516	0.82	5/3399 (0.1%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	A	5	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	10	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	315	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	10	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	ASN	Peptide

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	2410	0	2359	25	0
2	A	15	0	0	1	0
3	A	8	0	12	5	0
4	A	181	0	0	4	0
All	All	2614	0	2371	29	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 6.

All (29) 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:299:ARG:HB3	1:A:313[A]:MSE:HE3	1.61	0.82
3:A:334:TRS:C2	4:A:474:HOH:O	2.43	0.67
1:A:200:GLN:HG2	1:A:203[A]:MSE:CE	2.26	0.65
1:A:200:GLN:HG2	1:A:203[A]:MSE:HE2	1.81	0.62
1:A:218:LYS:HG3	1:A:238:ASP:HB3	1.82	0.62
1:A:299:ARG:CB	1:A:313[A]:MSE:HE3	2.33	0.59
1:A:316:ASN:OD1	1:A:317:PRO:HA	2.03	0.59
1:A:30[A]:GLN:NE2	4:A:371:HOH:O	2.36	0.58
1:A:227:GLN:O	1:A:231[A]:GLN:HG3	2.10	0.52
1:A:316:ASN:HA	1:A:317:PRO:C	2.31	0.51
1:A:54:PHE:HB3	1:A:55:PRO:HD3	1.92	0.51
1:A:271[A]:MSE:HG3	1:A:289:PHE:O	2.12	0.49
1:A:10:ARG:HD2	1:A:39:ASP:OD2	2.14	0.48
1:A:91[A]:ARG:NH2	2:A:331:PO4:O3	2.49	0.46
1:A:19:LEU:HD12	1:A:271[A]:MSE:HE1	1.97	0.46
1:A:199:HIS:O	1:A:203[A]:MSE:HG3	2.17	0.45
3:A:334:TRS:H22	4:A:474:HOH:O	2.13	0.45
3:A:334:TRS:H21	4:A:474:HOH:O	2.08	0.45
1:A:211:LEU:HD11	1:A:313[B]:MSE:SE	2.67	0.45
1:A:5:ARG:HD2	1:A:124:ASN:HD22	1.83	0.44
1:A:170:SER:O	1:A:217:VAL:HA	2.17	0.44
1:A:227:GLN:O	1:A:231[B]:GLN:HG3	2.18	0.43
1:A:313[A]:MSE:HE2	1:A:314:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:O	1:A:55:PRO:HD2	2.18	0.43
1:A:3:LYS:NZ	3:A:334:TRS:O2	2.45	0.42
3:A:334:TRS:O2	3:A:334:TRS:O3	2.24	0.42
1:A:271[B]:MSE:HG3	1:A:289:PHE:CE1	2.53	0.42
1:A:203[A]:MSE:HE3	1:A:303:PHE:CZ	2.56	0.41
1:A:299:ARG:HG2	1:A:313[A]:MSE:HE1	2.03	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	298/330 (90%)	294 (99%)	4 (1%)	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	265/276 (96%)	256 (97%)	9 (3%)	37	47

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30[A]	GLN
1	A	30[B]	GLN
1	A	102	GLU
1	A	116	GLN
1	A	193	ASP
1	A	218	LYS
1	A	266	SER
1	A	313[A]	MSE
1	A	313[B]	MSE

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	124	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	333	-	4,4,4	0.78	0	6,6,6	0.55	0
3	TRS	A	334	-	7,7,7	0.41	0	9,9,9	1.18	1 (11%)
2	PO4	A	332	-	4,4,4	0.80	0	6,6,6	1.01	0
2	PO4	A	331	-	4,4,4	0.81	0	6,6,6	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	A	334	-	-	9/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	334	TRS	O1-C1-C	2.63	119.33	111.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	334	TRS	C3-C-C1-O1
3	A	334	TRS	C3-C-C2-O2
3	A	334	TRS	N-C-C2-O2
3	A	334	TRS	C2-C-C1-O1
3	A	334	TRS	C2-C-C3-O3
3	A	334	TRS	N-C-C1-O1
3	A	334	TRS	C1-C-C2-O2
3	A	334	TRS	N-C-C3-O3
3	A	334	TRS	C1-C-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	334	TRS	5	0
2	A	331	PO4	1	0

5.7 Other polymers ⓘ

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	287/330 (86%)	-0.13	13 (4%)	33	32	26, 35, 48, 56	14 (4%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	PRO	5.3
1	A	192	ALA	5.0
1	A	306	SER	4.2
1	A	305	LEU	4.1
1	A	191	TRP	3.8
1	A	307	ASN	3.5
1	A	304	ASP	3.5
1	A	308	PRO	3.3
1	A	178	HIS	3.2
1	A	193	ASP	2.9
1	A	224	ASP	2.5
1	A	309	GLY	2.4
1	A	257	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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(Å^2)	Q<0.9
2	PO4	A	331	5/5	0.73	0.34	31,53,59,60	5
3	TRS	A	334	8/8	0.83	0.32	55,57,59,59	0
2	PO4	A	332	5/5	0.92	0.27	36,48,58,63	5
2	PO4	A	333	5/5	0.99	0.30	41,48,55,58	0

6.5   Other polymers ⓘ

There are no such residues in this entry.