



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:49 pm GMT

PDB ID : 2C25
Title : 1.8A Crystal Structure of Psathyrella velutina lectin in complex with N-acetylneuraminic acid
Authors : Cioci, G.; Mitchell, E.P.; Chazalet, V.; Gautier, C.; Oscarson, S.; Debray, H.; Perez, S.; Imberty, A.
Deposited on : 2005-09-26
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

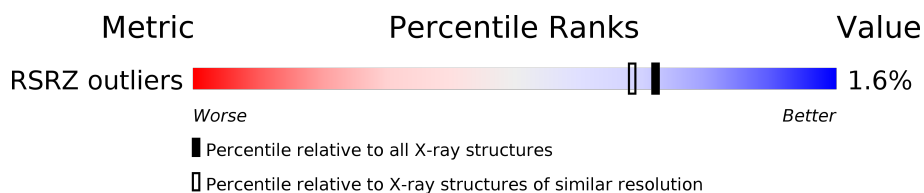
1 Overall quality at a glance

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))
RSRZ outliers	108989	5157 (1.80-1.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6661 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.

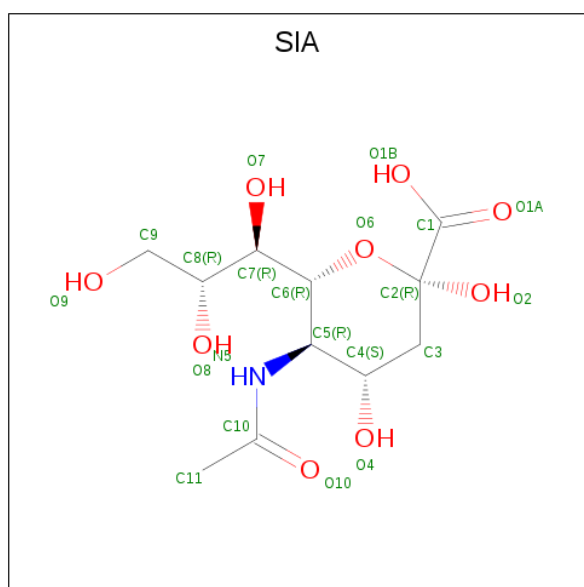
- Molecule 1 is a protein called PSATHYRELLA VELUTINA LECTIN PVL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	3	0
			3046	1934	546	557	9			
1	B	401	Total	C	N	O	S	0	1	0
			3041	1929	546	557	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

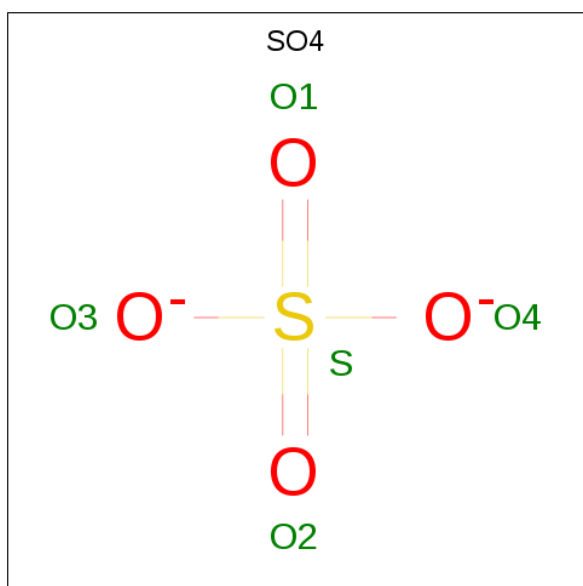
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is O-SIALIC ACID (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	267	Total	O	0	0
			267	267		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	180	Total 180	O 180	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.73Å 144.40Å 52.60Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	72.17 – 1.80 24.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.17-1.80) 99.8 (24.68-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.231 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for l,k,-h 0.047 for h,-k,-l 0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6661	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

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4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	401/401 (100%)	-0.22	4 (0%) 82 80	12, 19, 28, 39	0
1	B	401/401 (100%)	0.15	9 (2%) 62 57	15, 27, 39, 45	0
All	All	802/802 (100%)	-0.04	13 (1%) 72 68	12, 22, 36, 45	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	SER	8.0
1	A	2	VAL	4.5
1	A	1	SER	4.2
1	B	2	VAL	4.1
1	B	401	LEU	3.8
1	A	401	LEU	3.4
1	B	273	VAL	2.6
1	B	335	ASP	2.4
1	A	196	ILE	2.2
1	B	278	ARG	2.1
1	B	324	ASP	2.1
1	B	274	ASN	2.1
1	B	276	GLY	2.1

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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(Å ²)	Q<0.9
3	SIA	A	602	21/21	0.74	0.30	35,46,51,51	0
3	SIA	B	601	21/21	0.78	0.17	35,41,47,52	0
3	SIA	B	600	21/21	0.79	0.28	29,41,47,49	0
3	SIA	A	601	21/21	0.82	0.20	22,34,38,44	0
3	SIA	A	600	21/21	0.82	0.18	26,33,42,50	0
4	SO4	B	700	5/5	0.93	0.14	48,48,50,51	0
4	SO4	A	701	5/5	0.96	0.14	35,36,37,37	0
4	SO4	A	702	5/5	0.97	0.17	31,32,36,37	0
4	SO4	A	700	5/5	0.99	0.07	23,24,26,28	0
2	CA	A	500	1/1	1.00	0.05	16,16,16,16	0
2	CA	B	500	1/1	1.00	0.04	17,17,17,17	0

5.5 Other polymers [i](#)

There are no such residues in this entry.