



wwPDB X-ray Structure Validation Summary Report

Dec 14, 2023 – 04:57 am GMT

PDB ID : 3ZYB
Title : CRYSTAL STRUCTURE OF PA-IL LECTIN COMPLEXED WITH GALAG0 AT 2.3 Å RESOLUTION
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Deposited on : 2011-08-19
Resolution : 2.29 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  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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

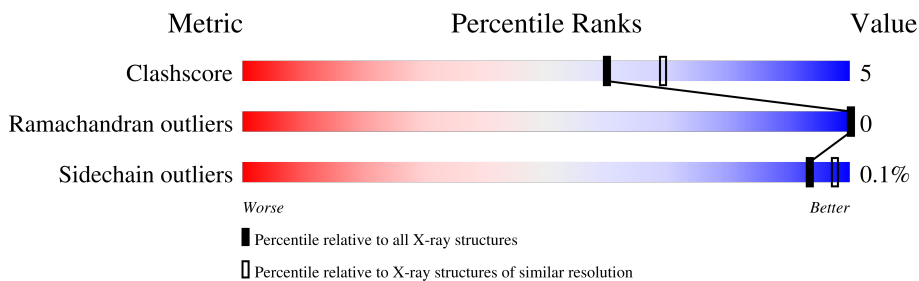
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)




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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	122	96% ..
1	B	122	86% 13% .
1	C	122	88% 11% .
1	D	122	91% 8% .
1	E	122	90% 9% .
1	F	122	84% 15% .
1	G	122	89% 11% .
1	H	122	88% 11% .

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Mol	Chain	Length	Quality of chain
2	I	4	 75% 25%
2	J	4	 50% 50%
2	N	4	 75% 25%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8394 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 PA-I galactophilic lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	121	901	567	156	175	3	0	0	0
1	B	121	901	567	156	175	3	0	0	0
1	C	121	901	567	156	175	3	0	0	0
1	D	121	901	567	156	175	3	0	0	0
1	E	121	901	567	156	175	3	0	0	0
1	F	121	901	567	156	175	3	0	0	0
1	G	121	901	567	156	175	3	0	0	0
1	H	121	901	567	156	175	3	0	0	0

- Molecule 2 is a protein called GALA-LYS-PRO-LEUNH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	4	25	17	5	3	0	0	1
2	J	4	25	17	5	3	0	0	1
2	N	4	25	17	5	3	0	0	1

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

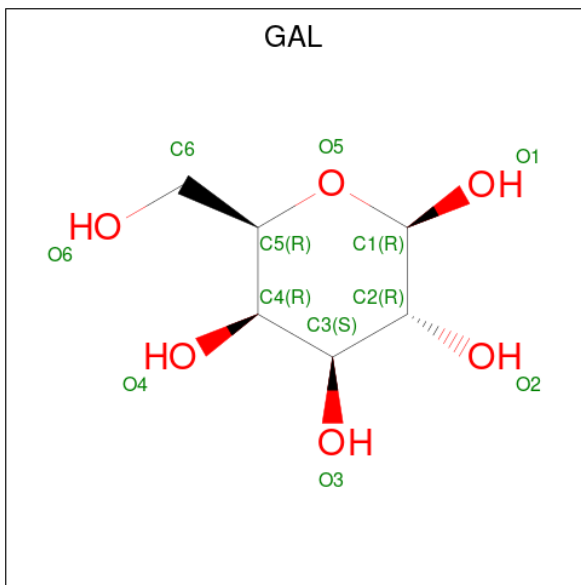
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆).



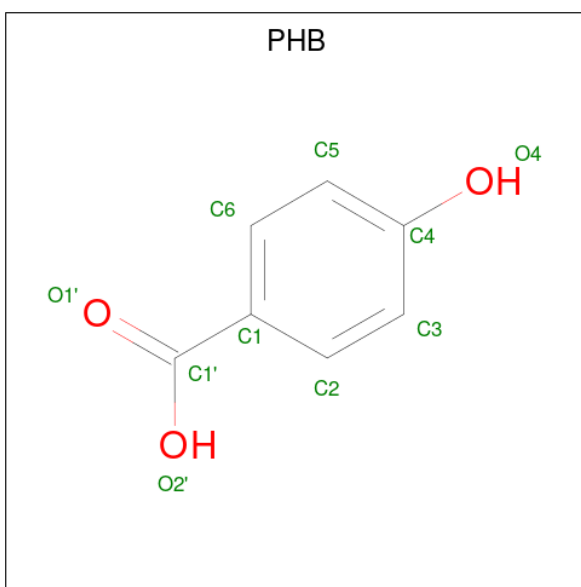
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			11	6	5		
4	F	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		
4	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is P-HYDROXYBENZOIC ACID (three-letter code: PHB) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	7	2		
5	B	1	Total	C	O	0	0
			9	7	2		
5	C	1	Total	C	O	0	0
			9	7	2		
5	D	1	Total	C	O	0	0
			9	7	2		
5	E	1	Total	C	O	0	0
			9	7	2		
5	F	1	Total	C	O	0	0
			9	7	2		
5	G	1	Total	C	O	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			9	7	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	115	Total	O	0	0
			115	115		
6	C	136	Total	O	0	0
			136	136		
6	D	149	Total	O	0	0
			149	149		
6	E	108	Total	O	0	0
			108	108		
6	F	98	Total	O	0	0
			98	98		
6	G	96	Total	O	0	0
			96	96		
6	H	105	Total	O	0	0
			105	105		
6	I	3	Total	O	0	0
			3	3		
6	J	4	Total	O	0	0
			4	4		
6	N	1	Total	O	0	0
			1	1		

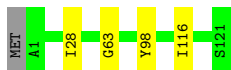
3 Residue-property plots [i](#)

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.


Note EDS failed to run properly.

- Molecule 1: PA-I galactophilic lectin

Chain A:  96%




- Molecule 1: PA-I galactophilic lectin

Chain B:  86% 13%



- Molecule 1: PA-I galactophilic lectin

Chain C:  88% 11%




- Molecule 1: PA-I galactophilic lectin

Chain D:  91% 8%




- Molecule 1: PA-I galactophilic lectin

Chain E:  90% 9%




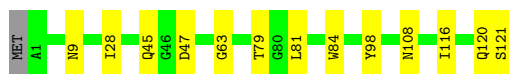
- Molecule 1: PA-I galactophilic lectin

Chain F:  84% 15%




- Molecule 1: PA-I galactophilic lectin

Chain G:  89% 11%



- Molecule 1: PA-I galactophilic lectin

Chain H:  88% 11%



- Molecule 2: GALA-LYS-PRO-LEUNH2

Chain I:  75% 25%



- Molecule 2: GALA-LYS-PRO-LEUNH2

Chain J:  50% 50%



- Molecule 2: GALA-LYS-PRO-LEUNH2

Chain N:  75% 25%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.33Å 128.56Å 146.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.29	Depositor
% Data completeness (in resolution range)	99.6 (49.26-2.29)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.07Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.214 , 0.240	Depositor
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	0.605	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8394	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0013e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, NH2, PHB, CA

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	0.21	0/924	0.38	0/1262
1	B	0.21	0/924	0.39	0/1262
1	C	0.21	0/924	0.39	0/1262
1	D	0.21	0/924	0.38	0/1262
1	E	0.21	0/924	0.38	0/1262
1	F	0.21	0/924	0.39	0/1262
1	G	0.20	0/924	0.38	0/1262
1	H	0.20	0/924	0.38	0/1262
2	I	0.21	0/24	0.38	0/31
2	J	0.19	0/24	0.38	0/31
2	N	0.25	0/24	0.43	0/31
All	All	0.21	0/7464	0.39	0/10189

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 [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	901	0	861	2	0
1	B	901	0	861	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	901	0	861	13	0
1	D	901	0	861	6	0
1	E	901	0	861	9	0
1	F	901	0	861	14	0
1	G	901	0	861	8	0
1	H	901	0	861	10	0
2	I	25	0	30	0	0
2	J	25	0	30	2	0
2	N	25	0	30	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	11	0	10	1	0
4	B	11	0	10	0	0
4	C	11	0	10	0	0
4	D	11	0	10	0	0
4	E	11	0	10	0	0
4	F	11	0	10	0	0
4	G	11	0	10	0	0
4	H	11	0	10	0	0
5	A	9	0	4	0	0
5	B	9	0	4	0	0
5	C	9	0	4	0	0
5	D	9	0	4	0	0
5	E	9	0	4	0	0
5	F	9	0	4	0	0
5	G	9	0	4	0	0
5	H	9	0	4	0	0
6	A	128	0	0	0	1
6	B	115	0	0	1	0
6	C	136	0	0	2	3
6	D	149	0	0	1	0
6	E	108	0	0	1	1
6	F	98	0	0	1	0
6	G	96	0	0	4	1
6	H	105	0	0	1	0
6	I	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	4	0	0	2	0
6	N	1	0	0	0	0
All	All	8394	0	7090	67	3

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 5.

The worst 5 of 67 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:B:32:GLY:H	1:C:45:GLN:HE22	1.10	0.99
1:B:45:GLN:HE22	1:C:32:GLY:H	1.12	0.97
1:E:32:GLY:H	1:F:45:GLN:HE22	1.17	0.92
1:E:45:GLN:HE22	1:F:32:GLY:H	1.24	0.85
2:J:301:LYS:HG2	6:J:402:HOH:O	1.89	0.71

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:330:HOH:O	6:E:377:HOH:O[1_455]	1.99	0.21
6:A:369:HOH:O	6:C:419:HOH:O[3_544]	2.03	0.17
6:C:374:HOH:O	6:G:305:HOH:O[2_454]	2.18	0.02

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	119/122 (98%)	116 (98%)	3 (2%)	0	100 100
1	B	119/122 (98%)	115 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	D	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	E	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	F	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
1	G	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
1	H	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
2	I	2/4 (50%)	2 (100%)	0	0	100	100
2	J	2/4 (50%)	2 (100%)	0	0	100	100
2	N	2/4 (50%)	2 (100%)	0	0	100	100
All	All	958/988 (97%)	929 (97%)	29 (3%)	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	Rotameric	Outliers	Percentiles	
1	A	94/95 (99%)	94 (100%)	0	100	100
1	B	94/95 (99%)	94 (100%)	0	100	100
1	C	94/95 (99%)	94 (100%)	0	100	100
1	D	94/95 (99%)	94 (100%)	0	100	100
1	E	94/95 (99%)	94 (100%)	0	100	100
1	F	94/95 (99%)	94 (100%)	0	100	100
1	G	94/95 (99%)	94 (100%)	0	100	100
1	H	94/95 (99%)	94 (100%)	0	100	100
2	I	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	J	3/3 (100%)	3 (100%)	0	100	100
2	N	3/3 (100%)	3 (100%)	0	100	100
All	All	761/769 (99%)	760 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	40	GLN
1	H	115	ASN
1	E	45	GLN
1	E	78	ASN
1	E	88	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.