

wwPDB X-ray Structure Validation Summary Report (i)

Dec 13, 2022 – 03:36 pm GMT

PDB ID : 8AIY

Title : STRUCTURE OF THE LECB LECTIN FROM PSEUDOMONAS AERUG-

INOSA STRAIN PAO1 IN COMPLEX WITH N-(beta-L-Fucopyranosyl)-bip

henyl-3-carboxamide (4i)

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Deposited on : 2022-07-27

Resolution : 1.55 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 : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

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)

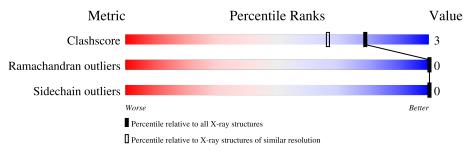
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.55 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	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain	
1	AAA	114	93%	7%
1	BBB	114	95%	5%
1	CCC	114	95%	5%
1	DDD	114	91%	9%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4094 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 Fucose-binding lectin PA-IIL.

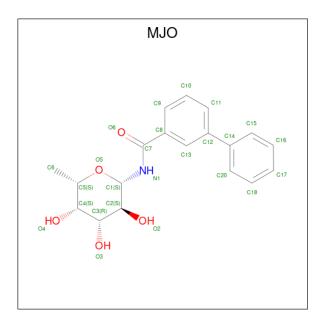
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
1	AAA	114	Total	С	N	О	0	1	0
1	АЛА	114	833	511	144	178	0	1	0
1	BBB	114	Total	С	N	О	0	2	0
1	מממ	114	833	513	145	175	0	2	0
1	CCC	114	Total	С	N	О	0	1	0
1		114	830	511	144	175	0	1	0
1	1 DDD	11/	Total	С	N	О	0	3	0
1 DDD	114	843	517	146	180	0	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	2	Total Ca 2 2	0	0
2	BBB	2	Total Ca 2 2	0	0
2	CCC	2	Total Ca 2 2	0	0
2	DDD	2	Total Ca 2 2	0	0

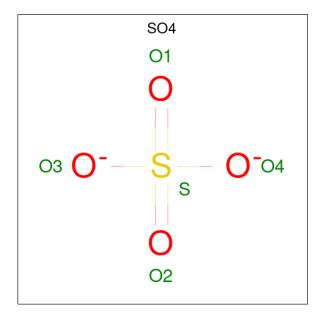
• Molecule 3 is N-(beta-L-Fucopyranosyl)-biphenyl-3-carboxamide (three-letter code: MJO) (formula: $C_{19}H_{21}NO_5$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	AAA	1	Total	С	N	О	0	0	
9	ААА	1	25	19	1	5	0		
3	BBB	1	Total	С	N	О	0	0	
3	ррр	1	25	19	1	5	0	0	
3	CCC	1	Total	С	N	О	0	0	
3	3 CCC		25	19	1	5	0	0	
3	3 DDD	1	Total	С	N	О	0	0	
3	עעע			19	1	5	0	U	

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$





Mo	l Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O S 5 4 1	0	0
4	CCC	1	Total O S 5 4 1	0	0

$\bullet\,$ Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	155	Total O 158 158	0	3
5	BBB	150	Total O 151 151	0	1
5	CCC	157	Total O 161 161	0	4
5	DDD	165	Total O 167 167	0	2

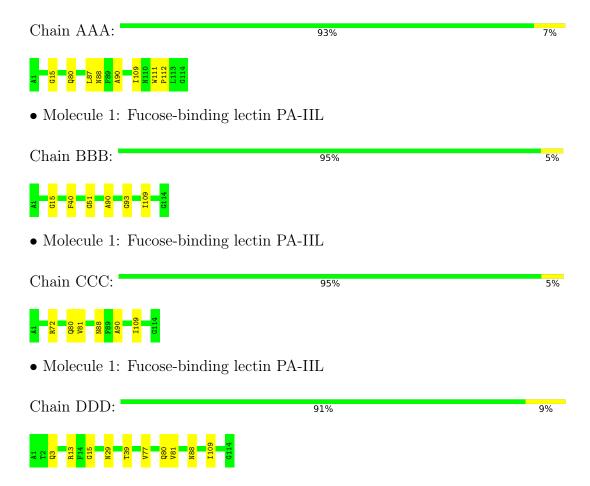


3 Residue-property plots (i)

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: Fucose-binding lectin PA-IIL





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	71.91Å 76.50Å 184.31Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.08 - 1.55	Depositor
% Data completeness	100.0 (46.08-1.55)	Depositor
(in resolution range)	,	_
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.02 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.142 , 0.166	Depositor
Wilson B-factor (\mathring{A}^2)	18.9	Xtriage
Anisotropy	0.046	Xtriage
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4094	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.30% 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: CA, MJO, SO4

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).

Mal	Chain	Bond	lengths	Bond angles		
Mol		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.80	0/843	0.83	0/1154	
1	BBB	0.80	0/843	0.86	0/1155	
1	CCC	0.75	0/840	0.87	1/1151 (0.1%)	
1	DDD	0.78	0/853	0.86	1/1168 (0.1%)	
All	All	0.78	0/3379	0.86	2/4628 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	DDD	13	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	CCC	72	ARG	NE-CZ-NH2	-5.17	117.71	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	AAA	833	0	804	5	0
1	BBB	833	0	806	4	0
1	CCC	830	0	804	5	0
1	DDD	843	0	812	9	0
2	AAA	2	0	0	0	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	2	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	2	0	0	0	0
3	AAA	25	0	0	0	0
3	BBB	25	0	0	0	0
3	CCC	25	0	0	0	0
3	DDD	25	0	0	0	0
4	AAA	5	0	0	0	0
4	CCC	5	0	0	0	0
5	AAA	158	0	0	0	0
5	BBB	151	0	0	0	0
5	CCC	161	0	0	0	0
5	DDD	167	0	0	1	0
All	All	4094	0	3226	19	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 3.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\left(\operatorname{\AA}\right)$	$\text{overlap } (\text{\AA})$
1:CCC:81[B]:VAL:HG21	1:DDD:81:VAL:HG21	1.30	1.05
1:DDD:39[A]:THR:HG22	5:DDD:359:HOH:O	1.85	0.74
1:CCC:81[B]:VAL:HG21	1:DDD:81:VAL:CG2	2.18	0.67
1:DDD:3:GLN:HE21	1:DDD:77:VAL:HA	1.69	0.57
1:CCC:80:GLN:HE21	1:CCC:88:ASN:HD22	1.53	0.56

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	Perce	entiles
1	AAA	$113/114\ (99\%)$	111 (98%)	2 (2%)	0	100	100
1	BBB	$114/114\ (100\%)$	112 (98%)	2 (2%)	0	100	100
1	CCC	$113/114\ (99\%)$	110 (97%)	3 (3%)	0	100	100
1	DDD	115/114 (101%)	112 (97%)	3 (3%)	0	100	100
All	All	455/456~(100%)	445 (98%)	10 (2%)	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	Perce	ntiles
1	AAA	94/93 (101%)	94 (100%)	0	100	100
1	BBB	93/93~(100%)	93 (100%)	0	100	100
1	CCC	93/93 (100%)	93 (100%)	0	100	100
1	DDD	95/93 (102%)	95 (100%)	0	100	100
All	All	375/372 (101%)	375 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	Trino	Chain	Chain	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
3	MJO	BBB	203	2	27,27,27	0.58	0	37,38,38	0.76	1 (2%)		
4	SO4	CCC	204	-	4,4,4	0.32	0	6,6,6	0.19	0		
3	MJO	CCC	201	2	27,27,27	0.67	1 (3%)	37,38,38	1.13	2 (5%)		
4	SO4	AAA	204	-	4,4,4	0.29	0	6,6,6	0.62	0		
3	MJO	DDD	203	2	27,27,27	0.75	0	37,38,38	0.85	2 (5%)		
3	MJO	AAA	203	2	27,27,27	0.65	0	37,38,38	1.02	1 (2%)		

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	MJO	DDD	203	2	-	0/12/32/32	0/3/3/3
3	MJO	BBB	203	2	-	0/12/32/32	0/3/3/3
3	MJO	CCC	201	2	-	0/12/32/32	0/3/3/3
3	MJO	AAA	203	2	-	6/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	CCC	201	MJO	C1-N1	-2.32	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
3	CCC	201	MJO	O2-C2-C1	3.52	115.69	109.39
3	AAA	203	MJO	O2-C2-C1	3.42	115.51	109.39
3	BBB	203	MJO	O2-C2-C1	3.08	114.90	109.39
3	DDD	203	MJO	O2-C2-C1	2.69	114.20	109.39
3	CCC	201	MJO	O5-C1-C2	-2.40	107.41	109.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

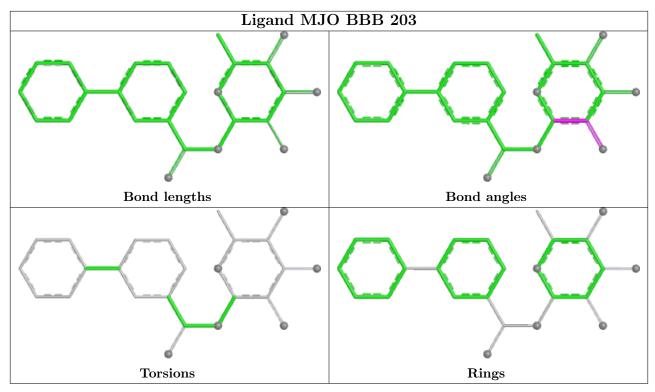
Mol	Chain	Res	Type	Atoms
3	AAA	203	MJO	O5-C1-N1-C7
3	AAA	203	MJO	N1-C7-C8-C13
3	AAA	203	MJO	C2-C1-N1-C7
3	AAA	203	MJO	O6-C7-C8-C13
3	AAA	203	MJO	N1-C7-C8-C9

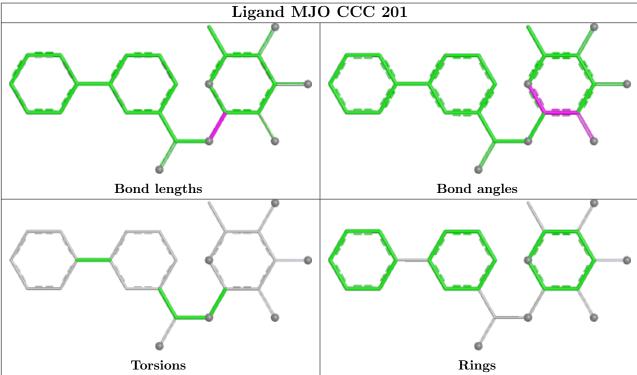
There are no ring outliers.

No monomer is involved in short contacts.

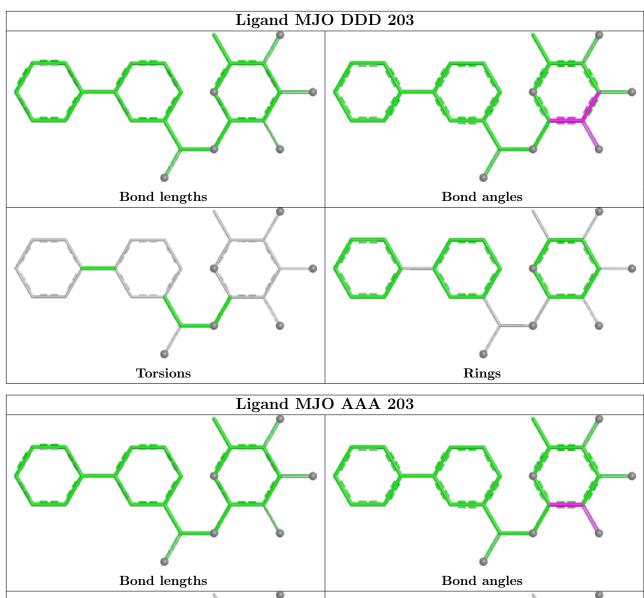
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

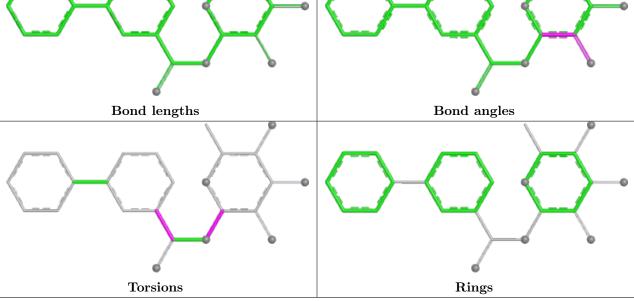












5.7 Other polymers (i)

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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

