



wwPDB X-ray Structure Validation Summary Report ⓘ

May 11, 2026 – 08:22 PM EDT

PDB ID : 9OT8 / pdb_00009ot8
Title : Crystal structure of Galectin-3 bound to FN3con-9 and FN3con-41, a cooperative binder that recognises the Galectin-3-FN3con-9 interface
Authors : Mutschler, R.; Caputo, A.T.; Guo, Z.; Fiorito, M.M.; Newton, S.; Zhang, X.; Karunathilaka, N.; Duval, C.; Brazel, H.; Abwanka, D.; Punyadeera, C.; Alexandrov, K.; Cui, Z.
Deposited on : 2025-05-26
Resolution : 1.96 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

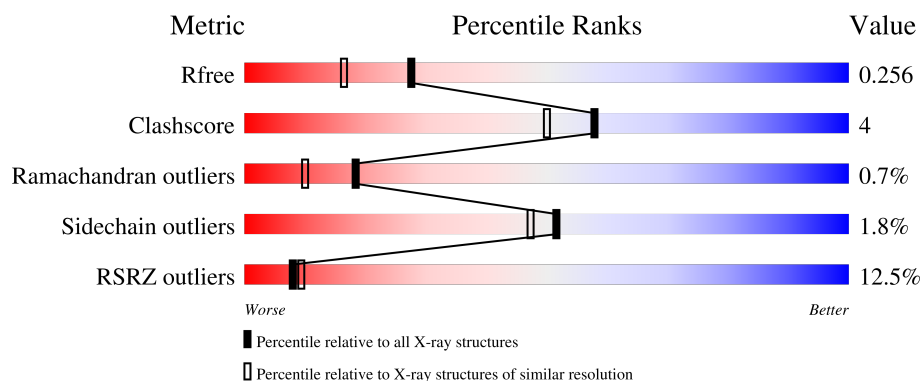
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	403	<div> <div>10%</div> <div>67%</div> <div>9%</div> <div>23%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4999 atoms, of which 2439 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 FN3con-9 - FN3con-41 fusion, Galectin-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	311	4929	1591	2439	434	462	3	0	0	0

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	linker	PDB ?
A	218	GLY	-	linker	PDB ?
A	219	GLY	-	linker	PDB ?
A	220	SER	-	linker	PDB ?
A	221	GLY	-	linker	PDB ?
A	222	GLY	-	linker	PDB ?
A	223	SER	-	linker	PDB ?
A	224	GLY	-	linker	PDB ?
A	225	GLY	-	linker	PDB ?
A	226	ASP	-	linker	PDB ?
A	227	GLY	-	linker	PDB ?
A	228	GLY	-	linker	PDB ?
A	229	GLY	-	linker	PDB ?
A	230	SER	-	linker	PDB ?
A	231	GLY	-	linker	PDB ?
A	232	ASP	-	linker	PDB ?
A	233	GLY	-	linker	PDB ?
A	234	GLY	-	linker	PDB ?
A	235	SER	-	linker	PDB ?
A	236	GLY	-	linker	PDB ?
A	237	SER	-	linker	PDB ?
A	238	GLY	-	linker	PDB ?
A	239	SER	-	linker	PDB ?
A	240	GLY	-	linker	PDB ?
A	241	GLY	-	linker	PDB ?
A	242	GLY	-	linker	PDB ?
A	243	GLY	-	linker	PDB ?

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ASP	-	linker	PDB ?
A	245	SER	-	linker	PDB ?
A	246	GLY	-	linker	PDB ?
A	247	SER	-	linker	PDB ?
A	248	SER	-	linker	PDB ?
A	249	GLY	-	linker	PDB ?
A	250	GLY	-	linker	PDB ?
A	251	SER	-	linker	PDB ?
A	252	GLY	-	linker	PDB ?
A	253	SER	-	linker	PDB ?
A	254	GLY	-	linker	PDB ?
A	255	GLY	-	linker	PDB ?
A	256	GLY	-	linker	PDB ?
A	257	GLY	-	linker	PDB ?
A	258	SER	-	linker	PDB ?
A	259	HIS	-	linker	PDB ?
A	260	MET	-	linker	PDB ?
A	401	GLY	-	expression tag	UNP P17931
A	402	LYS	-	expression tag	UNP P17931
A	403	LEU	-	expression tag	UNP P17931

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	70	Total O 70 70	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 68.31Å 171.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.48 – 1.96 63.48 – 1.96	Depositor EDS
% Data completeness (in resolution range)	45.8 (63.48-1.96) 44.0 (63.48-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.221 , 0.255 0.221 , 0.256	Depositor DCC
R_{free} test set	671 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4999	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/2554	0.51	0/3474

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ARG	Sidechain
1	A	72	ARG	Sidechain

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	2490	2439	2438	22	0
2	A	70	0	0	0	0
All	All	2560	2439	2438	22	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 4.

The worst 5 of 22 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:14:VAL:HG21	1:A:87:VAL:HG21	1.73	0.70
1:A:70:ARG:HD3	1:A:72:ARG:NH2	2.08	0.69
1:A:167:ALA:HB2	1:A:193:GLU:HG2	1.85	0.57
1:A:391:ASP:OD1	1:A:391:ASP:N	2.30	0.55
1:A:39:GLU:O	1:A:40:ALA:C	2.52	0.53

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	305/403 (76%)	290 (95%)	13 (4%)	2 (1%)	18 10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA
1	A	167	ALA

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	272/312 (87%)	267 (98%)	5 (2%)	51 47

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

Mol	Chain	Res	Type
1	A	52	LEU
1	A	157	SER
1	A	213	SER
1	A	293	ASN
1	A	329	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	135	ASN
1	A	303	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

6.1 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	311/403 (77%)	0.95	39 (12%) 8 9	18, 36, 70, 92	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	PRO	4.9
1	A	70	ARG	4.7
1	A	17	THR	4.5
1	A	61	LEU	4.5
1	A	270	LEU	4.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.