



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 07:15 AM UTC

PDB ID : 5NIJ / pdb_00005nij
Title : Crystal structure of arabidopsis thaliana legumain isoform gamma in two-chain activation state
Authors : Zauner, F.B.; Dall, E.; Brandstetter, H.
Deposited on : 2017-03-24
Resolution : 2.75 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 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
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

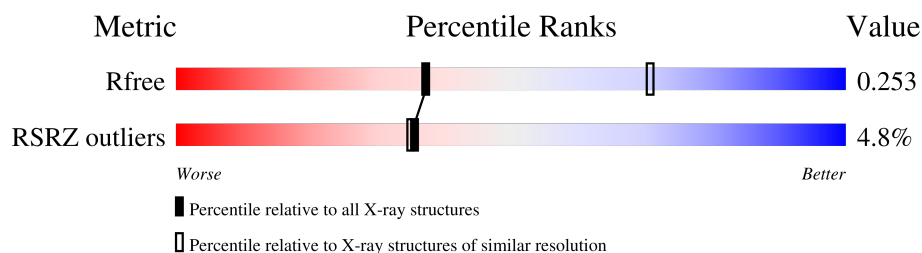
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13474 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 Vacuolar-processing enzyme gamma-isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3342	2099	578	646	19			
1	B	428	Total	C	N	O	S	0	0	0
			3338	2099	575	645	19			
1	C	429	Total	C	N	O	S	0	0	0
			3342	2099	578	646	19			
1	D	428	Total	C	N	O	S	0	0	0
			3335	2094	577	645	19			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	-	expression tag	UNP Q39119
A	42	LEU	-	expression tag	UNP Q39119
A	43	GLU	-	expression tag	UNP Q39119
A	44	HIS	-	expression tag	UNP Q39119
A	45	HIS	-	expression tag	UNP Q39119
A	46	HIS	-	expression tag	UNP Q39119
A	47	HIS	-	expression tag	UNP Q39119
A	48	HIS	-	expression tag	UNP Q39119
A	49	HIS	-	expression tag	UNP Q39119
A	50	GLU	-	expression tag	UNP Q39119
A	51	ASN	-	expression tag	UNP Q39119
A	52	LEU	-	expression tag	UNP Q39119
A	53	TYR	-	expression tag	UNP Q39119
A	54	PHE	-	expression tag	UNP Q39119
A	55	GLN	-	expression tag	UNP Q39119
B	41	SER	-	expression tag	UNP Q39119
B	42	LEU	-	expression tag	UNP Q39119
B	43	GLU	-	expression tag	UNP Q39119
B	44	HIS	-	expression tag	UNP Q39119
B	45	HIS	-	expression tag	UNP Q39119
B	46	HIS	-	expression tag	UNP Q39119

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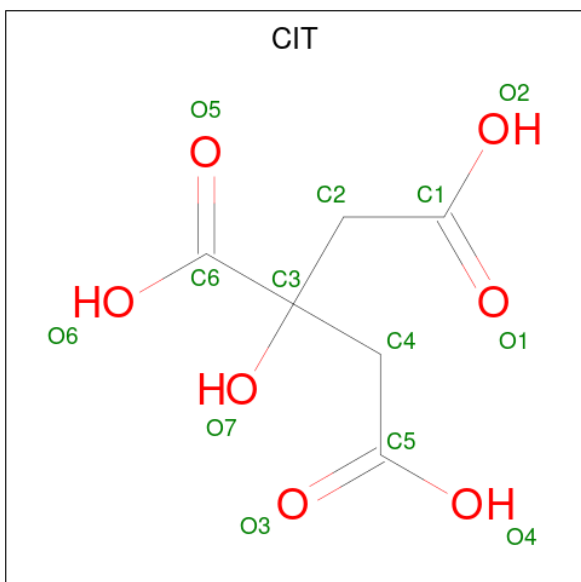
Chain	Residue	Modelled	Actual	Comment	Reference
B	47	HIS	-	expression tag	UNP Q39119
B	48	HIS	-	expression tag	UNP Q39119
B	49	HIS	-	expression tag	UNP Q39119
B	50	GLU	-	expression tag	UNP Q39119
B	51	ASN	-	expression tag	UNP Q39119
B	52	LEU	-	expression tag	UNP Q39119
B	53	TYR	-	expression tag	UNP Q39119
B	54	PHE	-	expression tag	UNP Q39119
B	55	GLN	-	expression tag	UNP Q39119
C	41	SER	-	expression tag	UNP Q39119
C	42	LEU	-	expression tag	UNP Q39119
C	43	GLU	-	expression tag	UNP Q39119
C	44	HIS	-	expression tag	UNP Q39119
C	45	HIS	-	expression tag	UNP Q39119
C	46	HIS	-	expression tag	UNP Q39119
C	47	HIS	-	expression tag	UNP Q39119
C	48	HIS	-	expression tag	UNP Q39119
C	49	HIS	-	expression tag	UNP Q39119
C	50	GLU	-	expression tag	UNP Q39119
C	51	ASN	-	expression tag	UNP Q39119
C	52	LEU	-	expression tag	UNP Q39119
C	53	TYR	-	expression tag	UNP Q39119
C	54	PHE	-	expression tag	UNP Q39119
C	55	GLN	-	expression tag	UNP Q39119
D	41	SER	-	expression tag	UNP Q39119
D	42	LEU	-	expression tag	UNP Q39119
D	43	GLU	-	expression tag	UNP Q39119
D	44	HIS	-	expression tag	UNP Q39119
D	45	HIS	-	expression tag	UNP Q39119
D	46	HIS	-	expression tag	UNP Q39119
D	47	HIS	-	expression tag	UNP Q39119
D	48	HIS	-	expression tag	UNP Q39119
D	49	HIS	-	expression tag	UNP Q39119
D	50	GLU	-	expression tag	UNP Q39119
D	51	ASN	-	expression tag	UNP Q39119
D	52	LEU	-	expression tag	UNP Q39119
D	53	TYR	-	expression tag	UNP Q39119
D	54	PHE	-	expression tag	UNP Q39119
D	55	GLN	-	expression tag	UNP Q39119

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	29	Total	O	0	0
			29	29		
4	C	12	Total	O	0	0
			12	12		
4	D	5	Total	O	0	0
			5	5		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	147.83Å 147.83Å 101.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.11 – 2.75 66.11 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.11-2.75) 99.9 (66.11-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.252 0.222 , 0.253	Depositor DCC
R_{free} test set	2711 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13474	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SNN	C	176	1	5,6,8	0.45	0	1,6,11	1.31	0
1	SCH	C	219	1	6,7,8	1.01	0	4,7,9	1.18	0
1	SNN	D	176	1	5,6,8	0.44	0	1,6,11	1.33	0
1	SNN	A	176	1	5,6,8	0.45	0	1,6,11	1.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SCH	D	219	1	6,7,8	0.99	0	4,7,9	0.97	0
1	SCH	A	219	1	6,7,8	0.96	0	4,7,9	1.36	1 (25%)
1	SCH	B	219	1	6,7,8	0.98	0	4,7,9	1.13	0
1	SNN	B	176	1	5,6,8	0.46	0	1,6,11	1.46	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
1	SNN	C	176	1	-	3/3/5/12	-
1	SCH	C	219	1	-	0/2/6/8	-
1	SNN	D	176	1	-	3/3/5/12	-
1	SNN	A	176	1	-	3/3/5/12	-
1	SCH	D	219	1	-	0/2/6/8	-
1	SCH	A	219	1	-	0/2/6/8	-
1	SCH	B	219	1	-	0/2/6/8	-
1	SNN	B	176	1	-	3/3/5/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	SCH	CB-SG-SD	2.38	110.02	103.86

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	176	SNN	O-C-CA-C4
1	A	176	SNN	C5-C4-CA-N
1	A	176	SNN	CA-C4-C5-O5
1	B	176	SNN	O-C-CA-C4
1	B	176	SNN	C5-C4-CA-N
1	B	176	SNN	CA-C4-C5-O5
1	C	176	SNN	O-C-CA-C4
1	C	176	SNN	C5-C4-CA-N
1	C	176	SNN	CA-C4-C5-O5
1	D	176	SNN	O-C-CA-C4

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Mol	Chain	Res	Type	Atoms
1	D	176	SNN	C5-C4-CA-N
1	D	176	SNN	CA-C4-C5-O5

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

6 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	SO4	C	501	-	4,4,4	0.44	0	6,6,6	0.07	0
2	SO4	B	502	-	4,4,4	0.45	0	6,6,6	0.08	0
2	SO4	B	501	-	4,4,4	0.42	0	6,6,6	0.09	0
2	SO4	A	501	-	4,4,4	0.43	0	6,6,6	0.08	0
2	SO4	D	501	-	4,4,4	0.44	0	6,6,6	0.07	0
3	CIT	A	502	-	12,12,12	1.16	0	17,17,17	1.38	3 (17%)

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	CIT	A	502	-	-	6/16/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	CIT	O6-C6-C3	3.30	119.47	113.14
3	A	502	CIT	C3-C2-C1	2.17	119.87	113.92
3	A	502	CIT	O4-C5-C4	2.14	121.13	114.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	CIT	O7-C3-C6-O5
3	A	502	CIT	O7-C3-C6-O6
3	A	502	CIT	C4-C3-C6-O5
3	A	502	CIT	C4-C3-C6-O6
3	A	502	CIT	O7-C3-C4-C5
3	A	502	CIT	C6-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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	427/454 (94%)	0.19	18 (4%) 40 39	29, 49, 79, 116	0
1	B	426/454 (93%)	0.25	22 (5%) 33 32	32, 48, 95, 155	0
1	C	427/454 (94%)	0.45	19 (4%) 39 38	32, 56, 97, 157	0
1	D	426/454 (93%)	0.60	23 (5%) 31 31	41, 66, 99, 129	0
All	All	1706/1816 (93%)	0.37	82 (4%) 35 35	29, 55, 95, 157	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	PHE	5.7
1	D	305	TYR	5.6
1	D	307	TYR	4.7
1	A	349	SER	4.6
1	B	262	GLU	4.5
1	A	348	PRO	4.4
1	A	258	SER	4.3
1	A	305	TYR	4.3
1	D	304	GLY	4.2
1	D	303	VAL	4.2
1	B	257	PRO	3.8
1	D	90	GLY	3.8
1	B	302	PRO	3.7
1	C	260	PRO	3.6
1	C	303	VAL	3.6
1	B	303	VAL	3.6
1	B	337	PHE	3.6
1	B	307	TYR	3.4
1	C	108	TYR	3.4
1	C	348	PRO	3.3
1	B	351	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	349	SER	3.3
1	D	482	THR	3.2
1	C	307	TYR	3.1
1	A	303	VAL	3.1
1	D	308	GLY	3.1
1	C	305	TYR	3.1
1	B	261	PRO	3.0
1	B	486	SER	3.0
1	B	258	SER	2.8
1	A	494	ALA	2.8
1	C	257	PRO	2.8
1	B	305	TYR	2.8
1	B	479	THR	2.8
1	A	261	PRO	2.7
1	D	262	GLU	2.7
1	C	337	PHE	2.7
1	A	333	ALA	2.7
1	C	273	VAL	2.7
1	B	485	TRP	2.6
1	B	492	PHE	2.6
1	D	333	ALA	2.6
1	C	333	ALA	2.5
1	C	306	SER	2.5
1	C	254	GLY	2.5
1	B	494	ALA	2.5
1	B	482	THR	2.5
1	D	258	SER	2.5
1	B	480	LEU	2.4
1	D	159	GLY	2.4
1	B	284	LEU	2.4
1	D	336	ASN	2.4
1	B	484	PRO	2.4
1	C	302	PRO	2.4
1	D	257	PRO	2.4
1	D	286	THR	2.4
1	C	261	PRO	2.3
1	D	261	PRO	2.3
1	C	482	THR	2.3
1	A	256	GLU	2.3
1	C	255	GLU	2.3
1	C	207	GLY	2.3
1	C	161	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	479	THR	2.3
1	A	482	THR	2.3
1	D	371	GLU	2.3
1	A	351	VAL	2.3
1	A	371	GLU	2.3
1	B	263	TYR	2.2
1	D	484	PRO	2.2
1	D	483	GLY	2.2
1	D	255	GLU	2.1
1	A	302	PRO	2.1
1	A	257	PRO	2.1
1	C	167	ASN	2.1
1	A	307	TYR	2.1
1	D	480	LEU	2.1
1	B	306	SER	2.1
1	A	350	ARG	2.0
1	D	94	GLU	2.0
1	A	306	SER	2.0
1	B	121	HIS	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [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
1	SCH	C	219	8/9	0.87	0.12	45,48,53,54	0
1	SNN	B	176	7/8	0.88	0.13	29,34,38,40	0
1	SNN	D	176	7/8	0.88	0.14	48,49,51,52	0
1	SNN	C	176	7/8	0.91	0.10	39,42,42,48	0
1	SNN	A	176	7/8	0.91	0.11	28,30,33,34	0
1	SCH	B	219	8/9	0.91	0.11	44,47,61,66	0
1	SCH	A	219	8/9	0.92	0.11	31,36,59,59	0
1	SCH	D	219	8/9	0.94	0.10	41,47,60,60	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	C	501	5/5	0.68	0.12	85,87,99,121	0
2	SO4	B	502	5/5	0.69	0.18	88,91,106,130	0
3	CIT	A	502	13/13	0.74	0.24	39,43,50,51	13
2	SO4	D	501	5/5	0.76	0.18	83,94,100,121	0
2	SO4	A	501	5/5	0.79	0.13	100,100,101,102	0
2	SO4	B	501	5/5	0.82	0.11	68,69,73,77	0

5.5 Other polymers [i](#)

There are no such residues in this entry.