



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 09:08 PM UTC

PDB ID : 9LJ7 / pdb_00009lj7
Title : Crystal structure of a leaf-branch compost cutinase variant, ICCG-H218S/F222I
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Deposited on : 2025-01-14
Resolution : 1.61 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	:	4-5-2 with Phenix2.0
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

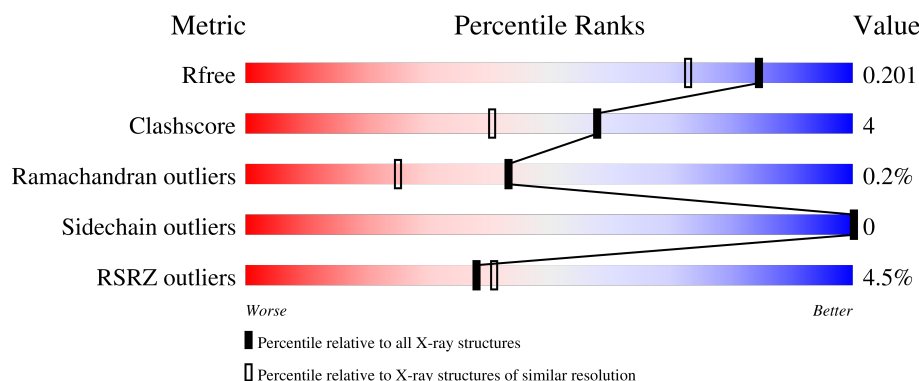
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	265	
1	B	265	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4567 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 Leaf-branch compost cutinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	4	0
			1957	1225	350	375	7			
1	B	258	Total	C	N	O	S	0	5	0
			1963	1228	351	377	7			

There are 26 discrepancies between the modelled and reference sequences:

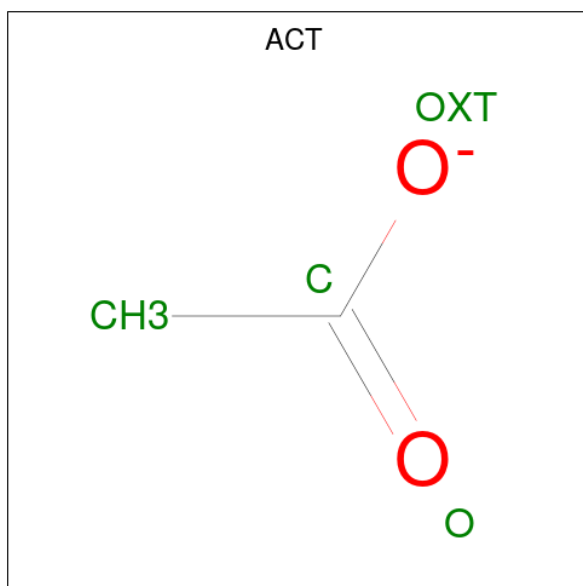
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP G9BY57
A	127	GLY	TYR	conflict	UNP G9BY57
A	218	SER	HIS	engineered mutation	UNP G9BY57
A	222	ILE	PHE	engineered mutation	UNP G9BY57
A	238	CYS	ASP	conflict	UNP G9BY57
A	243	ILE	PHE	conflict	UNP G9BY57
A	283	CYS	SER	conflict	UNP G9BY57
A	294	LEU	-	expression tag	UNP G9BY57
A	295	GLU	-	expression tag	UNP G9BY57
A	296	LEU	-	expression tag	UNP G9BY57
A	297	VAL	-	expression tag	UNP G9BY57
A	298	PRO	-	expression tag	UNP G9BY57
A	299	ARG	-	expression tag	UNP G9BY57
B	35	MET	-	initiating methionine	UNP G9BY57
B	127	GLY	TYR	conflict	UNP G9BY57
B	218	SER	HIS	engineered mutation	UNP G9BY57
B	222	ILE	PHE	engineered mutation	UNP G9BY57
B	238	CYS	ASP	conflict	UNP G9BY57
B	243	ILE	PHE	conflict	UNP G9BY57
B	283	CYS	SER	conflict	UNP G9BY57
B	294	LEU	-	expression tag	UNP G9BY57
B	295	GLU	-	expression tag	UNP G9BY57
B	296	LEU	-	expression tag	UNP G9BY57
B	297	VAL	-	expression tag	UNP G9BY57
B	298	PRO	-	expression tag	UNP G9BY57

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	ARG	-	expression tag	UNP G9BY57

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

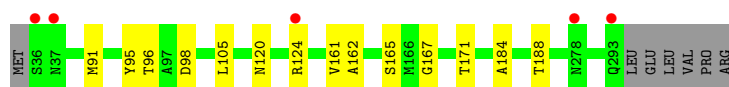
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	338	Total 338	O 338	0	0
4	B	287	Total 287	O 287	0	0

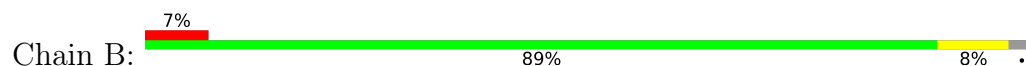
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Leaf-branch compost cutinase



- Molecule 1: Leaf-branch compost cutinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.66Å 101.66Å 98.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.17 – 1.61 45.17 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.17-1.61) 99.7 (45.17-1.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.15 (at 1.62Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.172 , 0.200 0.172 , 0.201	Depositor DCC
R_{free} test set	2000 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-l,-k 0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4567	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	0.26	0/2014	0.52	0/2757
1	B	0.26	0/2020	0.53	0/2765
All	All	0.26	0/4034	0.53	0/5522

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

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	1957	0	1917	13	0
1	B	1963	0	1921	21	0
2	A	8	0	6	0	0
2	B	12	0	9	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	338	0	0	2	1
4	B	287	0	0	1	1
All	All	4567	0	3853	35	1

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.

All (35) 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:165:SER:OG	1:B:190:TRP:NE1	2.17	0.77
1:B:69:SER:O	4:B:401:HOH:O	2.09	0.70
1:B:194:LYS:NZ	1:B:195:THR:O	2.25	0.69
1:A:96:THR:HA	1:A:124:ARG:HB3	1.78	0.65
1:A:161:VAL:HG23	1:A:171[A]:THR:HG23	1.78	0.64
1:B:161:VAL:HG23	1:B:171[A]:THR:HG23	1.77	0.64
1:A:91:MET:HE1	1:A:105:LEU:HD23	1.80	0.63
1:A:124:ARG:NE	1:A:124:ARG:H	1.98	0.60
1:B:91:MET:HE1	1:B:105:LEU:HD23	1.86	0.57
1:A:167:GLY:O	1:A:171[B]:THR:HG23	2.05	0.56
1:B:143:ARG:HH22	2:B:301:ACT:CH3	2.22	0.53
1:B:193:ASP:CG	1:B:194:LYS:H	2.08	0.51
1:B:196:PHE:O	1:B:227:PRO:HD3	2.13	0.49
4:A:433:HOH:O	2:B:301:ACT:H1	2.12	0.49
1:B:193:ASP:OD2	1:B:194:LYS:N	2.38	0.49
1:B:166:MET:HE3	1:B:190:TRP:CH2	2.49	0.48
1:B:59:ALA:HB2	1:B:80:THR:HG21	1.95	0.48
1:B:164:HIS:O	1:B:167:GLY:N	2.47	0.47
1:A:124:ARG:HD3	4:A:448:HOH:O	2.15	0.45
1:A:91:MET:HA	1:A:162:ALA:O	2.15	0.45
1:B:193:ASP:CG	1:B:194:LYS:N	2.74	0.45
1:A:171[A]:THR:HG22	1:A:184:ALA:HB1	1.99	0.44
1:B:171[A]:THR:CG2	1:B:184:ALA:HB1	2.48	0.44
1:B:70:GLY:O	1:B:134:GLN:HG2	2.18	0.44
1:B:143:ARG:HH22	2:B:301:ACT:H1	1.83	0.44
1:B:171[A]:THR:HG22	1:B:184:ALA:HB1	2.00	0.44
1:A:165:SER:HA	1:A:188:THR:O	2.18	0.43
1:B:165:SER:HG	1:B:190:TRP:HE1	1.63	0.42
1:A:162:ALA:C	1:A:171[B]:THR:HG21	2.44	0.42
1:A:98:ASP:HB2	1:A:120:ASN:OD1	2.20	0.42
1:B:91:MET:HB3	1:B:91:MET:HE2	1.76	0.42
1:B:91:MET:HE2	1:B:102:LEU:HD13	2.02	0.41
1:A:95:TYR:CD2	1:A:96:THR:HG23	2.55	0.41
1:A:91:MET:HB3	1:A:91:MET:HE2	1.78	0.41
1:B:194:LYS:HD2	1:B:195:THR:H	1.85	0.41

All (1) 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)
4:A:577:HOH:O	4:B:430:HOH:O[7_555]	2.19	0.01

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	260/265 (98%)	253 (97%)	7 (3%)	0	100	100
1	B	261/265 (98%)	252 (97%)	8 (3%)	1 (0%)	30	14
All	All	521/530 (98%)	505 (97%)	15 (3%)	1 (0%)	43	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	ASP

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	215/218 (99%)	215 (100%)	0	100	100
1	B	216/218 (99%)	216 (100%)	0	100	100
All	All	431/436 (99%)	431 (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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	B	140	ASN
1	B	272	GLN
1	B	289	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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	B	303	-	3,3,3	0.83	0	3,3,3	1.35	0
2	ACT	B	301	-	3,3,3	0.88	0	3,3,3	1.18	0
2	ACT	A	303	-	3,3,3	0.87	0	3,3,3	1.28	0
2	ACT	A	301	-	3,3,3	0.76	0	3,3,3	0.91	0
2	ACT	B	302	-	3,3,3	0.79	0	3,3,3	1.38	0

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ACT	3	0

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

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	258/265 (97%)	-0.18	5 (1%) 66 71	7, 17, 29, 232	4 (1%)
1	B	258/265 (97%)	0.15	18 (6%) 22 24	8, 19, 38, 239	5 (1%)
All	All	516/530 (97%)	-0.02	23 (4%) 38 41	7, 18, 34, 239	9 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	SER	8.6
1	A	278	ASN	8.0
1	B	36	SER	7.3
1	B	278	ASN	5.7
1	B	193	ASP	5.5
1	B	190	TRP	5.0
1	B	195	THR	4.4
1	B	194	LYS	4.4
1	B	192	THR	3.9
1	B	66	LEU	3.8
1	A	37	ASN	3.7
1	B	196	PHE	3.6
1	B	197	ASN	3.6
1	B	37	ASN	3.3
1	B	191	HIS	3.0
1	B	293	GLN	2.6
1	B	279	ASP	2.5
1	A	293	GLN	2.4
1	B	167	GLY	2.4
1	B	169	GLY	2.4
1	B	277	VAL	2.3
1	B	165	SER	2.3
1	A	124	ARG	2.1

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](#)

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	ACT	B	301	4/4	0.89	0.11	21,21,23,30	0
2	ACT	B	302	4/4	0.89	0.18	32,32,33,33	0
2	ACT	B	303	4/4	0.89	0.12	26,27,31,36	0
2	ACT	A	301	4/4	0.94	0.12	19,28,30,32	0
2	ACT	A	303	4/4	0.96	0.06	20,20,24,26	0
3	CA	A	302	1/1	0.98	0.18	29,29,29,29	0
3	CA	B	304	1/1	0.98	0.23	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.