



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:52 AM UTC

PDB ID : 1XZK / pdb_00001xzk
Title : FUSARIUM SOLANI CUTINASE COMPLEX WITH DI(ISOPROPYL)PHOSPHATE
Authors : Martinez, C.; Cambillau, C.
Deposited on : 1995-11-28
Resolution : 2.01 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

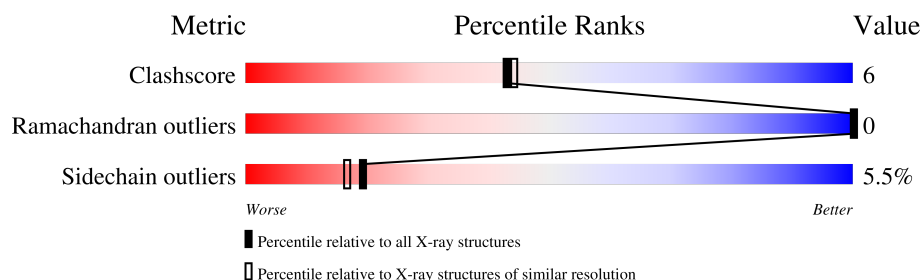
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	 76% 13% • 8%
1	B	214	 79% 11% • 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4357 atoms, of which 1196 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.

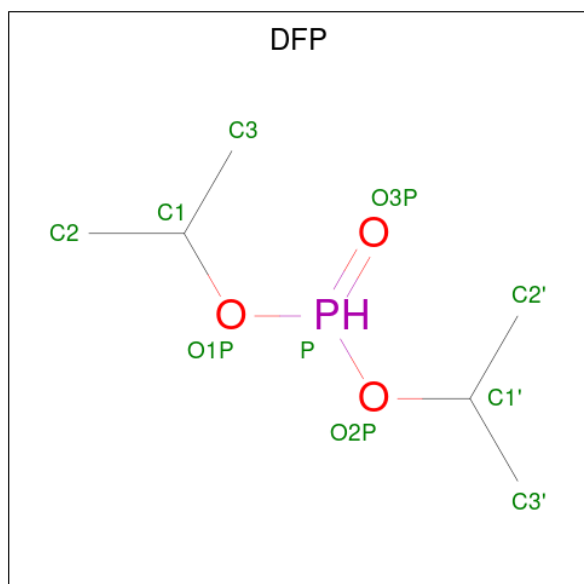
- Molecule 1 is a protein called CUTINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			1774	893	335	260	281	5			
1	B	197	Total	C	H	N	O	S	0	0	0
			1774	893	335	260	281	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLU	GLY	conflict	UNP P00590
A	32	ALA	ARG	cloning artifact	UNP P00590
B	16	GLU	GLY	conflict	UNP P00590
B	32	ALA	ARG	cloning artifact	UNP P00590

- Molecule 2 is DIISOPROPYL PHOSPHONATE (CCD ID: DFP) (formula: $C_6H_{15}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	6	3	1		
2	B	1	Total	C	O	P	0	0
			10	6	3	1		

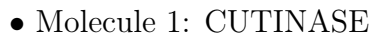
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	119	Total	H	O	0	0
			357	238	119		
3	B	144	Total	H	O	0	0
			432	288	144		

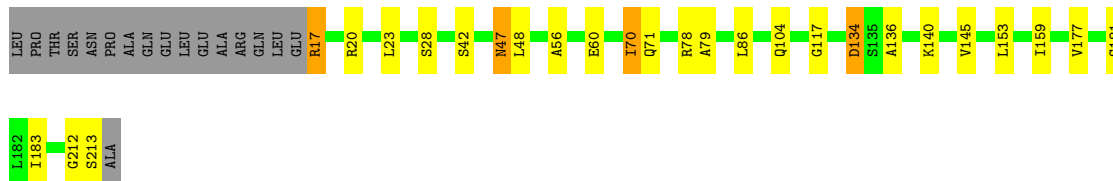
i

Note EDS was not executed.

Chain A: 76% 13% • 8%



Chain B: 79% 11% • 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.20Å 94.80Å 55.00Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	6.00 – 2.01	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.01)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4357	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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: DFP

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	0.64	0/1462	1.04	2/1984 (0.1%)
1	B	0.71	0/1462	1.05	1/1984 (0.1%)
All	All	0.68	0/2924	1.05	3/3968 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	PHE	N-CA-C	-9.48	95.73	110.42
1	B	159	ILE	N-CA-C	-7.46	99.23	107.73
1	A	180	GLY	N-CA-C	5.42	122.26	115.21

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	1439	335	1423	20	2
1	B	1439	335	1423	16	0
2	A	10	0	14	0	0
2	B	10	0	14	0	0
3	A	119	238	0	3	0
3	B	144	288	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3161	1196	2874	36	2

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 6.

All (36) 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:140:LYS:HD3	3:B:477:HOH:O	1.82	0.79
1:B:20:ARG:H	1:B:47:ASN:HD21	1.34	0.75
1:A:20:ARG:H	1:A:47:ASN:HD21	1.42	0.66
1:A:83:ASP:HA	1:A:86:LEU:HD13	1.82	0.62
1:A:61:SER:HB2	3:A:403:HOH:O	2.01	0.59
1:B:20:ARG:HH22	1:B:60:GLU:CD	2.16	0.54
1:B:177:VAL:HA	1:B:181:SER:O	2.08	0.53
1:A:24:ILE:H	1:A:71:GLN:NE2	2.07	0.52
1:A:23:LEU:HB3	1:A:71:GLN:HE21	1.74	0.52
1:A:78:ARG:NE	1:A:78:ARG:HA	2.25	0.51
1:A:181:SER:HB2	1:A:183:ILE:HG13	1.93	0.51
1:B:42:SER:HA	1:B:79:ALA:HB1	1.93	0.50
1:A:60:GLU:O	1:A:63:PHE:O	2.29	0.50
1:B:48:LEU:HD11	1:B:70:ILE:HD11	1.94	0.50
1:B:104:GLN:NE2	3:B:475:HOH:O	2.44	0.50
1:A:17:ARG:N	3:A:453:HOH:O	2.45	0.49
1:B:181:SER:HB3	1:B:183:ILE:HG13	1.94	0.49
1:B:17:ARG:N	1:B:17:ARG:HD3	2.27	0.49
1:B:23:LEU:HB3	1:B:71:GLN:HE21	1.79	0.48
1:A:45:THR:HG22	1:A:46:GLY:N	2.29	0.48
1:B:212:GLY:O	1:B:213:SER:HB2	2.14	0.46
1:A:78:ARG:HA	1:A:78:ARG:CZ	2.47	0.45
1:A:28:SER:HA	1:A:31:CYS:SG	2.56	0.45
1:A:197:GLY:O	1:A:201:GLU:HB2	2.17	0.44
1:A:168:LYS:HG2	1:A:170:PHE:CE2	2.52	0.44
1:B:48:LEU:HD21	1:B:70:ILE:HD11	2.00	0.44
1:B:56:ALA:O	1:B:60:GLU:HG3	2.18	0.43
1:A:78:ARG:HD2	3:A:491:HOH:O	2.17	0.43
1:B:47:ASN:HD22	1:B:47:ASN:C	2.26	0.42
1:B:134:ASP:OD2	1:B:136:ALA:HB3	2.19	0.42
1:A:177:VAL:HA	1:A:181:SER:O	2.21	0.41
1:A:47:ASN:C	1:A:47:ASN:HD22	2.28	0.41
1:A:86:LEU:HB3	1:A:87:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:O	1:A:206:LYS:HG2	2.20	0.41
1:A:152:ASN:ND2	1:A:157:GLY:HA2	2.36	0.41
1:B:117:GLY:HA2	1:B:145:VAL:O	2.21	0.40

All (2) 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)
1:A:103:GLN:HE21	3:B:524:HOH:H2[1_556]	1.22	0.38
1:A:96:ARG:HH22	3:B:456:HOH:H2[1_556]	1.28	0.32

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	195/214 (91%)	190 (97%)	5 (3%)	0	100	100
1	B	195/214 (91%)	191 (98%)	4 (2%)	0	100	100
All	All	390/428 (91%)	381 (98%)	9 (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	Percentiles	
1	A	146/160 (91%)	138 (94%)	8 (6%)	19	17
1	B	146/160 (91%)	138 (94%)	8 (6%)	19	17
All	All	292/320 (91%)	276 (94%)	16 (6%)	19	17

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	78	ARG
1	A	139	ASP
1	A	168	LYS
1	A	177	VAL
1	A	183	ILE
1	A	189	LEU
1	A	208	ARG
1	B	17	ARG
1	B	28	SER
1	B	47	ASN
1	B	70	ILE
1	B	78	ARG
1	B	86	LEU
1	B	134	ASP
1	B	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	71	GLN
1	A	121	GLN
1	A	152	ASN
1	B	27	ASN
1	B	47	ASN
1	B	71	GLN
1	B	121	GLN

5.3.3 RNA ⓘ

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](#)

2 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	DFP	B	401	1	6,9,9	2.44	2 (33%)	6,11,11	1.82	1 (16%)
2	DFP	A	401	1	6,9,9	1.90	2 (33%)	6,11,11	0.61	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
2	DFP	B	401	1	-	2/4/8/8	-
2	DFP	A	401	1	-	0/4/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	DFP	O2P-C1'	-5.06	1.36	1.45
2	A	401	DFP	O2P-C1'	-3.63	1.39	1.45
2	B	401	DFP	O1P-C1	-2.92	1.40	1.45
2	A	401	DFP	O1P-C1	-2.39	1.41	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	401	DFP	O1P-C1-C3	-4.08	93.64	107.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	DFP	C3'-C1'-O2P-P
2	B	401	DFP	C2'-C1'-O2P-P

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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.