



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 4FC9 / pdb\_00004fc9  
Title : Structure of the C-terminal domain of the type III effector Xcv3220 (XopL)  
Authors : Singer, A.U.; Xu, X.; Cui, H.; Tan, K.; Joachimiak, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2012-05-24  
Resolution : 1.80 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](mailto: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>.

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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

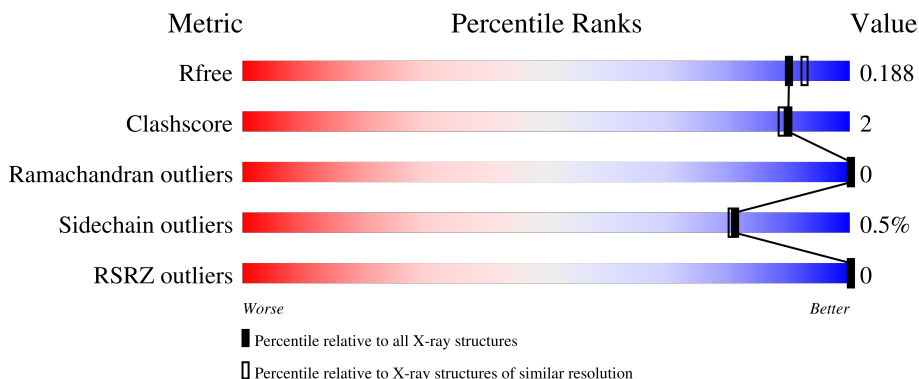
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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  $\geq 3$ , 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	208	 79% 18%
1	B	208	 81% 16%
1	C	208	 75% 6% 19%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4543 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 uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	B	175	1377	866	243	263	5	0	2	0
1	A	171	1405	881	253	266	5	0	6	0
1	C	169	1337	844	238	251	4	0	2	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	453	MSE	-	expression tag	UNP Q3BQL2
B	454	GLY	-	expression tag	UNP Q3BQL2
B	455	SER	-	expression tag	UNP Q3BQL2
B	456	SER	-	expression tag	UNP Q3BQL2
B	457	HIS	-	expression tag	UNP Q3BQL2
B	458	HIS	-	expression tag	UNP Q3BQL2
B	459	HIS	-	expression tag	UNP Q3BQL2
B	460	HIS	-	expression tag	UNP Q3BQL2
B	461	HIS	-	expression tag	UNP Q3BQL2
B	462	HIS	-	expression tag	UNP Q3BQL2
B	463	SER	-	expression tag	UNP Q3BQL2
B	464	SER	-	expression tag	UNP Q3BQL2
B	465	GLY	-	expression tag	UNP Q3BQL2
B	466	ARG	-	expression tag	UNP Q3BQL2
B	467	GLU	-	expression tag	UNP Q3BQL2
B	468	ASN	-	expression tag	UNP Q3BQL2
B	469	LEU	-	expression tag	UNP Q3BQL2
B	470	TYR	-	expression tag	UNP Q3BQL2
B	471	PHE	-	expression tag	UNP Q3BQL2
B	472	GLN	-	expression tag	UNP Q3BQL2
B	473	GLY	-	expression tag	UNP Q3BQL2
A	453	MSE	-	expression tag	UNP Q3BQL2
A	454	GLY	-	expression tag	UNP Q3BQL2

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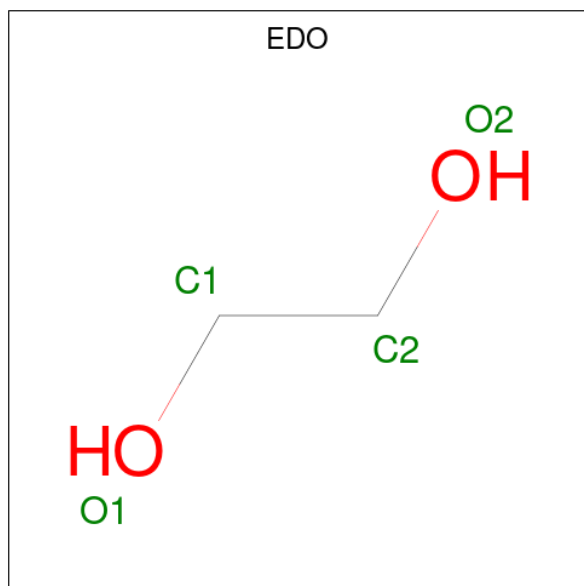
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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	SER	-	expression tag	UNP Q3BQL2
A	456	SER	-	expression tag	UNP Q3BQL2
A	457	HIS	-	expression tag	UNP Q3BQL2
A	458	HIS	-	expression tag	UNP Q3BQL2
A	459	HIS	-	expression tag	UNP Q3BQL2
A	460	HIS	-	expression tag	UNP Q3BQL2
A	461	HIS	-	expression tag	UNP Q3BQL2
A	462	HIS	-	expression tag	UNP Q3BQL2
A	463	SER	-	expression tag	UNP Q3BQL2
A	464	SER	-	expression tag	UNP Q3BQL2
A	465	GLY	-	expression tag	UNP Q3BQL2
A	466	ARG	-	expression tag	UNP Q3BQL2
A	467	GLU	-	expression tag	UNP Q3BQL2
A	468	ASN	-	expression tag	UNP Q3BQL2
A	469	LEU	-	expression tag	UNP Q3BQL2
A	470	TYR	-	expression tag	UNP Q3BQL2
A	471	PHE	-	expression tag	UNP Q3BQL2
A	472	GLN	-	expression tag	UNP Q3BQL2
A	473	GLY	-	expression tag	UNP Q3BQL2
C	453	MSE	-	expression tag	UNP Q3BQL2
C	454	GLY	-	expression tag	UNP Q3BQL2
C	455	SER	-	expression tag	UNP Q3BQL2
C	456	SER	-	expression tag	UNP Q3BQL2
C	457	HIS	-	expression tag	UNP Q3BQL2
C	458	HIS	-	expression tag	UNP Q3BQL2
C	459	HIS	-	expression tag	UNP Q3BQL2
C	460	HIS	-	expression tag	UNP Q3BQL2
C	461	HIS	-	expression tag	UNP Q3BQL2
C	462	HIS	-	expression tag	UNP Q3BQL2
C	463	SER	-	expression tag	UNP Q3BQL2
C	464	SER	-	expression tag	UNP Q3BQL2
C	465	GLY	-	expression tag	UNP Q3BQL2
C	466	ARG	-	expression tag	UNP Q3BQL2
C	467	GLU	-	expression tag	UNP Q3BQL2
C	468	ASN	-	expression tag	UNP Q3BQL2
C	469	LEU	-	expression tag	UNP Q3BQL2
C	470	TYR	-	expression tag	UNP Q3BQL2
C	471	PHE	-	expression tag	UNP Q3BQL2
C	472	GLN	-	expression tag	UNP Q3BQL2
C	473	GLY	-	expression tag	UNP Q3BQL2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	165	Total O 172 172	0	7
4	A	159	Total O 165 165	0	6
4	C	68	Total O 72 72	0	4



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.20Å 119.20Å 38.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.63 – 1.80 28.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (28.63-1.80) 91.0 (28.63-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.80Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.152 , 0.196 0.147 , 0.188	Depositor DCC
$R_{free}$ test set	1972 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.065 for -h,-k,l 0.277 for h,-h-k,-l 0.058 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO

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	0.36	0/1433	0.70	0/1939
1	B	0.38	0/1405	0.73	0/1905
1	C	0.37	0/1365	0.75	2/1850 (0.1%)
All	All	0.37	0/4203	0.73	2/5694 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	530	VAL	CA-C-N	5.43	124.89	119.24
1	C	530	VAL	C-N-CA	5.43	124.89	119.24

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	1405	0	1374	5	0
1	B	1377	0	1337	3	0
1	C	1337	0	1298	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	6	0	0
3	B	8	0	12	0	0
4	A	165	0	0	2	0
4	B	172	0	0	0	0
4	C	72	0	0	0	0
All	All	4543	0	4027	15	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 2.

The worst 5 of 15 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:569[B]:ARG:NH1	4:A:959:HOH:O	2.32	0.62
1:A:526:THR:HG21	1:C:523:ASP:HB3	1.82	0.62
1:C:499:THR:O	1:C:503:GLU:HB2	2.14	0.47
1:C:506:ASN:O	1:C:512:ALA:HA	2.16	0.46
1:B:511:GLY:HA3	1:C:511:GLY:HA3	1.98	0.45

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	176/208 (85%)	175 (99%)	1 (1%)	0	100	100
1	B	175/208 (84%)	174 (99%)	1 (1%)	0	100	100
1	C	167/208 (80%)	163 (98%)	4 (2%)	0	100	100
All	All	518/624 (83%)	512 (99%)	6 (1%)	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	150/172 (87%)	150 (100%)	0	100	100
1	B	146/172 (85%)	144 (99%)	2 (1%)	59	52
1	C	141/172 (82%)	141 (100%)	0	100	100
All	All	437/516 (85%)	435 (100%)	2 (0%)	81	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	502	ASP
1	B	636	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	624	HIS
1	C	547	GLN

### 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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
3	EDO	B	702	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	A	702	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	B	703	-	3,3,3	0.43	0	2,2,2	0.37	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	A	702	-	-	0/1/1/1	-
3	EDO	B	703	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	703	EDO	O1-C1-C2-O2

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	167/208 (80%)	-1.38	0 100 100	7, 27, 45, 60	5 (2%)
1	B	171/208 (82%)	-1.38	0 100 100	12, 27, 48, 80	1 (0%)
1	C	165/208 (79%)	-1.07	0 100 100	18, 40, 65, 86	2 (1%)
All	All	503/624 (80%)	-1.28	0 100 100	7, 32, 58, 86	8 (1%)

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	B	702	4/4	0.97	0.07	39,39,40,41	0
3	EDO	B	703	4/4	0.98	0.04	42,42,43,45	0
2	CL	C	701	1/1	0.99	0.03	46,46,46,46	0
3	EDO	A	702	4/4	0.99	0.05	38,39,40,43	0
2	CL	B	701	1/1	1.00	0.01	30,30,30,30	0
2	CL	A	701	1/1	1.00	0.02	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.