



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 12:03 am BST

PDB ID : 6K94  
Title : Crystal structure of the type III effector XopAI from *Xanthomonas axonopodis* pv. citri - a 70 residue N-terminal truncation  
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Deposited on : 2019-06-14  
Resolution : 2.26 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

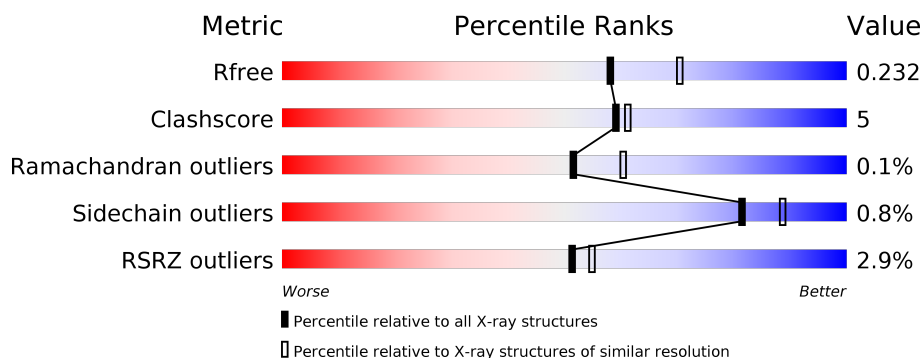
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	247	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>
1	B	247	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	247	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	D	247	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14908 atoms, of which 6996 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 Type III effector XopAI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	224	Total	C	H	N	O	S	0	0	0
			3626	1164	1774	331	349	8			
1	B	226	Total	C	H	N	O	S	0	0	0
			3598	1157	1755	329	349	8			
1	C	224	Total	C	H	N	O	S	0	0	0
			3583	1155	1744	326	350	8			
1	D	224	Total	C	H	N	O	S	0	0	0
			3543	1147	1723	321	344	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP Q8PHM1
A	51	GLY	-	expression tag	UNP Q8PHM1
A	52	SER	-	expression tag	UNP Q8PHM1
A	53	SER	-	expression tag	UNP Q8PHM1
A	54	HIS	-	expression tag	UNP Q8PHM1
A	55	HIS	-	expression tag	UNP Q8PHM1
A	56	HIS	-	expression tag	UNP Q8PHM1
A	57	HIS	-	expression tag	UNP Q8PHM1
A	58	HIS	-	expression tag	UNP Q8PHM1
A	59	HIS	-	expression tag	UNP Q8PHM1
A	60	SER	-	expression tag	UNP Q8PHM1
A	61	SER	-	expression tag	UNP Q8PHM1
A	62	GLY	-	expression tag	UNP Q8PHM1
A	63	LEU	-	expression tag	UNP Q8PHM1
A	64	VAL	-	expression tag	UNP Q8PHM1
A	65	PRO	-	expression tag	UNP Q8PHM1
A	66	ARG	-	expression tag	UNP Q8PHM1
A	67	GLY	-	expression tag	UNP Q8PHM1
A	68	SER	-	expression tag	UNP Q8PHM1
A	69	HIS	-	expression tag	UNP Q8PHM1
A	70	MET	-	expression tag	UNP Q8PHM1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	50	MET	-	expression tag	UNP Q8PHM1
B	51	GLY	-	expression tag	UNP Q8PHM1
B	52	SER	-	expression tag	UNP Q8PHM1
B	53	SER	-	expression tag	UNP Q8PHM1
B	54	HIS	-	expression tag	UNP Q8PHM1
B	55	HIS	-	expression tag	UNP Q8PHM1
B	56	HIS	-	expression tag	UNP Q8PHM1
B	57	HIS	-	expression tag	UNP Q8PHM1
B	58	HIS	-	expression tag	UNP Q8PHM1
B	59	HIS	-	expression tag	UNP Q8PHM1
B	60	SER	-	expression tag	UNP Q8PHM1
B	61	SER	-	expression tag	UNP Q8PHM1
B	62	GLY	-	expression tag	UNP Q8PHM1
B	63	LEU	-	expression tag	UNP Q8PHM1
B	64	VAL	-	expression tag	UNP Q8PHM1
B	65	PRO	-	expression tag	UNP Q8PHM1
B	66	ARG	-	expression tag	UNP Q8PHM1
B	67	GLY	-	expression tag	UNP Q8PHM1
B	68	SER	-	expression tag	UNP Q8PHM1
B	69	HIS	-	expression tag	UNP Q8PHM1
B	70	MET	-	expression tag	UNP Q8PHM1
C	50	MET	-	expression tag	UNP Q8PHM1
C	51	GLY	-	expression tag	UNP Q8PHM1
C	52	SER	-	expression tag	UNP Q8PHM1
C	53	SER	-	expression tag	UNP Q8PHM1
C	54	HIS	-	expression tag	UNP Q8PHM1
C	55	HIS	-	expression tag	UNP Q8PHM1
C	56	HIS	-	expression tag	UNP Q8PHM1
C	57	HIS	-	expression tag	UNP Q8PHM1
C	58	HIS	-	expression tag	UNP Q8PHM1
C	59	HIS	-	expression tag	UNP Q8PHM1
C	60	SER	-	expression tag	UNP Q8PHM1
C	61	SER	-	expression tag	UNP Q8PHM1
C	62	GLY	-	expression tag	UNP Q8PHM1
C	63	LEU	-	expression tag	UNP Q8PHM1
C	64	VAL	-	expression tag	UNP Q8PHM1
C	65	PRO	-	expression tag	UNP Q8PHM1
C	66	ARG	-	expression tag	UNP Q8PHM1
C	67	GLY	-	expression tag	UNP Q8PHM1
C	68	SER	-	expression tag	UNP Q8PHM1
C	69	HIS	-	expression tag	UNP Q8PHM1
C	70	MET	-	expression tag	UNP Q8PHM1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	50	MET	-	expression tag	UNP Q8PHM1
D	51	GLY	-	expression tag	UNP Q8PHM1
D	52	SER	-	expression tag	UNP Q8PHM1
D	53	SER	-	expression tag	UNP Q8PHM1
D	54	HIS	-	expression tag	UNP Q8PHM1
D	55	HIS	-	expression tag	UNP Q8PHM1
D	56	HIS	-	expression tag	UNP Q8PHM1
D	57	HIS	-	expression tag	UNP Q8PHM1
D	58	HIS	-	expression tag	UNP Q8PHM1
D	59	HIS	-	expression tag	UNP Q8PHM1
D	60	SER	-	expression tag	UNP Q8PHM1
D	61	SER	-	expression tag	UNP Q8PHM1
D	62	GLY	-	expression tag	UNP Q8PHM1
D	63	LEU	-	expression tag	UNP Q8PHM1
D	64	VAL	-	expression tag	UNP Q8PHM1
D	65	PRO	-	expression tag	UNP Q8PHM1
D	66	ARG	-	expression tag	UNP Q8PHM1
D	67	GLY	-	expression tag	UNP Q8PHM1
D	68	SER	-	expression tag	UNP Q8PHM1
D	69	HIS	-	expression tag	UNP Q8PHM1
D	70	MET	-	expression tag	UNP Q8PHM1

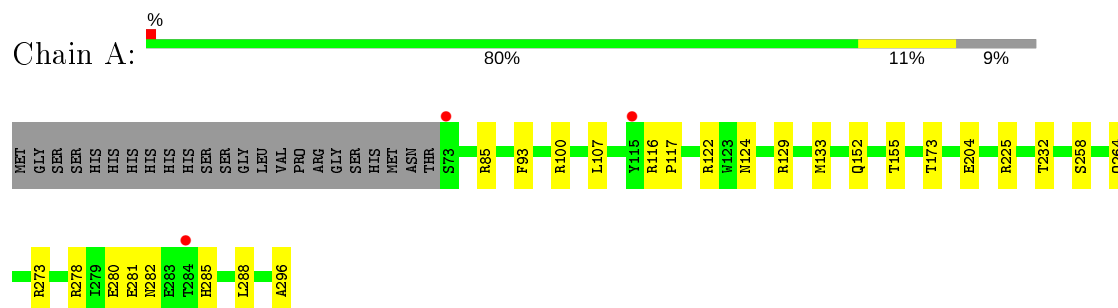
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	173	Total	O	0	0
			173	173		
2	B	150	Total	O	0	0
			150	150		
2	C	136	Total	O	0	0
			136	136		
2	D	99	Total	O	0	0
			99	99		

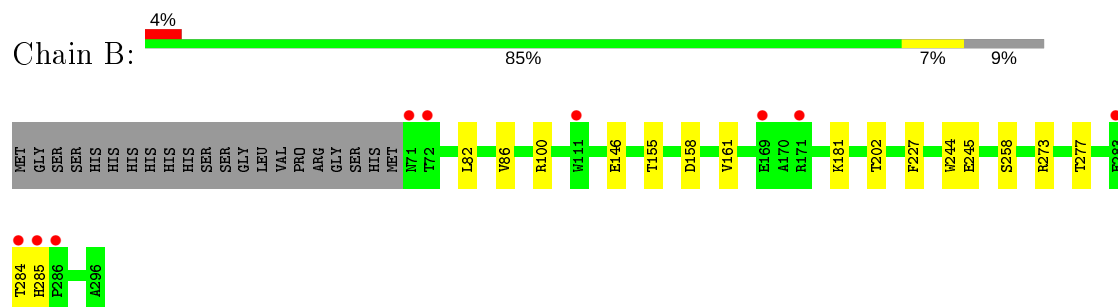
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

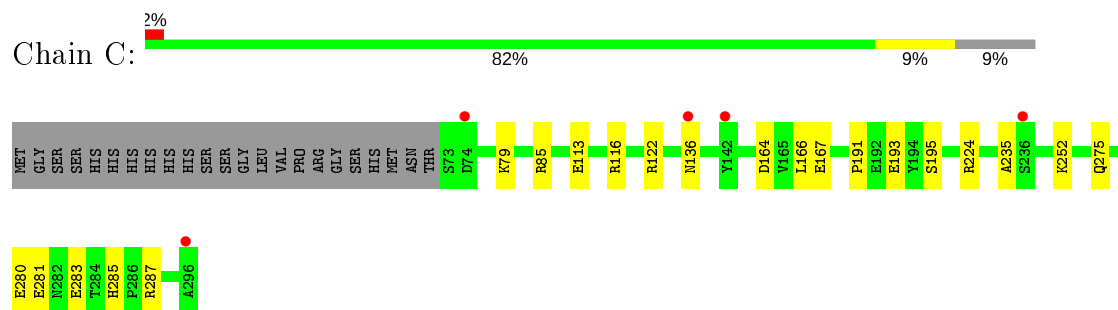
#### • Molecule 1: Type III effector XopAI



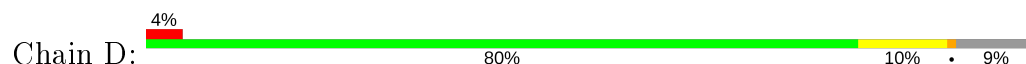
#### • Molecule 1: Type III effector XopAI

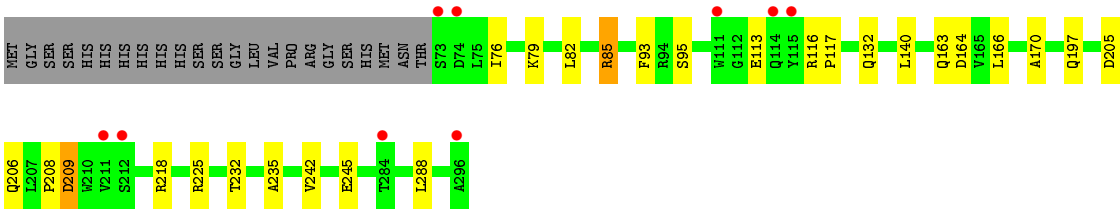


#### • Molecule 1: Type III effector XopAI



#### • Molecule 1: Type III effector XopAI





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.78Å 98.76Å 77.45Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	31.53 – 2.26 31.53 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.4 (31.53-2.26) 99.4 (31.53-2.26)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, $R_{free}$	0.189 , 0.232 0.189 , 0.232	Depositor DCC
$R_{free}$ test set	2222 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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](#)

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	0/1898	0.43	0/2567
1	B	0.29	0/1887	0.46	0/2552
1	C	0.27	0/1885	0.44	0/2553
1	D	0.25	0/1866	0.42	0/2529
All	All	0.27	0/7536	0.44	0/10201

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 [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	1852	1774	1774	17	0
1	B	1843	1755	1755	15	0
1	C	1839	1744	1744	14	0
1	D	1820	1723	1723	24	0
2	A	173	0	0	5	3
2	B	150	0	0	6	4
2	C	136	0	0	8	1
2	D	99	0	0	13	0
All	All	7912	6996	6996	68	4

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 5.

The worst 5 of 68 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:173:THR:OG1	2:A:301:HOH:O	1.55	1.22
1:C:287:ARG:NH1	2:C:301:HOH:O	1.75	1.16
1:D:132:GLN:OE1	2:D:302:HOH:O	1.74	1.06
1:D:85:ARG:NH2	2:D:303:HOH:O	1.93	0.99
1:A:100:ARG:NH2	2:A:302:HOH:O	2.03	0.90

All (4) 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)
2:A:400:HOH:O	2:B:310:HOH:O[2_545]	2.02	0.18
2:A:403:HOH:O	2:B:386:HOH:O[2_545]	2.06	0.14
2:B:432:HOH:O	2:C:331:HOH:O[1_565]	2.07	0.13
2:A:453:HOH:O	2:B:400:HOH:O[2_545]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	222/247 (90%)	220 (99%)	2 (1%)	0	100	100
1	B	224/247 (91%)	220 (98%)	4 (2%)	0	100	100
1	C	222/247 (90%)	219 (99%)	3 (1%)	0	100	100
1	D	222/247 (90%)	217 (98%)	4 (2%)	1 (0%)	29	29
All	All	890/988 (90%)	876 (98%)	13 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	209	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	195/219 (89%)	194 (100%)	1 (0%)	88	92
1	B	192/219 (88%)	192 (100%)	0	100	100
1	C	193/219 (88%)	190 (98%)	3 (2%)	62	73
1	D	189/219 (86%)	187 (99%)	2 (1%)	73	82
All	All	769/876 (88%)	763 (99%)	6 (1%)	81	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	275	GLN
1	D	206	GLN
1	C	285	HIS
1	C	136	ASN
1	D	85	ARG

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

Mol	Chain	Res	Type
1	A	264	GLN
1	D	137	HIS

### 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 carbohydrates 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 [i](#)

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	224/247 (90%)	-0.22	3 (1%) 77 79	14, 26, 54, 70	0
1	B	226/247 (91%)	0.08	9 (3%) 38 40	14, 30, 63, 93	0
1	C	224/247 (90%)	-0.21	5 (2%) 62 65	16, 31, 54, 77	0
1	D	224/247 (90%)	0.10	9 (4%) 38 40	18, 38, 65, 81	0
All	All	898/988 (90%)	-0.06	26 (2%) 51 55	14, 32, 61, 93	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	GLU	4.5
1	B	285	HIS	4.3
1	D	115	TYR	4.1
1	A	73	SER	3.7
1	B	72	THR	3.4

### 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 carbohydrates 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.