



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 12:10 pm BST

PDB ID : 5VFX  
Title : Structure of an accessory protein of the pCW3 relaxosome in complex with the origin of transfer (oriT) DNA  
Authors : Traore, D.A.K.; Wisniewski, J.A.; Flanigan, S.F.; Conroy, P.J.; Panjikar, S.; Mok, Y.-F.; Lao, C.; Griffin, M.D.W.; Adams, V.; Rood, J.I.; Whisstock, J.C.  
Deposited on : 2017-04-10  
Resolution : 2.81 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

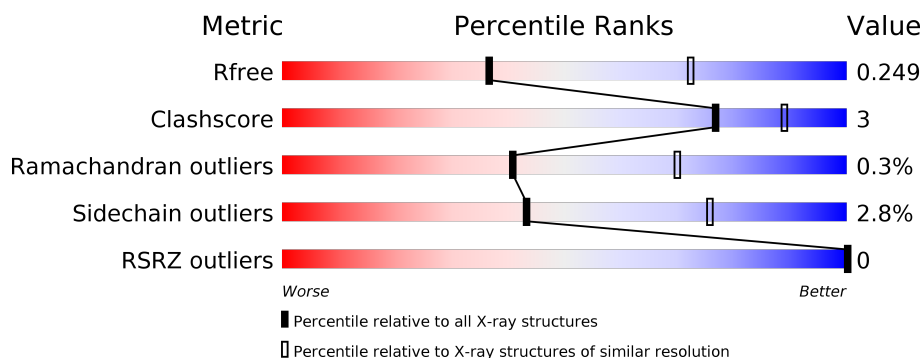
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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.








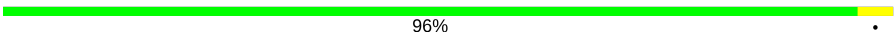



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 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	107	
1	B	107	
1	C	107	
1	D	107	
1	E	107	
1	F	107	

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Mol	Chain	Length	Quality of chain
1	G	107	 83%7%7%
1	H	107	 81%11%7%
2	I	23	 74%26%
2	K	23	 78%22%
2	N	23	 65%30%.
2	O	23	 74%22%.
3	J	23	 96%.
3	L	23	 83%17%
3	M	23	 83%17%
3	P	23	 87%13%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10251 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 TcpK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			821	535	134	149	3			
1	B	100	Total	C	N	O	S	0	0	0
			817	532	135	146	4			
1	C	100	Total	C	N	O	S	0	0	0
			826	537	134	151	4			
1	D	99	Total	C	N	O	S	0	0	0
			808	525	137	142	4			
1	E	100	Total	C	N	O	S	0	0	0
			779	501	130	146	2			
1	F	101	Total	C	N	O	S	0	0	0
			822	533	138	147	4			
1	G	100	Total	C	N	O	S	0	0	0
			823	531	137	151	4			
1	H	99	Total	C	N	O	S	0	0	0
			776	504	124	144	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLN	-	expression tag	UNP Q1PLI2
A	-3	ASN	-	expression tag	UNP Q1PLI2
A	-2	SER	-	expression tag	UNP Q1PLI2
A	-1	HIS	-	expression tag	UNP Q1PLI2
A	0	MET	-	expression tag	UNP Q1PLI2
A	1	VAL	-	expression tag	UNP Q1PLI2
B	-4	GLN	-	expression tag	UNP Q1PLI2
B	-3	ASN	-	expression tag	UNP Q1PLI2
B	-2	SER	-	expression tag	UNP Q1PLI2
B	-1	HIS	-	expression tag	UNP Q1PLI2
B	0	MET	-	expression tag	UNP Q1PLI2
B	1	VAL	-	expression tag	UNP Q1PLI2
C	-4	GLN	-	expression tag	UNP Q1PLI2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ASN	-	expression tag	UNP Q1PLI2
C	-2	SER	-	expression tag	UNP Q1PLI2
C	-1	HIS	-	expression tag	UNP Q1PLI2
C	0	MET	-	expression tag	UNP Q1PLI2
C	1	VAL	-	expression tag	UNP Q1PLI2
D	-4	GLN	-	expression tag	UNP Q1PLI2
D	-3	ASN	-	expression tag	UNP Q1PLI2
D	-2	SER	-	expression tag	UNP Q1PLI2
D	-1	HIS	-	expression tag	UNP Q1PLI2
D	0	MET	-	expression tag	UNP Q1PLI2
D	1	VAL	-	expression tag	UNP Q1PLI2
E	-4	GLN	-	expression tag	UNP Q1PLI2
E	-3	ASN	-	expression tag	UNP Q1PLI2
E	-2	SER	-	expression tag	UNP Q1PLI2
E	-1	HIS	-	expression tag	UNP Q1PLI2
E	0	MET	-	expression tag	UNP Q1PLI2
E	1	VAL	-	expression tag	UNP Q1PLI2
F	-4	GLN	-	expression tag	UNP Q1PLI2
F	-3	ASN	-	expression tag	UNP Q1PLI2
F	-2	SER	-	expression tag	UNP Q1PLI2
F	-1	HIS	-	expression tag	UNP Q1PLI2
F	0	MET	-	expression tag	UNP Q1PLI2
F	1	VAL	-	expression tag	UNP Q1PLI2
G	-4	GLN	-	expression tag	UNP Q1PLI2
G	-3	ASN	-	expression tag	UNP Q1PLI2
G	-2	SER	-	expression tag	UNP Q1PLI2
G	-1	HIS	-	expression tag	UNP Q1PLI2
G	0	MET	-	expression tag	UNP Q1PLI2
G	1	VAL	-	expression tag	UNP Q1PLI2
H	-4	GLN	-	expression tag	UNP Q1PLI2
H	-3	ASN	-	expression tag	UNP Q1PLI2
H	-2	SER	-	expression tag	UNP Q1PLI2
H	-1	HIS	-	expression tag	UNP Q1PLI2
H	0	MET	-	expression tag	UNP Q1PLI2
H	1	VAL	-	expression tag	UNP Q1PLI2

- Molecule 2 is a DNA chain called oriT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	23	Total	C	N	O	P	0	0	0
			473	227	91	133	22			
2	K	23	Total	C	N	O	P	0	0	0
			473	227	91	133	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	23	Total	C	N	O	P	0	0	0
			472	227	91	132	22			
2	O	23	Total	C	N	O	P	0	0	0
			472	227	91	132	22			

- Molecule 3 is a DNA chain called oriT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	23	Total	C	N	O	P	0	0	0
			467	225	78	141	23			
3	L	23	Total	C	N	O	P	0	0	0
			464	225	78	139	22			
3	M	23	Total	C	N	O	P	0	0	0
			467	225	78	141	23			
3	P	23	Total	C	N	O	P	0	0	0
			464	225	78	139	22			


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	8	Total	O	0	0
			8	8		
4	C	3	Total	O	0	0
			3	3		
4	D	4	Total	O	0	0
			4	4		
4	F	7	Total	O	0	0
			7	7		
4	G	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		

### 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.

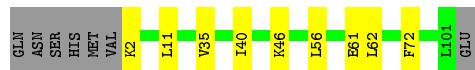
#### • Molecule 1: TcpK

Chain A:  84% 7% • 7%




#### • Molecule 1: TcpK

Chain B:  85% 8% 7%




#### • Molecule 1: TcpK

Chain C:  87% 5% • 7%




#### • Molecule 1: TcpK

Chain D:  87% 5% • 7%




#### • Molecule 1: TcpK

Chain E:  89% 5% 7%

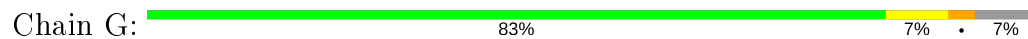


#### • Molecule 1: TcpK

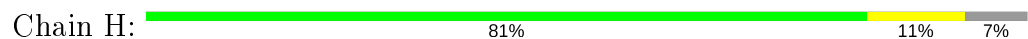
Chain F:  87% 7% 6%



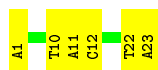
- Molecule 1: TcpK



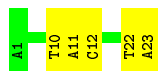
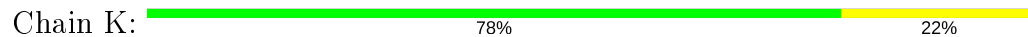
- Molecule 1: TcpK



- Molecule 2: oriT



- Molecule 2: oriT



- Molecule 2: oriT



- Molecule 2: oriT



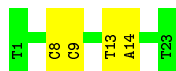
- Molecule 3: oriT





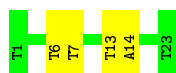
- Molecule 3: oriT

Chain L:   
83% 17%



- Molecule 3: oriT

Chain M:   
83% 17%



- Molecule 3: oriT

Chain P:   
87% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.50Å 109.89Å 122.78Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	43.08 – 2.81 41.48 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.08-2.81) 98.5 (41.48-2.81)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.198 , 0.233 0.217 , 0.249	Depositor DCC
$R_{free}$ test set	2236 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.50	0/836	0.69	0/1129
1	B	0.56	0/831	0.71	1/1120 (0.1%)
1	C	0.55	0/841	0.69	1/1136 (0.1%)
1	D	0.50	0/823	0.64	0/1109
1	E	0.47	0/793	0.63	0/1075
1	F	0.48	0/837	0.65	0/1130
1	G	0.48	0/838	0.65	0/1132
1	H	0.49	0/791	0.66	0/1074
2	I	1.05	0/532	1.06	1/820 (0.1%)
2	K	1.06	0/532	1.02	1/820 (0.1%)
2	N	1.04	0/531	1.01	1/819 (0.1%)
2	O	1.05	0/531	1.03	2/819 (0.2%)
3	J	1.12	0/521	1.00	0/801
3	L	1.14	0/518	1.04	0/797
3	M	1.03	0/521	1.02	0/801
3	P	1.19	0/518	0.97	0/797
All	All	0.78	0/10794	0.83	7/15379 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	12	DC	O4'-C4'-C3'	-8.16	101.10	106.00
2	K	12	DC	O4'-C4'-C3'	-6.69	101.82	104.50
2	O	12	DC	O4'-C4'-C3'	-6.54	101.89	104.50
2	N	12	DC	O4'-C4'-C3'	-6.32	101.97	104.50
1	B	72	PHE	C-N-CA	5.97	136.63	121.70

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	821	0	793	7	0
1	B	817	0	801	6	0
1	C	826	0	807	3	0
1	D	808	0	785	3	0
1	E	779	0	698	5	0
1	F	822	0	797	6	0
1	G	823	0	793	9	0
1	H	776	0	712	5	0
2	I	473	0	261	4	0
2	K	473	0	261	2	0
2	N	472	0	258	5	0
2	O	472	0	258	4	0
3	J	467	0	263	3	0
3	L	464	0	264	2	0
3	M	467	0	263	2	0
3	P	464	0	264	2	0
4	A	2	0	0	0	0
4	B	8	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	F	7	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
All	All	10251	0	8278	55	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 3.

The worst 5 of 55 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:G:37:THR:HG21	1:G:73:ASN:HD22	1.37	0.87
2:I:1:DA:H2	3:J:23:DT:H3	1.29	0.79
1:D:31:LYS:HZ3	1:D:91:SER:H	1.36	0.73
1:A:95:ILE:HG12	1:B:61:GLU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:VAL:HG13	1:G:34:TYR:HB2	1.77	0.65

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	98/107 (92%)	94 (96%)	3 (3%)	1 (1%)	15	42
1	B	98/107 (92%)	94 (96%)	4 (4%)	0	100	100
1	C	98/107 (92%)	94 (96%)	4 (4%)	0	100	100
1	D	97/107 (91%)	91 (94%)	5 (5%)	1 (1%)	15	42
1	E	98/107 (92%)	94 (96%)	4 (4%)	0	100	100
1	F	99/107 (92%)	92 (93%)	7 (7%)	0	100	100
1	G	98/107 (92%)	94 (96%)	4 (4%)	0	100	100
1	H	97/107 (91%)	93 (96%)	4 (4%)	0	100	100
All	All	783/856 (92%)	746 (95%)	35 (4%)	2 (0%)	41	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	69	GLU
1	A	22	ASN

### 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	81/102 (79%)	78 (96%)	3 (4%)	34	66
1	B	81/102 (79%)	78 (96%)	3 (4%)	34	66
1	C	85/102 (83%)	83 (98%)	2 (2%)	49	80
1	D	81/102 (79%)	79 (98%)	2 (2%)	47	78
1	E	70/102 (69%)	69 (99%)	1 (1%)	67	89
1	F	83/102 (81%)	83 (100%)	0	100	100
1	G	85/102 (83%)	81 (95%)	4 (5%)	26	57
1	H	74/102 (72%)	71 (96%)	3 (4%)	30	63
All	All	640/816 (78%)	622 (97%)	18 (3%)	43	76

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	40	ILE
1	D	100	TYR
1	G	101	LEU
1	C	40	ILE
1	C	95	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	5	ASN
1	F	82	ASN
1	G	82	ASN
1	H	29	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 ⓘ

### 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, 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	100/107 (93%)	-0.22	0 100 100	43, 62, 80, 93	0
1	B	100/107 (93%)	-0.33	0 100 100	38, 51, 78, 92	0
1	C	100/107 (93%)	-0.33	0 100 100	34, 47, 64, 78	0
1	D	99/107 (92%)	-0.47	0 100 100	41, 58, 79, 93	0
1	E	100/107 (93%)	-0.24	0 100 100	58, 77, 95, 104	0
1	F	101/107 (94%)	-0.24	0 100 100	45, 60, 88, 114	0
1	G	100/107 (93%)	-0.31	0 100 100	44, 69, 88, 100	0
1	H	99/107 (92%)	-0.36	0 100 100	54, 73, 91, 99	0
2	I	23/23 (100%)	-0.48	0 100 100	48, 62, 93, 107	0
2	K	23/23 (100%)	-0.49	0 100 100	41, 58, 77, 95	0
2	N	23/23 (100%)	-0.32	0 100 100	75, 106, 137, 142	0
2	O	23/23 (100%)	-0.54	0 100 100	49, 61, 77, 81	0
3	J	23/23 (100%)	-0.41	0 100 100	49, 66, 87, 108	0
3	L	23/23 (100%)	-0.52	0 100 100	47, 56, 79, 89	0
3	M	23/23 (100%)	-0.07	0 100 100	76, 99, 127, 146	0
3	P	23/23 (100%)	-0.52	0 100 100	53, 63, 74, 83	0
All	All	983/1040 (94%)	-0.33	0 100 100	34, 63, 95, 146	0

There are no RSRZ outliers to report.

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

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.