



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:23 PM GMT

PDB ID : 3TU3  
Title : 1.92 Angstrom resolution crystal structure of the full-length SpcU in complex with full-length ExoU from the type III secretion system of *Pseudomonas aeruginosa*  
Authors : Halavaty, A.S.; Borek, D.; Otwinowski, Z.; Minasov, G.; Veesenmeyer, J.L.; Tyson, G.; Shuvalova, L.; Hauser, A.R.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-09-15  
Resolution : 1.92 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

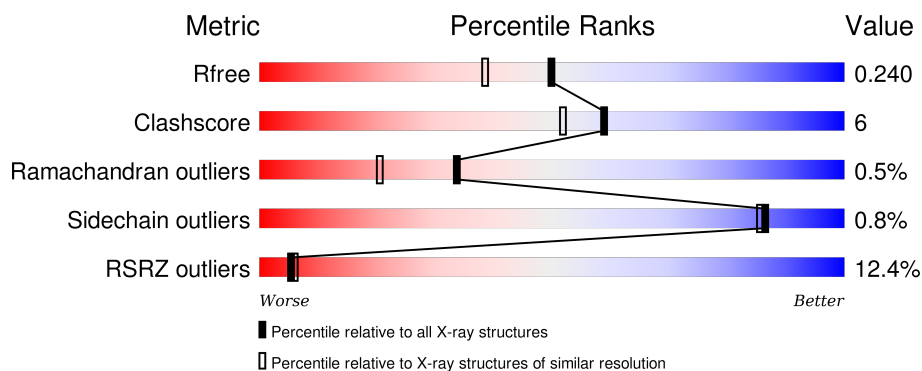
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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. 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	161	<div> <div>9%</div> <div>61%</div> <div>12%</div> <div>•</div> <div>26%</div> </div>
2	B	711	<div> <div>9%</div> <div>66%</div> <div>8%</div> <div>26%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5674 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 ExoU chaperone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	4	0
			958	610	169	177	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP O66100
A	-22	HIS	-	EXPRESSION TAG	UNP O66100
A	-21	HIS	-	EXPRESSION TAG	UNP O66100
A	-20	HIS	-	EXPRESSION TAG	UNP O66100
A	-19	HIS	-	EXPRESSION TAG	UNP O66100
A	-18	HIS	-	EXPRESSION TAG	UNP O66100
A	-17	HIS	-	EXPRESSION TAG	UNP O66100
A	-16	SER	-	EXPRESSION TAG	UNP O66100
A	-15	SER	-	EXPRESSION TAG	UNP O66100
A	-14	GLY	-	EXPRESSION TAG	UNP O66100
A	-13	VAL	-	EXPRESSION TAG	UNP O66100
A	-12	ASP	-	EXPRESSION TAG	UNP O66100
A	-11	LEU	-	EXPRESSION TAG	UNP O66100
A	-10	GLY	-	EXPRESSION TAG	UNP O66100
A	-9	THR	-	EXPRESSION TAG	UNP O66100
A	-8	GLU	-	EXPRESSION TAG	UNP O66100
A	-7	ASN	-	EXPRESSION TAG	UNP O66100
A	-6	LEU	-	EXPRESSION TAG	UNP O66100
A	-5	TYR	-	EXPRESSION TAG	UNP O66100
A	-4	PHE	-	EXPRESSION TAG	UNP O66100
A	-3	GLN	-	EXPRESSION TAG	UNP O66100
A	-2	SER	-	EXPRESSION TAG	UNP O66100
A	-1	ASN	-	EXPRESSION TAG	UNP O66100
A	0	ALA	-	EXPRESSION TAG	UNP O66100

- Molecule 2 is a protein called ExoU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	526	Total	C	N	O	S	0	24	0
			4215	2610	767	826	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	EXPRESSION TAG	UNP O34208
B	-22	HIS	-	EXPRESSION TAG	UNP O34208
B	-21	HIS	-	EXPRESSION TAG	UNP O34208
B	-20	HIS	-	EXPRESSION TAG	UNP O34208
B	-19	HIS	-	EXPRESSION TAG	UNP O34208
B	-18	HIS	-	EXPRESSION TAG	UNP O34208
B	-17	HIS	-	EXPRESSION TAG	UNP O34208
B	-16	SER	-	EXPRESSION TAG	UNP O34208
B	-15	SER	-	EXPRESSION TAG	UNP O34208
B	-14	GLY	-	EXPRESSION TAG	UNP O34208
B	-13	VAL	-	EXPRESSION TAG	UNP O34208
B	-12	ASP	-	EXPRESSION TAG	UNP O34208
B	-11	LEU	-	EXPRESSION TAG	UNP O34208
B	-10	GLY	-	EXPRESSION TAG	UNP O34208
B	-9	THR	-	EXPRESSION TAG	UNP O34208
B	-8	GLU	-	EXPRESSION TAG	UNP O34208
B	-7	ASN	-	EXPRESSION TAG	UNP O34208
B	-6	LEU	-	EXPRESSION TAG	UNP O34208
B	-5	TYR	-	EXPRESSION TAG	UNP O34208
B	-4	PHE	-	EXPRESSION TAG	UNP O34208
B	-3	GLN	-	EXPRESSION TAG	UNP O34208
B	-2	SER	-	EXPRESSION TAG	UNP O34208
B	-1	ASN	-	EXPRESSION TAG	UNP O34208
B	0	ALA	-	EXPRESSION TAG	UNP O34208

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	3
			56	56		
3	B	436	Total	O	0	18
			445	445		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.14Å 52.58Å 119.54Å 90.00° 126.59° 90.00°	Depositor
Resolution (Å)	29.17 – 1.92 27.13 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.17-1.92) 99.8 (27.13-1.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.191 , 0.225 0.210 , 0.240	Depositor DCC
$R_{free}$ test set	2975 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 58993 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.41	0/977	0.73	0/1332
2	B	0.44	0/4272	0.67	0/5776
All	All	0.43	0/5249	0.68	0/7108

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	958	0	969	19	0
2	B	4215	0	4206	47	0
3	A	56	0	0	0	0
3	B	445	0	0	4	0
All	All	5674	0	5175	60	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 6.

All (60) 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:76:LEU:HD11	1:A:84[B]:LEU:HD21	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD11	1:A:84[B]:LEU:CD2	1.94	0.97
2:B:287:THR:HG23	2:B:351:VAL:HG22	1.75	0.68
2:B:186:ILE:HG22	2:B:186:ILE:O	1.94	0.65
2:B:209:LEU:C	2:B:209:LEU:HD23	2.21	0.61
1:A:16:SER:O	1:A:18:ASP:N	2.34	0.60
1:A:45:GLU:CG	1:A:83:ARG:HD3	2.33	0.59
2:B:175:SER:O	2:B:176:SER:C	2.41	0.59
2:B:425:VAL:HG13	2:B:426:PRO:HD2	1.86	0.57
1:A:76:LEU:CD1	1:A:84[B]:LEU:CD2	2.75	0.56
2:B:59:VAL:O	2:B:59:VAL:HG22	2.04	0.56
2:B:186:ILE:CG2	2:B:186:ILE:O	2.56	0.53
2:B:175:SER:O	2:B:177:ASN:N	2.42	0.53
1:A:118:LEU:O	1:A:119:GLU:C	2.47	0.53
2:B:376:PHE:O	2:B:377:GLU:HB2	2.09	0.53
2:B:146:ILE:HG23	2:B:227:LEU:HD21	1.92	0.52
2:B:361:PHE:O	2:B:362[B]:ASP:OD2	2.28	0.52
1:A:45:GLU:HG3	1:A:83:ARG:HD3	1.90	0.52
2:B:571:VAL:O	2:B:575[A]:GLN:HG3	2.10	0.52
2:B:632[A]:ARG:NH1	3:B:1118[A]:HOH:O	2.42	0.51
1:A:24:GLN:HB2	2:B:65:SER:HB3	1.93	0.51
1:A:106[A]:ARG:NH1	1:A:109[A]:GLU:HG2	2.26	0.51
2:B:289:MET:HG2	2:B:349:ILE:CD1	2.42	0.50
2:B:67:PRO:HB2	2:B:477:THR:HG22	1.92	0.50
2:B:241[B]:THR:HG22	2:B:241[B]:THR:O	2.11	0.50
1:A:108:ARG:HH11	2:B:58:SER:CB	2.25	0.49
1:A:108:ARG:HH11	2:B:58:SER:HB2	1.77	0.49
2:B:177:ASN:OD1	2:B:178:LYS:HE3	2.13	0.49
2:B:617[A]:SER:OG	2:B:674:THR:OG1	2.24	0.49
1:A:108:ARG:NH1	2:B:58:SER:HB2	2.27	0.49
2:B:614:ILE:HD12	2:B:638:LEU:HD12	1.95	0.48
2:B:212:VAL:HG12	2:B:215:ARG:NH1	2.28	0.48
2:B:180:LEU:HD12	2:B:180:LEU:N	2.29	0.48
2:B:362[A]:ASP:OD2	3:B:1051:HOH:O	2.20	0.47
2:B:376:PHE:O	2:B:377:GLU:CB	2.62	0.47
2:B:141:SER:HB3	2:B:356:MET:SD	2.54	0.47
2:B:102:PRO:HB2	2:B:369:ASN:HA	1.96	0.47
2:B:362[A]:ASP:OD2	3:B:935:HOH:O	2.21	0.46
1:A:106[A]:ARG:NE	1:A:106[A]:ARG:HA	2.30	0.46
2:B:357:ILE:CD1	2:B:418:LEU:HD22	2.46	0.46
1:A:76:LEU:CD1	1:A:84[B]:LEU:HD21	2.25	0.46
2:B:114:ALA:HB2	2:B:170:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ILE:HD13	2:B:205:PHE:CE1	2.53	0.44
2:B:623:GLN:OE1	2:B:624:PRO:HD2	2.18	0.44
2:B:209:LEU:O	2:B:212:VAL:HG22	2.17	0.44
1:A:18:ASP:OD1	1:A:19:ALA:N	2.51	0.44
2:B:209:LEU:HD23	2:B:209:LEU:O	2.17	0.43
2:B:615:PHE:HB3	2:B:616:PRO:HD3	2.00	0.43
1:A:85:VAL:HG21	2:B:397:TRP:CH2	2.54	0.43
2:B:147:THR:HG23	2:B:160:PHE:CZ	2.55	0.42
2:B:289:MET:CG	2:B:349:ILE:HD13	2.50	0.42
2:B:468:LYS:HB2	2:B:468:LYS:HE3	1.86	0.41
1:A:46:LEU:HD12	1:A:84[B]:LEU:HD22	2.02	0.41
2:B:357:ILE:CD1	2:B:418:LEU:CD2	2.99	0.41
1:A:36:LEU:O	1:A:38:GLY:N	2.54	0.41
2:B:425:VAL:CG1	2:B:426:PRO:HD2	2.50	0.40
2:B:213:LEU:N	2:B:214:PRO:CD	2.85	0.40
2:B:141:SER:HA	2:B:285:THR:O	2.22	0.40
2:B:226:LEU:CD1	3:B:1020:HOH:O	2.68	0.40
1:A:81:ALA:HB1	2:B:636:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

## 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	121/161 (75%)	118 (98%)	2 (2%)	1 (1%)	24	11
2	B	536/711 (75%)	526 (98%)	8 (2%)	2 (0%)	39	27
All	All	657/872 (75%)	644 (98%)	10 (2%)	3 (0%)	34	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
2	B	176	SER
2	B	178	LYS

### 5.3.2 Protein sidechains ⓘ

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	103/135 (76%)	100 (97%)	3 (3%)	50	39
2	B	456/575 (79%)	454 (100%)	2 (0%)	93	94
All	All	559/710 (79%)	554 (99%)	5 (1%)	86	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	106[A]	ARG
1	A	106[B]	ARG
2	B	74	ARG
2	B	178	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	295	GLN
2	B	350	ASN
2	B	500	ASN
2	B	649	GLN
2	B	657	ASN

### 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 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	119/161 (73%)	0.78	15 (12%) <b>5</b> <b>6</b>	27, 37, 63, 68	0
2	B	526/711 (73%)	0.58	65 (12%) <b>5</b> <b>6</b>	15, 32, 67, 94	0
All	All	645/872 (73%)	0.62	80 (12%) <b>5</b> <b>6</b>	15, 33, 66, 94	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	182	LEU	8.5
2	B	415	LEU	8.2
2	B	180	LEU	8.0
2	B	529	ASN	7.0
1	A	19	ALA	6.2
2	B	183	PHE	6.1
2	B	186	ILE	6.0
2	B	216	ILE	5.9
2	B	449	GLU	5.3
2	B	448	ASP	4.9
2	B	114	ALA	4.9
1	A	18	ASP	4.8
2	B	215	ARG	4.7
2	B	683	ASN	4.5
2	B	416	GLU	4.2
2	B	450	ILE	4.2
1	A	17	ASN	4.2
2	B	179	LYS	4.1
2	B	178	LYS	3.9
2	B	184	GLN	3.8
2	B	185	HIS	3.7
2	B	107	LEU	3.7
2	B	176	SER	3.6
2	B	55	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	37	GLU	3.6
2	B	349	ILE	3.5
2	B	112	GLY	3.4
2	B	170	ILE	3.4
2	B	419	ARG	3.3
2	B	452	ALA	3.3
1	A	91	ARG	3.3
2	B	401	VAL	3.2
2	B	377	GLU	3.2
1	A	93	GLY	3.2
2	B	109	LEU	3.1
2	B	214	PRO	3.1
2	B	457	ARG	3.1
2	B	188	SER	3.1
2	B	659	SER	3.1
2	B	181	LYS	3.0
2	B	57	GLU	2.9
2	B	424	VAL	2.9
2	B	426	PRO	2.9
2	B	361	PHE	2.9
1	A	16	SER	2.8
2	B	122	ALA	2.8
2	B	207	GLU	2.7
1	A	119	GLU	2.7
2	B	204	GLY	2.6
2	B	119	TYR	2.6
2	B	350	ASN	2.6
2	B	177	ASN	2.6
1	A	94	VAL	2.6
2	B	402	PRO	2.5
1	A	85	VAL	2.5
2	B	530	GLY	2.5
2	B	208	LEU	2.5
2	B	174	ASP	2.4
2	B	56	PRO	2.4
2	B	639[A]	ARG	2.4
2	B	357	ILE	2.4
2	B	147	THR	2.4
1	A	76	LEU	2.3
1	A	102	ARG	2.3
2	B	396	GLY	2.3
1	A	20	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	481	LEU	2.2
1	A	95	ASP	2.2
2	B	138	MET	2.2
2	B	108	VAL	2.2
2	B	149	ALA	2.1
2	B	175	SER	2.1
2	B	374	LEU	2.1
2	B	59	VAL	2.1
2	B	140	GLY	2.1
1	A	86	LEU	2.1
2	B	454	LEU	2.1
2	B	212	VAL	2.1
2	B	187	SER	2.1
2	B	417	GLU	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.