



# Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2021 – 02:37 PM JST

PDB ID : 7CQC  
Title : The NZ-1 Fab complexed with the PDZ tandem fragment of A. aeolicus S2P homolog with the PA14 tag inserted between the residues 181 and 184  
Authors : Aruga, R.; Tamura-Sakaguchi, R.; Nogi, T.  
Deposited on : 2020-08-10  
Resolution : 2.50 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

<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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

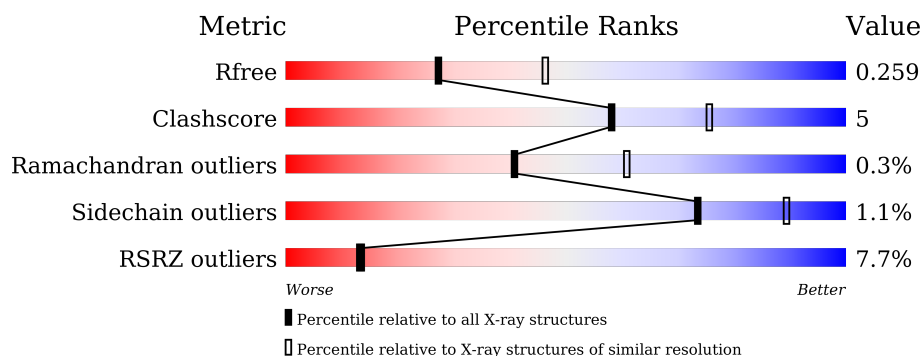
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	H	219	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
2	L	214	<div> <div>%</div> <div>88%</div> <div>12%</div> </div>
3	A	192	<div> <div>21%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4740 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 Heavy chain of antigen binding fragment, Fab of NZ-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1597	1009	265	314	9			

- Molecule 2 is a protein called Light chain of antigen binding fragment, Fab of NZ-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1641	1017	284	334	6			

- Molecule 3 is a protein called Putative zinc metalloprotease aq\_1964,PA14 from Podoplanin,Putative zinc metalloprotease aq\_1964.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	187	Total	C	N	O	S	0	0	0
			1452	940	245	265	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	expression tag	UNP O67776
A	114	SER	-	expression tag	UNP O67776

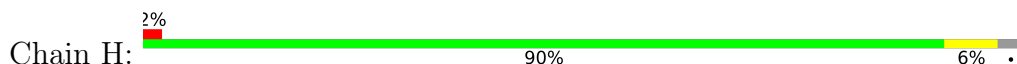
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	24	Total	O	0	0
			24	24		
4	L	15	Total	O	0	0
			15	15		
4	A	11	Total	O	0	0
			11	11		

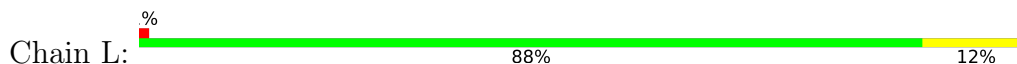
### 3 Residue-property plots

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

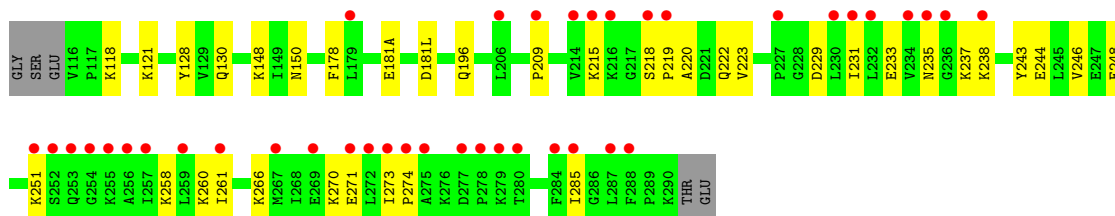
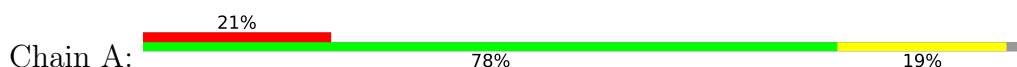
- Molecule 1: Heavy chain of antigen binding fragment, Fab of NZ-1



- Molecule 2: Light chain of antigen binding fragment, Fab of NZ-1



- Molecule 3: Putative zinc metalloprotease aq\_1964, PA14 from Podoplanin, Putative zinc metalloprotease aq\_1964



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.36Å 75.20Å 172.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.97 – 2.50 45.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.97-2.50) 99.9 (45.68-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998+SVN	Depositor
R, $R_{free}$	0.230 , 0.258 0.234 , 0.259	Depositor DCC
$R_{free}$ test set	1186 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

### 5.1 Standard geometry

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

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	H	0.25	0/1636	0.46	0/2229
2	L	0.25	0/1669	0.44	0/2272
3	A	0.26	0/1467	0.44	0/1977
All	All	0.25	0/4772	0.45	0/6478

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	H	1597	0	1555	9	0
2	L	1641	0	1576	14	0
3	A	1452	0	1546	25	0
4	A	11	0	0	0	0
4	H	24	0	0	0	0
4	L	15	0	0	0	0
All	All	4740	0	4677	45	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 5.

All (45) 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:H:120:ARG:NH1	3:A:181(L):ASP:O	2.26	0.68
3:A:118:LYS:HD2	3:A:118:LYS:H	1.59	0.68
1:H:142:PRO:HB3	1:H:168:TYR:HB3	1.78	0.65
3:A:219:PRO:HA	3:A:222:GLN:HB2	1.80	0.64
3:A:209:PRO:HB2	3:A:231:ILE:HB	1.80	0.64
3:A:223:VAL:HG11	3:A:270:LYS:HB3	1.81	0.62
3:A:231:ILE:HD13	3:A:261:ILE:HG12	1.82	0.62
3:A:215:LYS:HD3	3:A:218:SER:HB3	1.81	0.61
1:H:66:TRP:CE2	2:L:117:ILE:HD12	2.36	0.60
3:A:128:TYR:HE1	3:A:130:GLN:OE1	1.88	0.56
3:A:223:VAL:HG21	3:A:271:GLU:O	2.07	0.54
2:L:114:SER:OG	2:L:115:SER:N	2.41	0.54
2:L:46:GLY:O	2:L:91:ASN:ND2	2.40	0.53
2:L:182:ASP:OD1	2:L:200:ARG:NH1	2.42	0.51
3:A:233:GLU:HG2	3:A:238:LYS:HA	1.94	0.50
2:L:81:ARG:NH1	2:L:104:ASP:OD2	2.44	0.49
3:A:274:PRO:HG2	3:A:285:ILE:HD13	1.95	0.48
2:L:166:VAL:HG12	2:L:218:HIS:HB2	1.96	0.48
3:A:118:LYS:HD2	3:A:118:LYS:N	2.28	0.47
2:L:143:SER:HB2	2:L:145:GLU:OE1	2.15	0.47
1:H:20:GLU:OE2	1:H:22:GLN:NE2	2.32	0.46
3:A:218:SER:O	3:A:220:ALA:N	2.42	0.46
2:L:145:GLU:H	2:L:145:GLU:CD	2.19	0.46
3:A:219:PRO:HB2	3:A:274:PRO:HG3	1.98	0.46
2:L:162:TYR:CD2	2:L:163:PRO:HA	2.50	0.45
1:H:102:MET:HB3	1:H:105:LEU:HD21	1.99	0.45
3:A:223:VAL:HG12	3:A:270:LYS:HD2	1.98	0.45
2:L:31:THR:OG1	2:L:35:SER:OG	2.32	0.45
3:A:235:ASN:ND2	3:A:258:LYS:H	2.15	0.45
2:L:144:THR:O	2:L:148:GLN:HG3	2.16	0.45
3:A:235:ASN:HD22	3:A:258:LYS:HE2	1.83	0.44
1:H:120:ARG:NH2	3:A:181(A):GLU:OE1	2.51	0.44
1:H:120:ARG:HG3	1:H:121:VAL:HG13	1.99	0.44
3:A:223:VAL:CG1	3:A:270:LYS:HD2	2.47	0.44
1:H:92:ASP:OD2	1:H:95:LYS:NZ	2.31	0.44
3:A:148:LYS:HB3	3:A:178:PHE:HB2	2.00	0.44
3:A:243:TYR:O	3:A:246:VAL:HG22	2.19	0.43
1:H:91:ARG:HA	1:H:98:HIS:HA	2.00	0.42
3:A:229:ASP:HB3	3:A:261:ILE:HG21	2.02	0.42
2:L:40:SER:HA	2:L:94:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:244:GLU:O	3:A:248:GLU:HG3	2.21	0.41
3:A:233:GLU:HB2	3:A:260:LYS:NZ	2.36	0.41
3:A:237:LYS:HD3	3:A:248:GLU:OE1	2.20	0.41
2:L:209:ARG:HD3	2:L:209:ARG:HA	1.89	0.40
2:L:100:VAL:CG1	2:L:127:VAL:HG21	2.52	0.40

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	H	208/219 (95%)	200 (96%)	8 (4%)	0	100	100
2	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	48
3	A	182/192 (95%)	170 (93%)	11 (6%)	1 (0%)	29	48
All	All	602/625 (96%)	573 (95%)	27 (4%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	114	SER
3	A	273	ILE

### 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	H	178/183 (97%)	177 (99%)	1 (1%)	86	95
2	L	187/187 (100%)	186 (100%)	1 (0%)	88	96
3	A	158/162 (98%)	154 (98%)	4 (2%)	47	73
All	All	523/532 (98%)	517 (99%)	6 (1%)	73	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	128	GLN
2	L	228	SER
3	A	121	LYS
3	A	196	GLN
3	A	251	LYS
3	A	266	LYS

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

Mol	Chain	Res	Type
2	L	91	ASN
3	A	235	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
3	SNN	A	150	3	7,8,8	5.34	5 (71%)	7,11,11	1.52	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PCA	L	20	2	7,8,9	1.81	1 (14%)	9,10,12	2.14	5 (55%)

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
3	SNN	A	150	3	-	-	0/1/1/1
2	PCA	L	20	2	-	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	150	SNN	C2-N1	9.62	1.50	1.37
3	A	150	SNN	C4-C5	8.93	1.63	1.51
2	L	20	PCA	CD-N	4.69	1.46	1.34
3	A	150	SNN	C5-N1	4.09	1.43	1.37
3	A	150	SNN	O2-C2	-2.29	1.18	1.23
3	A	150	SNN	O5-C5	-2.20	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	150	SNN	O5-C5-C4	3.13	130.53	126.39
2	L	20	PCA	OE-CD-CG	-3.10	121.36	126.76
2	L	20	PCA	CA-N-CD	-2.97	103.40	113.58
2	L	20	PCA	CB-CA-N	2.67	110.97	103.30
2	L	20	PCA	CG-CD-N	2.44	114.70	108.39
2	L	20	PCA	CB-CA-C	-2.38	109.43	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

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

### 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	H	212/219 (96%)	0.15	4 (1%) 66 69	42, 58, 97, 123	0
2	L	213/214 (99%)	0.26	3 (1%) 75 77	47, 67, 89, 117	0
3	A	186/192 (96%)	1.11	40 (21%) 0 0	45, 77, 143, 162	0
All	All	611/625 (97%)	0.48	47 (7%) 13 13	42, 66, 132, 162	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	254	GLY	9.7
3	A	216	LYS	7.6
3	A	275	ALA	6.3
3	A	238	LYS	5.5
3	A	255	LYS	5.4
3	A	252	SER	5.3
3	A	261	ILE	5.2
3	A	278	PRO	5.0
3	A	235	ASN	4.8
3	A	253	GLN	4.7
2	L	230	ALA	4.3
3	A	215	LYS	4.2
3	A	259	LEU	4.0
3	A	272	LEU	4.0
3	A	274	PRO	4.0
3	A	214	VAL	3.8
3	A	219	PRO	3.7
3	A	284	PHE	3.7
3	A	267	MET	3.6
3	A	256	ALA	3.5
3	A	273	ILE	3.4
3	A	231	ILE	3.3
3	A	257	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	211	TRP	3.2
3	A	218	SER	3.1
3	A	269	GLU	3.1
3	A	288	PHE	3.0
3	A	287	LEU	3.0
3	A	279	LYS	2.9
3	A	280	THR	2.9
3	A	230	LEU	2.8
2	L	231	GLU	2.8
3	A	277	ASP	2.6
3	A	251	LYS	2.4
3	A	232	LEU	2.4
1	H	212	SER	2.4
3	A	285	ILE	2.3
1	H	236	ARG	2.3
1	H	148	ALA	2.3
3	A	271	GLU	2.2
3	A	234	VAL	2.2
3	A	179	LEU	2.2
2	L	126	THR	2.2
3	A	236	GLY	2.2
3	A	206	LEU	2.1
3	A	209	PRO	2.0
3	A	227	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
2	PCA	L	20	8/9	0.86	0.25	76,82,88,89	0
3	SNN	A	150	8/8	0.98	0.15	46,48,51,55	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.