



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 10:35 PM EST

PDB ID : 6EOO  
Title : DPP8 - Apo, space group 20  
Authors : Ross, B.R.; Huber, R.  
Deposited on : 2017-10-10  
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

<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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

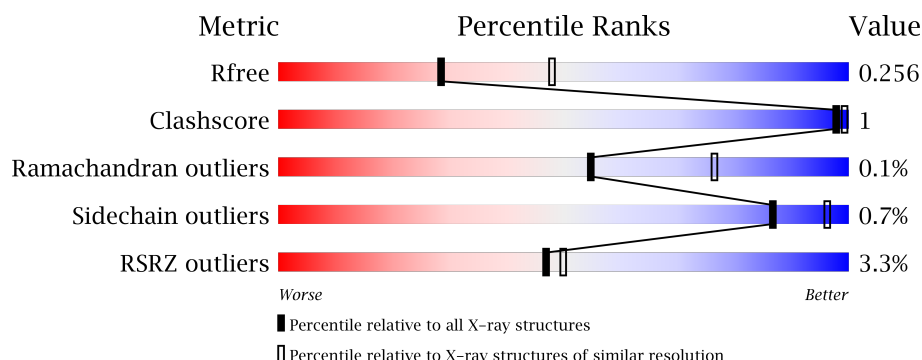
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 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	898	 3% 88% 9%
1	B	898	 2% 89% 9%
1	C	898	 3% 89% 9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20373 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 Dipeptidyl peptidase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	1	0
			6674	4292	1117	1239	26			
1	B	819	Total	C	N	O	S	0	1	0
			6663	4283	1116	1238	26			
1	C	820	Total	C	N	O	S	0	1	0
			6670	4288	1117	1239	26			

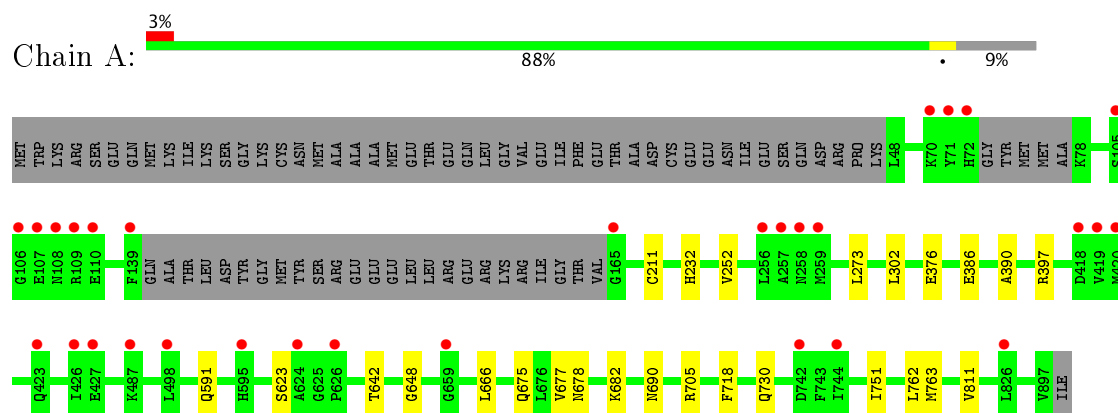
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	131	Total	O	0	0
			131	131		
2	C	103	Total	O	0	0
			103	103		

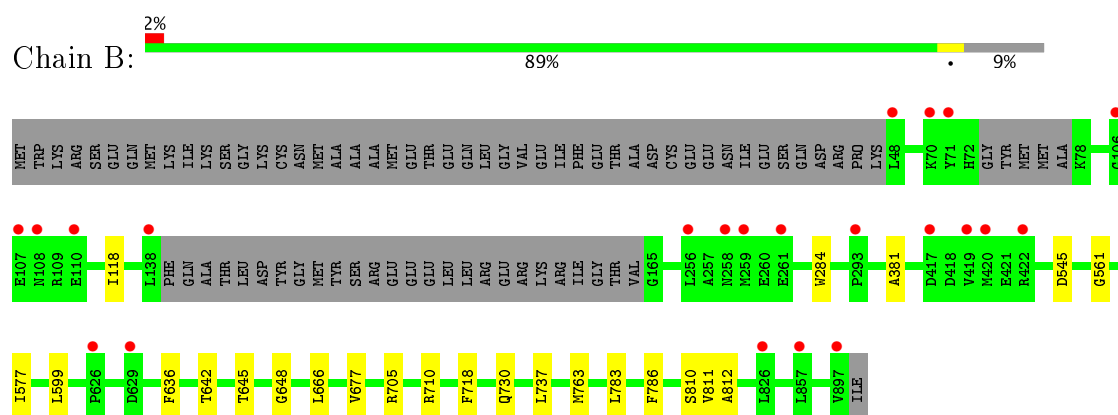
### 3 Residue-property plots [i](#)

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.

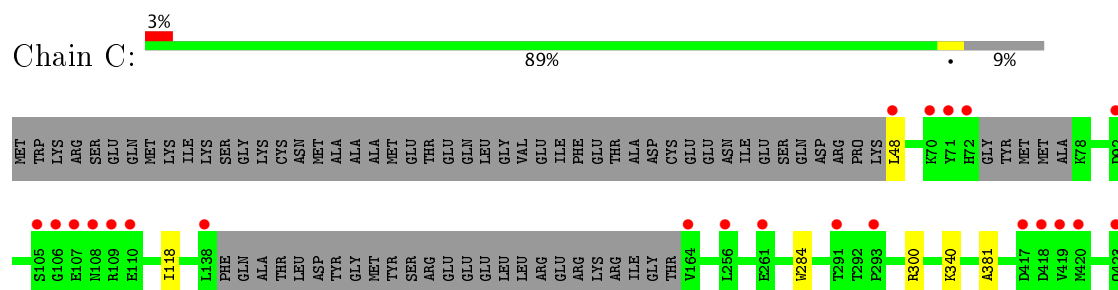
#### • Molecule 1: Dipeptidyl peptidase 8



#### • Molecule 1: Dipeptidyl peptidase 8



#### • Molecule 1: Dipeptidyl peptidase 8





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.84Å 247.06Å 260.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.65 – 2.50 44.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.65-2.50) 99.9 (44.65-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.229 , 0.254 0.232 , 0.256	Depositor DCC
$R_{free}$ test set	9013 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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	0.36	0/6862	0.58	0/9311
1	B	0.36	0/6850	0.58	0/9295
1	C	0.36	0/6857	0.58	0/9305
All	All	0.36	0/20569	0.58	0/27911

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	6674	0	6485	12	0
1	B	6663	0	6476	13	0
1	C	6670	0	6485	12	0
2	A	132	0	0	0	0
2	B	131	0	0	0	0
2	C	103	0	0	0	0
All	All	20373	0	19446	37	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 1.

All (37) 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:C:642:THR:HG21	1:C:705:ARG:NH1	2.11	0.65
1:B:642:THR:HG21	1:B:705:ARG:NH1	2.11	0.64
1:A:642:THR:HG21	1:A:705:ARG:NH1	2.14	0.62
1:B:783:LEU:HD13	1:B:812:ALA:HB3	1.88	0.53
1:A:666:LEU:HD21	1:A:730:GLN:HE21	1.75	0.51
1:C:783:LEU:HD13	1:C:812:ALA:HB3	1.92	0.51
1:C:675:GLN:HE21	1:C:678:ASN:HD22	1.58	0.50
1:A:675:GLN:HE21	1:A:678:ASN:HD22	1.59	0.50
1:A:666:LEU:HD23	1:A:751:ILE:HD12	1.94	0.49
1:A:648:GLY:HA2	1:A:677:VAL:HG21	1.94	0.49
1:B:118:ILE:HD12	1:B:599:LEU:HD22	1.96	0.48
1:C:762:LEU:HD13	1:C:811:VAL:HG21	1.94	0.48
1:B:763:MET:SD	1:B:811:VAL:HG12	2.54	0.48
1:C:118:ILE:HD12	1:C:599:LEU:HD22	1.95	0.47
1:B:648:GLY:HA2	1:B:677:VAL:HG21	1.95	0.47
1:A:591:GLN:HE22	1:A:682:LYS:HG2	1.81	0.46
1:C:118:ILE:HD12	1:C:599:LEU:CD2	2.45	0.46
1:B:284:TRP:CZ2	1:B:381:ALA:HB3	2.51	0.46
1:C:666:LEU:HD21	1:C:730:GLN:HE21	1.82	0.45
1:B:577:ILE:HD12	1:B:577:ILE:N	2.32	0.45
1:B:666:LEU:HD21	1:B:730:GLN:HE21	1.83	0.44
1:B:118:ILE:HD12	1:B:599:LEU:CD2	2.48	0.43
1:C:782:THR:HA	1:C:811:VAL:HG22	2.01	0.43
1:B:636:PHE:CZ	1:B:737:LEU:HD11	2.53	0.43
1:C:284:TRP:CZ2	1:C:381:ALA:HB3	2.54	0.42
1:A:302:LEU:HD22	1:A:390:ALA:HB1	2.00	0.42
1:A:763:MET:SD	1:A:811:VAL:HG12	2.60	0.42
1:C:705:ARG:NH1	1:C:729:ASP:OD1	2.53	0.42
1:A:211:CYS:HB3	1:A:232:HIS:CE1	2.55	0.42
1:A:376:GLU:HG3	1:A:397:ARG:HB2	2.01	0.41
1:A:591:GLN:HE22	1:A:682:LYS:CG	2.33	0.41
1:B:645:THR:O	1:B:710:ARG:NH1	2.50	0.41
1:B:783:LEU:HD12	1:B:810:SER:HB3	2.02	0.41
1:C:804:GLN:HE21	1:C:804:GLN:HA	1.85	0.41
1:A:762:LEU:HD13	1:A:811:VAL:HG21	2.03	0.40
1:B:783:LEU:HD23	1:B:786:PHE:CE1	2.56	0.40
1:C:675:GLN:NE2	1:C:678:ASN:HD22	2.20	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	815/898 (91%)	795 (98%)	20 (2%)	0	100	100
1	B	814/898 (91%)	790 (97%)	23 (3%)	1 (0%)	55	76
1	C	815/898 (91%)	789 (97%)	25 (3%)	1 (0%)	55	76
All	All	2444/2694 (91%)	2374 (97%)	68 (3%)	2 (0%)	55	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	839	ALA
1	B	561	GLY

### 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	729/795 (92%)	723 (99%)	6 (1%)	85	95
1	B	728/795 (92%)	726 (100%)	2 (0%)	94	98
1	C	729/795 (92%)	722 (99%)	7 (1%)	80	93
All	All	2186/2385 (92%)	2171 (99%)	15 (1%)	87	96

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	VAL

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	386	GLU
1	A	623	SER
1	A	690	ASN
1	A	718	PHE
1	B	545	ASP
1	B	718	PHE
1	C	48	LEU
1	C	300	ARG
1	C	340	LYS
1	C	545	ASP
1	C	614	LYS
1	C	718	PHE
1	C	804	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	199	GLN
1	A	232	HIS
1	A	274	GLN
1	A	403	GLN
1	A	550	HIS
1	A	573	HIS
1	A	579	GLN
1	A	591	GLN
1	A	675	GLN
1	A	704	ASN
1	A	730	GLN
1	A	814	GLN
1	A	829	HIS
1	A	862	GLN
1	A	885	GLN
1	B	274	GLN
1	B	403	GLN
1	B	573	HIS
1	B	591	GLN
1	B	675	GLN
1	B	704	ASN
1	B	730	GLN
1	B	829	HIS

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Mol	Chain	Res	Type
1	B	885	GLN
1	C	173	GLN
1	C	274	GLN
1	C	403	GLN
1	C	573	HIS
1	C	579	GLN
1	C	591	GLN
1	C	675	GLN
1	C	704	ASN
1	C	730	GLN
1	C	804	GLN
1	C	814	GLN
1	C	829	HIS
1	C	837	HIS
1	C	885	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 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	820/898 (91%)	0.18	30 (3%) 42 44	40, 58, 93, 133	0
1	B	819/898 (91%)	0.19	22 (2%) 55 58	43, 60, 95, 142	0
1	C	820/898 (91%)	0.22	30 (3%) 42 44	43, 62, 98, 146	0
All	All	2459/2694 (91%)	0.20	82 (3%) 47 50	40, 60, 96, 146	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	TYR	8.5
1	A	71	TYR	7.2
1	B	71	TYR	6.5
1	C	108	ASN	6.1
1	A	108	ASN	6.1
1	A	106	GLY	5.7
1	C	107	GLU	5.6
1	C	106	GLY	5.5
1	A	110	GLU	5.2
1	B	420	MET	4.4
1	A	256	LEU	4.3
1	C	70	LYS	4.1
1	A	109	ARG	4.1
1	A	107	GLU	4.0
1	A	70	LYS	4.0
1	B	108	ASN	3.8
1	C	293	PRO	3.8
1	C	164	VAL	3.7
1	A	420	MET	3.6
1	A	626	PRO	3.5
1	B	417	ASP	3.5
1	C	417	ASP	3.4
1	C	48	LEU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	139	PHE	3.3
1	A	165	GLY	3.3
1	C	740	ARG	3.2
1	B	419	VAL	3.2
1	B	138	LEU	3.2
1	A	426	ILE	3.1
1	B	106	GLY	3.1
1	C	420	MET	3.0
1	B	70	LYS	3.0
1	C	138	LEU	3.0
1	C	419	VAL	3.0
1	A	105	SER	2.9
1	B	293	PRO	2.9
1	B	48	LEU	2.9
1	A	72	HIS	2.9
1	B	261	GLU	2.9
1	A	259	MET	2.8
1	B	259	MET	2.8
1	B	107	GLU	2.8
1	A	423	GLN	2.7
1	C	105	SER	2.7
1	C	256	LEU	2.6
1	C	261	GLU	2.6
1	C	72	HIS	2.6
1	C	508	ILE	2.6
1	C	92	ASP	2.5
1	C	110	GLU	2.5
1	C	490	LYS	2.5
1	A	826	LEU	2.5
1	C	423	GLN	2.5
1	B	626	PRO	2.4
1	A	659	GLY	2.4
1	B	258	ASN	2.4
1	A	427	GLU	2.4
1	A	258	ASN	2.3
1	B	110	GLU	2.3
1	B	422	ARG	2.3
1	C	626	PRO	2.2
1	A	487	LYS	2.2
1	B	629	ASP	2.2
1	B	897	VAL	2.2
1	C	595	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	418	ASP	2.2
1	A	498	LEU	2.2
1	C	891	ARG	2.2
1	A	742	ASP	2.2
1	C	291	THR	2.2
1	B	256	LEU	2.2
1	A	419	VAL	2.1
1	A	595	HIS	2.1
1	C	418	ASP	2.1
1	C	109	ARG	2.1
1	C	825	LEU	2.1
1	A	744	ILE	2.1
1	C	826	LEU	2.1
1	A	257	ALA	2.1
1	A	624	ALA	2.0
1	B	826	LEU	2.0
1	B	857	LEU	2.0

## 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.