



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2025 – 12:07 pm GMT

PDB ID : 9H3I  
Title : trans-aconitate decarboxylase Tad1- wild type  
Authors : Zheng, L.; Bang, G.  
Deposited on : 2024-10-16  
Resolution : 2.31 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

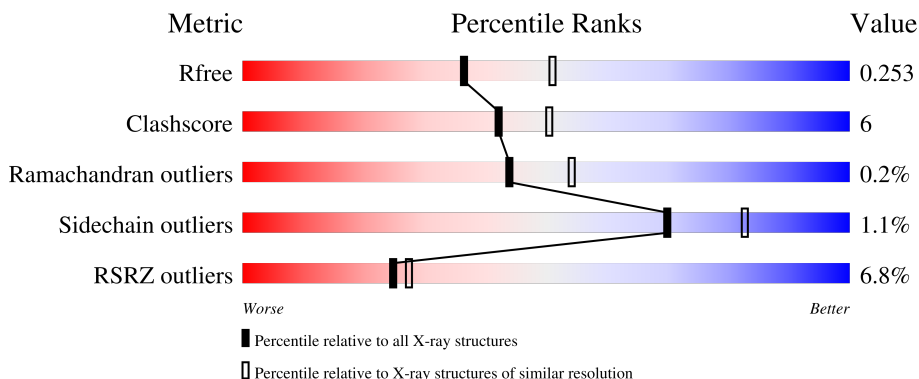
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	A	493	<div> <div>5%</div> <div> <div>73%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	493	<div> <div>12%</div> <div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	493	<div> <div>4%</div> <div> <div>76%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	493	<div> <div>3%</div> <div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13546 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 Trans-aconitate decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	437	Total	C	N	O	S	0	0	0
			3379	2126	596	635	22			
1	A	436	Total	C	N	O	S	0	0	0
			3368	2124	593	629	22			
1	B	434	Total	C	N	O	S	0	0	0
			3361	2117	592	630	22			
1	C	439	Total	C	N	O	S	0	0	0
			3384	2132	595	635	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	489	PRO	ARG	conflict	UNP A0A0U2UYC4
A	489	PRO	ARG	conflict	UNP A0A0U2UYC4
B	489	PRO	ARG	conflict	UNP A0A0U2UYC4
C	489	PRO	ARG	conflict	UNP A0A0U2UYC4

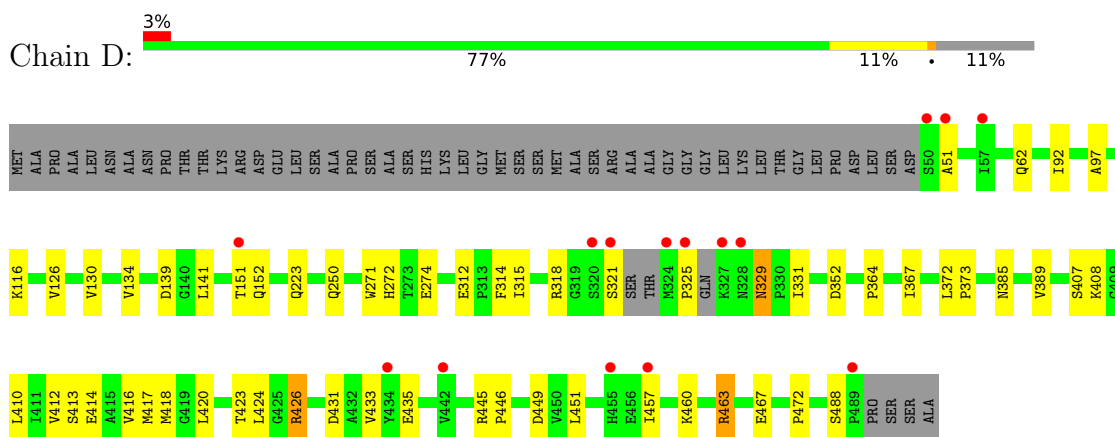
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	21	Total	O	0	0
			21	21		
2	A	16	Total	O	0	0
			16	16		
2	B	4	Total	O	0	0
			4	4		
2	C	13	Total	O	0	0
			13	13		

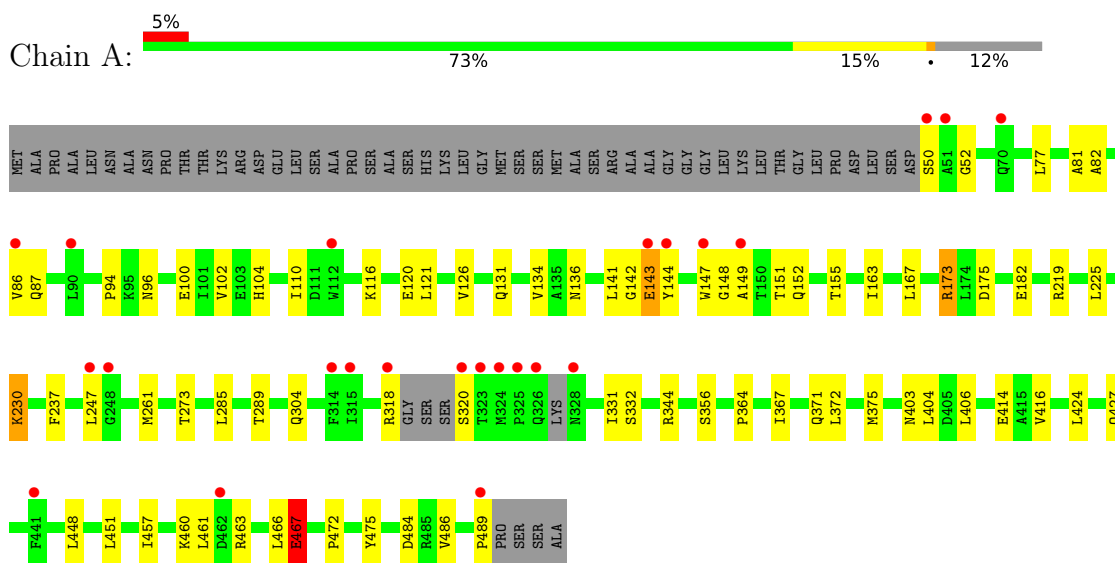
### 3 Residue-property plots [i](#)

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: Trans-aconitate decarboxylase 1

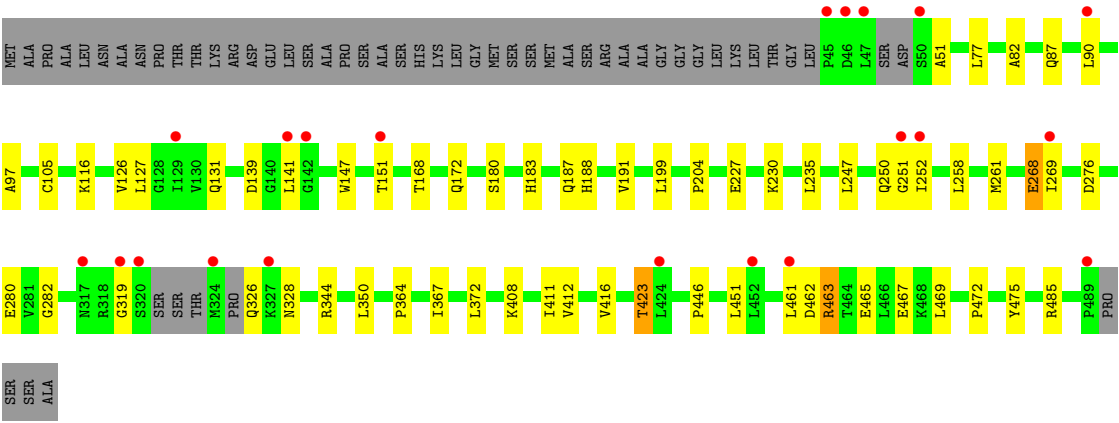
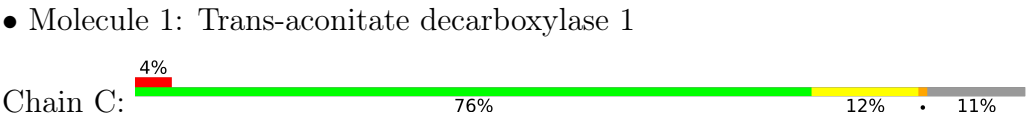
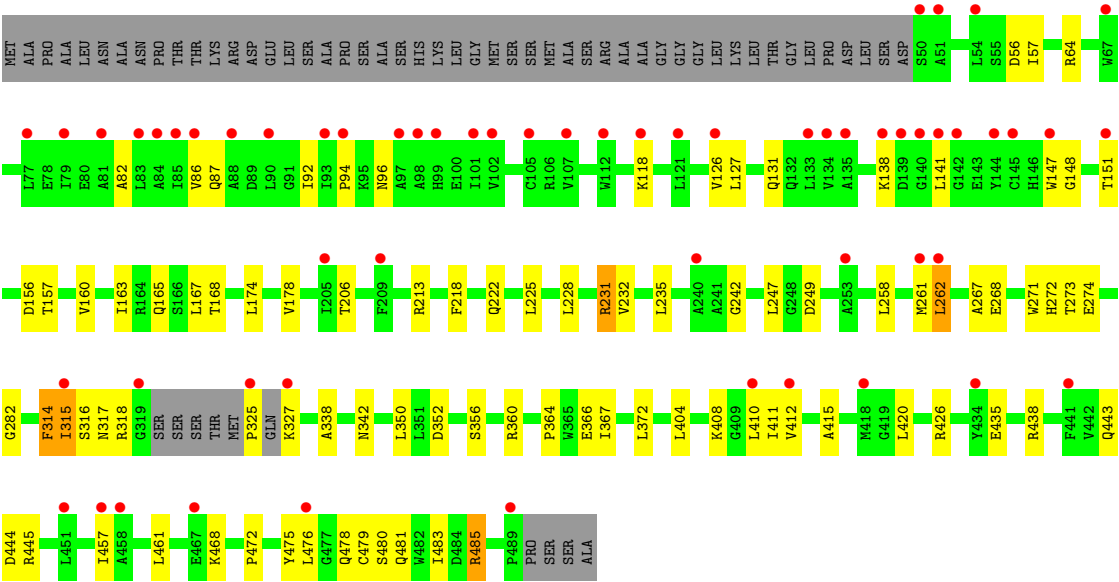


- Molecule 1: Trans-aconitate decarboxylase 1



- Molecule 1: Trans-aconitate decarboxylase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.62Å 164.69Å 208.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.31 49.72 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.72-2.31) 97.8 (49.72-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.227 , 0.257 0.225 , 0.253	Depositor DCC
$R_{free}$ test set	8322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.1	Xtrriage
Anisotropy	0.324	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.33	0/3430	0.55	1/4656 (0.0%)
1	B	0.30	0/3424	0.55	0/4648
1	C	0.31	0/3447	0.53	0/4680
1	D	0.31	0/3442	0.55	0/4672
All	All	0.31	0/13743	0.55	1/18656 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	GLU	CA-CB-CG	5.62	125.76	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Peptide
1	A	467	GLU	Peptide
1	D	426	ARG	Sidechain
1	D	463	ARG	Sidechain

## 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	3368	0	3329	46	2
1	B	3361	0	3324	60	0
1	C	3384	0	3334	41	2
1	D	3379	0	3337	37	0
2	A	16	0	0	1	0
2	B	4	0	0	1	0
2	C	13	0	0	1	0
2	D	21	0	0	0	0
All	All	13546	0	13324	167	2

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.

The worst 5 of 167 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:B:338:ALA:O	1:B:342:ASN:ND2	2.16	0.79
1:D:423:THR:HG21	1:D:460:LYS:HB3	1.68	0.76
1:A:219:ARG:NH1	1:A:486:VAL:O	2.20	0.74
1:A:182:GLU:OE2	1:A:219:ARG:NH2	2.25	0.70
1:A:371:GLN:O	1:A:375:MET:HG3	1.93	0.68

All (2) 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)
1:A:427:GLN:OE1	1:C:250:GLN:NE2[8_545]	2.10	0.10
1:A:427:GLN:NE2	1:C:90:LEU:O[8_545]	2.18	0.02



## 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	429/493 (87%)	410 (96%)	18 (4%)	1 (0%)	44	54
1	B	429/493 (87%)	412 (96%)	17 (4%)	0	100	100
1	C	433/493 (88%)	414 (96%)	18 (4%)	1 (0%)	44	54
1	D	431/493 (87%)	414 (96%)	16 (4%)	1 (0%)	44	54
All	All	1722/1972 (87%)	1650 (96%)	69 (4%)	3 (0%)	44	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLN
1	D	329	ASN
1	A	142	GLY

### 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	355/404 (88%)	350 (99%)	5 (1%)	62	77
1	B	356/404 (88%)	350 (98%)	6 (2%)	56	71
1	C	356/404 (88%)	353 (99%)	3 (1%)	79	88
1	D	358/404 (89%)	356 (99%)	2 (1%)	84	92
All	All	1425/1616 (88%)	1409 (99%)	16 (1%)	70	83

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	423	THR
1	C	268	GLU
1	B	262	LEU
1	B	485	ARG
1	B	231	ARG

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

Mol	Chain	Res	Type
1	D	190	ASN
1	B	104	HIS
1	B	478	GLN
1	C	328	ASN
1	C	430	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	320:SER	C	323:THR	N	6.43

## 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	436/493 (88%)	0.51	24 (5%) 32 34	51, 68, 94, 138	0
1	B	434/493 (88%)	1.03	59 (13%) 8 9	55, 81, 109, 122	0
1	C	439/493 (89%)	0.53	21 (4%) 36 39	53, 72, 98, 127	0
1	D	437/493 (88%)	0.38	15 (3%) 48 51	50, 68, 102, 126	0
All	All	1746/1972 (88%)	0.61	119 (6%) 25 27	50, 72, 104, 138	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	MET	7.9
1	B	325	PRO	7.6
1	C	324	MET	7.2
1	B	457	ILE	6.2
1	A	320	SER	6.1

### 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 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.