



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:09 AM GMT

PDB ID : 2QZ9  
Title : crystal structure of aspartate semialdehyde dehydrogenase II from vibrio cholerae  
Authors : Viola, R.E.; Liu, X.; Ohren, J.F.; Faehnle, C.R.  
Deposited on : 2007-08-16  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

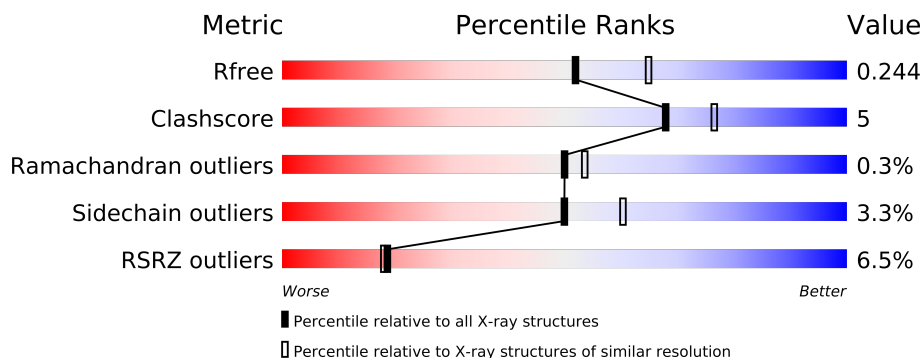
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	
1	C	336	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8266 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Aspartate-semialdehydedehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	2	0
			2617	1655	447	504	11			
1	B	335	Total	C	N	O	S	0	2	0
			2611	1652	446	502	11			
1	C	336	Total	C	N	O	S	0	3	0
			2621	1657	447	506	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	153	Total	O	0	0
			153	153		
2	B	103	Total	O	0	0
			103	103		
2	C	161	Total	O	0	0
			161	161		

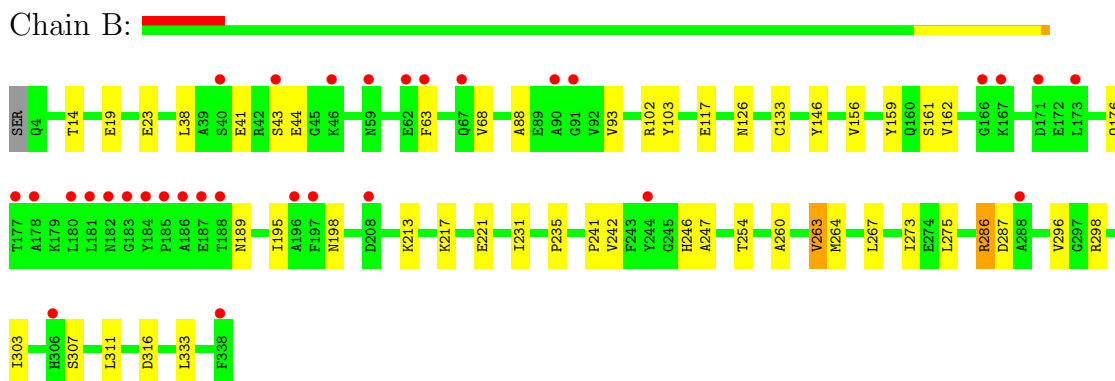
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

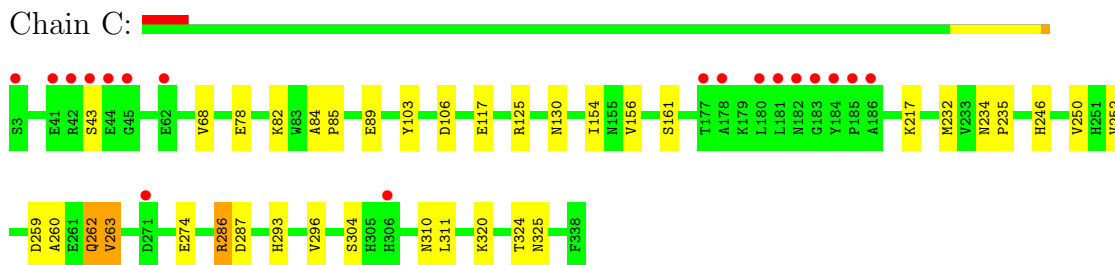
#### • Molecule 1: Aspartate-semialdehydedehydrogenase



#### • Molecule 1: Aspartate-semialdehydedehydrogenase



#### • Molecule 1: Aspartate-semialdehydedehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.33Å 85.66Å 116.10Å 90.00° 103.69° 90.00°	Depositor
Resolution (Å)	37.61 – 2.20 37.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.61-2.20) 99.2 (37.60-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.198 , 0.250 0.196 , 0.244	Depositor DCC
$R_{free}$ test set	2914 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57269 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.48	0/2671	0.60	0/3633
1	B	0.45	0/2665	0.57	0/3625
1	C	0.47	0/2680	0.60	0/3645
All	All	0.47	0/8016	0.59	0/10903

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2538	32	0
1	B	2611	0	2533	27	0
1	C	2621	0	2540	25	0
2	A	153	0	0	3	0
2	B	103	0	0	2	0
2	C	161	0	0	2	0
All	All	8266	0	7611	75	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (75) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:ASN:HD21	1:C:310:ASN:HD21	1.00	0.93
1:B:103:TYR:OH	1:B:217:LYS:HG2	1.72	0.89
1:A:310:ASN:HD21	1:C:234:ASN:HD21	1.29	0.81
1:A:234:ASN:ND2	1:C:310:ASN:HD21	1.80	0.77
1:B:14:THR:HG21	1:B:43:SER:HB3	1.66	0.77
1:A:133:CYS:HB2	2:A:339:HOH:O	1.85	0.75
1:A:130:ASN:ND2	1:A:325:ASN:HD22	1.88	0.70
1:C:130:ASN:ND2	1:C:325:ASN:HD22	1.90	0.69
1:A:176:GLN:HE22	1:A:195:ILE:H	1.42	0.68
1:B:316:ASP:HB3	2:B:440:HOH:O	1.93	0.67
1:C:130:ASN:HD21	1:C:325:ASN:HD22	1.42	0.66
1:B:103:TYR:HH	1:B:217:LYS:HG2	1.59	0.65
1:A:310:ASN:HD21	1:C:234:ASN:ND2	1.95	0.64
1:B:102:ARG:HD3	1:B:221:GLU:OE2	1.98	0.64
1:A:103:TYR:OH	1:A:217:LYS:HG2	1.97	0.63
1:A:234:ASN:HD21	1:C:310:ASN:ND2	1.84	0.63
1:A:310:ASN:ND2	1:C:234:ASN:HD21	1.97	0.61
1:A:232:MET:HB3	1:C:304:SER:HB2	1.83	0.61
1:A:286:ARG:HD2	1:A:287:ASP:OD1	2.02	0.59
1:A:228:ASP:HB3	1:A:231:ILE:HD11	1.83	0.59
1:B:176:GLN:HE22	1:B:195:ILE:H	1.50	0.58
1:A:130:ASN:HD21	1:A:325:ASN:HD22	1.50	0.58
1:C:260:ALA:HA	1:C:263:VAL:CG1	2.34	0.57
1:B:254:THR:OG1	1:B:307:SER:HB3	2.05	0.57
1:A:304:SER:HB2	1:C:232:MET:HB3	1.87	0.56
1:C:78:GLU:CD	1:C:78:GLU:H	2.09	0.55
1:A:161:SER:H	1:A:246:HIS:HD2	1.56	0.53
1:B:198:ASN:O	1:B:241:PRO:HD3	2.07	0.53
1:B:156:VAL:O	1:B:235:PRO:HA	2.09	0.53
1:C:286:ARG:HD2	1:C:287:ASP:OD1	2.10	0.52
1:B:161:SER:H	1:B:246:HIS:HD2	1.58	0.50
1:A:133:CYS:SG	2:A:492:HOH:O	2.60	0.50
1:B:286:ARG:NH1	1:B:287:ASP:OD1	2.44	0.50
1:B:264:MET:O	1:B:275:LEU:HD22	2.11	0.50
1:B:267:LEU:HD22	1:B:273:ILE:HD13	1.93	0.50
1:C:103:TYR:OH	1:C:217:LYS:HG2	2.11	0.50
1:A:161:SER:H	1:A:246:HIS:CD2	2.32	0.48
1:B:146:TYR:HE1	1:B:231:ILE:HD11	1.79	0.47
1:C:274:GLU:HB2	1:C:293:HIS:CD2	2.49	0.47
1:C:246:HIS:HE1	2:C:418:HOH:O	1.98	0.47
1:B:286:ARG:HH11	1:B:287:ASP:CG	2.18	0.47
1:C:156:VAL:O	1:C:235:PRO:HA	2.15	0.47
1:B:260:ALA:HA	1:B:263:VAL:HG13	1.96	0.47

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:275:LEU:HD12	1:B:296:VAL:HG23	1.97	0.46
1:A:162:VAL:HA	1:A:239:ARG:HD2	1.97	0.46
1:C:161:SER:H	1:C:246:HIS:HD2	1.63	0.46
1:A:246:HIS:HE1	2:A:492:HOH:O	1.99	0.46
1:B:159:TYR:HB2	1:B:247:ALA:HB3	1.97	0.46
1:A:14:THR:HG21	1:A:43:SER:HB3	1.97	0.46
1:B:267:LEU:HD13	1:B:296:VAL:HG21	1.97	0.45
1:B:38:LEU:HD21	1:B:63:PHE:CD1	2.51	0.45
1:B:162:VAL:HG22	1:B:242:VAL:O	2.16	0.45
1:B:133:CYS:HB2	2:B:340:HOH:O	2.16	0.45
1:C:250:VAL:HG12	1:C:252:VAL:HG13	1.99	0.45
1:A:263:VAL:HG23	1:A:299:VAL:HG11	1.98	0.45
1:A:78:GLU:HG3	1:B:213:LYS:HG2	1.98	0.44
1:C:320:LYS:HA	1:C:324:THR:HB	2.00	0.44
1:A:176:GLN:HG2	1:A:186:ALA:HB1	2.00	0.44
1:A:250:VAL:HG12	1:A:252:VAL:HG13	2.00	0.44
1:C:89[B]:GLU:HG2	2:C:468:HOH:O	2.17	0.44
1:B:19:GLU:O	1:B:23:GLU:HG3	2.17	0.44
1:A:263:VAL:CG2	1:A:299:VAL:HG11	2.48	0.43
1:C:154:ILE:HG12	1:C:252:VAL:HG12	2.01	0.43
1:A:262:GLN:O	1:A:266:MET:HG3	2.19	0.43
1:A:158:THR:HG22	1:A:248:GLU:HG2	2.01	0.43
1:A:114:VAL:HG13	1:A:143:LYS:HD3	2.01	0.43
1:C:106:ASP:OD2	1:C:125:ARG:HD3	2.20	0.42
1:C:84:ALA:HB3	1:C:85:PRO:HD3	2.01	0.42
1:A:288:ALA:HB2	1:A:314:VAL:HG12	2.02	0.42
1:B:146:TYR:CE1	1:B:231:ILE:HD11	2.54	0.41
1:C:259:ASP:H	1:C:262:GLN:NE2	2.18	0.41
1:B:88:ALA:HB1	1:B:126:ASN:HB2	2.02	0.41
1:A:143:LYS:HB3	1:A:144:PRO:HD3	2.02	0.40
1:B:93:VAL:HG11	1:B:333:LEU:HD21	2.02	0.40
1:A:41:GLU:O	1:A:44:GLU:HB3	2.21	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	334/336 (99%)	318 (95%)	15 (4%)	1 (0%)	50	53
1	B	333/336 (99%)	314 (94%)	17 (5%)	2 (1%)	33	32
1	C	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
All	All	1002/1008 (99%)	953 (95%)	46 (5%)	3 (0%)	50	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLU
1	A	322	ALA
1	B	44	GLU

### 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	279/280 (100%)	268 (96%)	11 (4%)	43	52
1	B	278/280 (99%)	270 (97%)	8 (3%)	55	66
1	C	280/280 (100%)	271 (97%)	9 (3%)	51	62
All	All	837/840 (100%)	809 (97%)	28 (3%)	50	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	53	LYS
1	A	132	ASN
1	A	179	LYS
1	A	187	GLU
1	A	213	LYS
1	A	231	ILE
1	A	271	ASP
1	A	286	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	296	VAL
1	A	307	SER
1	B	68	VAL
1	B	117	GLU
1	B	189	ASN
1	B	263	VAL
1	B	286	ARG
1	B	298	ARG
1	B	303	ILE
1	B	311	LEU
1	C	43	SER
1	C	68	VAL
1	C	82	LYS
1	C	117	GLU
1	C	262	GLN
1	C	263	VAL
1	C	286	ARG
1	C	296	VAL
1	C	311	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	155	ASN
1	A	176	GLN
1	A	202	GLN
1	A	234	ASN
1	A	246	HIS
1	B	176	GLN
1	B	194	GLN
1	B	202	GLN
1	B	234	ASN
1	B	246	HIS
1	C	130	ASN
1	C	155	ASN
1	C	176	GLN
1	C	193	GLN
1	C	234	ASN
1	C	246	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates 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	A	336/336 (100%)	0.27	16 (4%)	29 29	22, 37, 60, 75	2 (0%)
1	B	335/336 (99%)	0.44	31 (9%)	9 8	29, 44, 75, 90	2 (0%)
1	C	336/336 (100%)	0.04	18 (5%)	25 25	23, 35, 56, 67	2 (0%)
All	All	1007/1008 (99%)	0.25	65 (6%)	18 18	22, 39, 64, 90	6 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	TYR	7.6
1	B	186	ALA	6.7
1	A	3	SER	6.2
1	A	184	TYR	6.2
1	B	185	PRO	5.7
1	C	43	SER	5.1
1	C	184	TYR	5.1
1	C	182	ASN	4.3
1	B	171	ASP	4.2
1	C	3	SER	4.2
1	B	244	TYR	4.1
1	A	182	ASN	3.9
1	B	181	LEU	3.8
1	C	42	ARG	3.8
1	B	182	ASN	3.7
1	A	181	LEU	3.7
1	B	173	LEU	3.7
1	B	306	HIS	3.6
1	A	338	PHE	3.5
1	C	41	GLU	3.4
1	A	179	LYS	3.4
1	A	180	LEU	3.3
1	B	166	GLY	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	185	PRO	3.3
1	B	183	GLY	3.1
1	A	4	GLN	3.0
1	B	188	THR	3.0
1	A	45	GLY	2.9
1	B	178	ALA	2.9
1	C	185	PRO	2.9
1	B	177	THR	2.8
1	C	178	ALA	2.8
1	C	183	GLY	2.8
1	B	338	PHE	2.8
1	C	271	ASP	2.7
1	B	196	ALA	2.7
1	B	288	ALA	2.7
1	B	91	GLY	2.7
1	B	180	LEU	2.6
1	B	90	ALA	2.6
1	B	167	LYS	2.6
1	A	183	GLY	2.6
1	B	62	GLU	2.6
1	B	187	GLU	2.5
1	B	67	GLN	2.5
1	B	40	SER	2.4
1	C	186	ALA	2.4
1	A	203	ILE	2.4
1	C	177	THR	2.3
1	C	180	LEU	2.3
1	C	45	GLY	2.3
1	A	56	ARG	2.3
1	C	44	GLU	2.2
1	A	49	ARG	2.2
1	C	306	HIS	2.2
1	C	181	LEU	2.2
1	B	208	ASP	2.2
1	B	63	PHE	2.1
1	B	197	PHE	2.1
1	B	59	ASN	2.1
1	A	53	LYS	2.1
1	B	43	SER	2.1
1	B	46	LYS	2.0
1	C	62	GLU	2.0
1	A	62	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.