



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:01 PM UTC

PDB ID : 1GQN / pdb_00001gqn
Title : Native 3-dehydroquinase from Salmonella typhi
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Deposited on : 2001-11-26
Resolution : 1.78 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

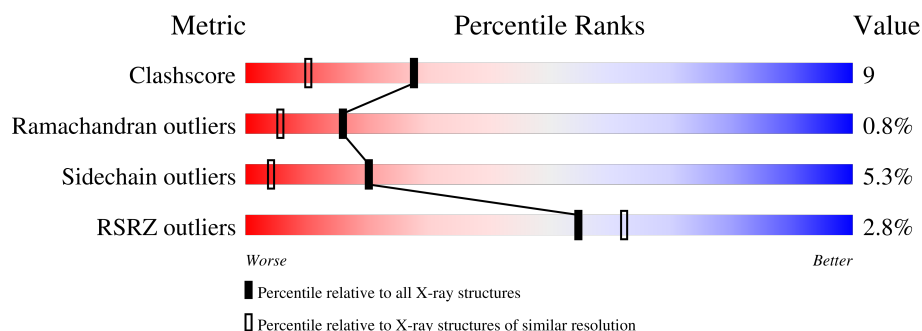
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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))
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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 ≥ 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	252	3% 63% 31% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2115 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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1934	1219	335	366	14			

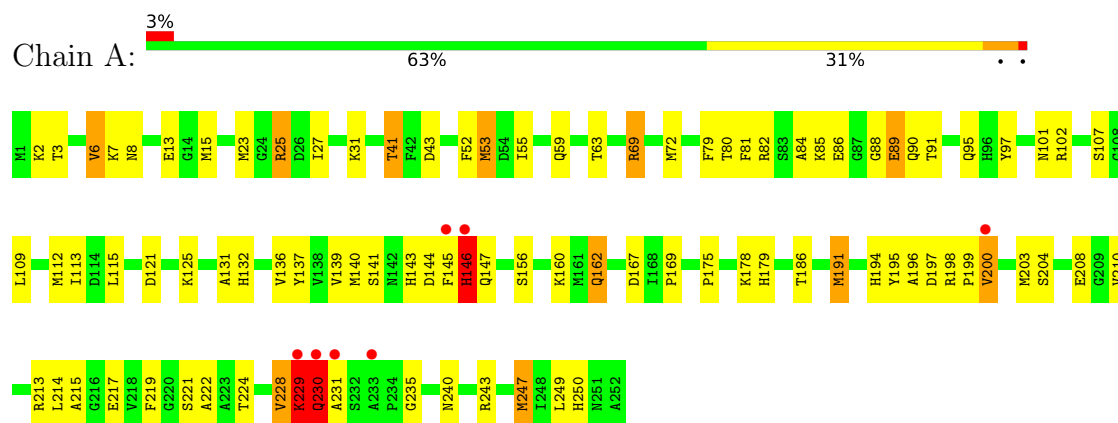
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	181	Total	O	0	0
			181	181		

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: 3-DEHYDROQUINATE DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	48.78Å 112.33Å 42.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.75 – 1.78 11.75 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.2 (11.75-1.78) 96.7 (11.75-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.247 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2115	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.26	3/1965 (0.2%)	2.30	96/2661 (3.6%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	PRO	C-N	-10.71	1.19	1.33
1	A	200	VAL	C-N	-10.05	1.20	1.33
1	A	247	MET	C-N	-9.90	1.21	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	PRO	CA-C-N	18.02	148.03	122.99
1	A	199	PRO	C-N-CA	18.02	148.03	122.99
1	A	145	PHE	CA-CB-CG	-12.00	101.80	113.80
1	A	102	ARG	CD-NE-CZ	11.81	140.93	124.40
1	A	131	ALA	CA-C-O	10.54	131.89	120.82
1	A	199	PRO	O-C-N	-9.79	111.02	123.06
1	A	115	LEU	CA-C-O	-9.47	110.20	120.24
1	A	131	ALA	O-C-N	-9.09	112.70	122.07
1	A	101	ASN	CA-CB-CG	-8.84	103.76	112.60
1	A	140	MET	CA-C-O	-8.47	111.20	120.43
1	A	197	ASP	N-CA-C	-8.31	101.61	112.41
1	A	200	VAL	CA-C-O	-8.06	111.81	120.36
1	A	175	PRO	CA-C-O	-8.04	111.83	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	HIS	N-CA-C	7.90	124.50	114.31
1	A	141	SER	N-CA-C	7.76	121.21	109.41
1	A	146	HIS	N-CA-C	7.73	123.29	113.55
1	A	69	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	A	102	ARG	NE-CZ-NH2	7.54	125.99	119.20
1	A	247	MET	O-C-N	-7.52	114.15	122.12
1	A	81	PHE	CA-C-O	-7.29	112.96	120.54
1	A	167	ASP	CA-CB-CG	-7.07	105.53	112.60
1	A	115	LEU	O-C-N	7.02	131.48	123.27
1	A	113	ILE	O-C-N	6.96	130.45	123.00
1	A	199	PRO	CA-C-O	-6.69	113.51	121.67
1	A	178	LYS	CA-C-O	6.65	127.62	119.97
1	A	146	HIS	CB-CA-C	-6.55	99.19	109.34
1	A	231	ALA	N-CA-C	-6.53	99.38	109.76
1	A	6	VAL	CA-C-O	6.48	126.81	120.27
1	A	167	ASP	CA-C-O	6.44	127.39	120.24
1	A	139	VAL	N-CA-C	-6.44	97.92	107.51
1	A	249	LEU	O-C-N	-6.42	115.31	122.12
1	A	221	SER	CA-C-O	-6.37	113.49	120.43
1	A	186	THR	CA-C-O	6.35	127.28	120.55
1	A	136	VAL	CA-C-O	-6.29	113.55	120.72
1	A	136	VAL	CA-CB-CG1	6.28	121.08	110.40
1	A	52	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	90	GLN	CA-C-N	-6.00	113.72	122.65
1	A	90	GLN	C-N-CA	-6.00	113.72	122.65
1	A	191	MET	CA-CB-CG	5.95	126.00	114.10
1	A	224	THR	CA-C-O	-5.94	115.09	121.45
1	A	219	PHE	CA-C-O	-5.93	112.39	119.15
1	A	27	ILE	CB-CA-C	-5.93	104.30	111.88
1	A	175	PRO	O-C-N	5.92	130.52	123.06
1	A	146	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	43	ASP	N-CA-C	5.87	120.57	113.41
1	A	89	GLU	N-CA-C	5.85	120.48	113.23
1	A	89	GLU	N-CA-CB	-5.84	101.33	110.44
1	A	7	LYS	CA-C-N	-5.83	113.94	122.86
1	A	7	LYS	C-N-CA	-5.83	113.94	122.86
1	A	140	MET	O-C-N	5.74	129.75	123.27
1	A	132	HIS	O-C-N	5.74	128.20	122.12
1	A	109	LEU	CA-C-N	-5.66	113.16	122.67
1	A	109	LEU	C-N-CA	-5.66	113.16	122.67
1	A	107	SER	CA-C-N	5.65	132.66	121.53
1	A	107	SER	C-N-CA	5.65	132.66	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	SER	N-CA-CB	-5.65	102.45	111.43
1	A	97	TYR	CA-C-O	5.64	126.74	120.82
1	A	231	ALA	CA-C-O	-5.61	114.30	120.69
1	A	215	ALA	N-CA-C	5.59	119.10	112.72
1	A	139	VAL	CA-C-O	-5.57	114.28	120.74
1	A	25	ARG	CA-CB-CG	5.57	125.24	114.10
1	A	41	THR	CA-C-O	-5.55	114.42	120.36
1	A	121	ASP	N-CA-C	5.53	118.02	111.33
1	A	169	PRO	CA-C-O	-5.52	114.68	121.31
1	A	109	LEU	O-C-N	5.51	130.01	122.46
1	A	235	GLY	CA-C-N	-5.50	113.30	122.64
1	A	235	GLY	C-N-CA	-5.50	113.30	122.64
1	A	63	THR	N-CA-C	-5.44	105.43	111.36
1	A	224	THR	O-C-N	5.39	129.30	123.10
1	A	69	ARG	CA-C-O	-5.38	114.85	120.55
1	A	194	HIS	CB-CA-C	-5.35	100.04	109.02
1	A	228	VAL	CB-CA-C	5.32	116.97	111.23
1	A	194	HIS	N-CA-CB	-5.31	103.83	110.90
1	A	222	ALA	N-CA-C	5.27	119.56	113.18
1	A	79	PHE	CA-C-O	-5.17	114.64	120.43
1	A	81	PHE	N-CA-C	-5.16	99.38	108.20
1	A	90	GLN	N-CA-C	5.15	117.22	109.23
1	A	145	PHE	CB-CA-C	-5.12	100.37	110.11
1	A	53	MET	N-CA-C	5.12	116.94	111.36
1	A	121	ASP	O-C-N	5.12	127.55	122.12
1	A	125	LYS	O-C-N	5.11	127.54	122.12
1	A	15	MET	CA-C-N	5.09	125.10	119.90
1	A	15	MET	C-N-CA	5.09	125.10	119.90
1	A	214	LEU	CA-C-O	5.09	124.74	119.14
1	A	204	SER	N-CA-C	-5.08	100.89	109.07
1	A	146	HIS	CB-CG-ND1	5.06	130.29	122.70
1	A	210	VAL	N-CA-C	5.06	116.39	110.62
1	A	72	MET	CA-C-O	5.06	127.09	121.22
1	A	162	GLN	N-CA-CB	5.06	117.56	110.12
1	A	80	THR	N-CA-C	5.06	116.63	108.34
1	A	23	MET	O-C-N	5.03	129.89	123.24
1	A	249	LEU	CA-C-O	5.03	125.88	120.55
1	A	198	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	147	GLN	N-CA-C	5.02	115.16	108.38
1	A	86	GLU	CA-CB-CG	-5.02	104.06	114.10
1	A	195	TYR	N-CA-C	5.02	120.93	114.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	VAL	Mainchain

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	1934	0	1962	35	0
2	A	181	0	0	12	0
All	All	2115	0	1962	35	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 9.

All (35) 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:156:SER:OG	2:A:2117:HOH:O	1.87	0.91
1:A:162:GLN:HE22	1:A:196:ALA:HA	1.47	0.77
1:A:240:ASN:HD22	1:A:243:ARG:HH11	1.39	0.69
1:A:3:THR:HG21	1:A:13:GLU:HG3	1.75	0.68
1:A:240:ASN:ND2	1:A:243:ARG:HH11	1.92	0.67
1:A:240:ASN:HB2	2:A:2177:HOH:O	1.96	0.65
1:A:112:MET:HG2	1:A:137:TYR:HB2	1.78	0.65
1:A:217:GLU:OE2	1:A:250:HIS:HD2	1.80	0.64
1:A:89:GLU:O	2:A:2072:HOH:O	2.14	0.64
1:A:84:ALA:HB3	1:A:91:THR:HG22	1.81	0.62
1:A:146:HIS:HE1	2:A:2104:HOH:O	1.83	0.61
1:A:247:MET:SD	2:A:2071:HOH:O	2.56	0.60
1:A:229:LYS:O	1:A:230:GLN:C	2.44	0.60
1:A:146:HIS:CE1	2:A:2104:HOH:O	2.56	0.58
1:A:25:ARG:HB3	1:A:53:MET:HG2	1.91	0.53
1:A:41:THR:HB	1:A:243:ARG:NH1	2.24	0.53
1:A:179:HIS:HB3	2:A:2135:HOH:O	2.08	0.52
1:A:53:MET:HE3	1:A:53:MET:HA	1.91	0.52
1:A:203:MET:HE3	2:A:2163:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:HG23	2:A:2037:HOH:O	2.11	0.50
1:A:84:ALA:CB	1:A:91:THR:HG22	2.42	0.49
1:A:208:GLU:HB2	2:A:2151:HOH:O	2.14	0.47
1:A:144:ASP:OD1	1:A:146:HIS:ND1	2.47	0.46
1:A:228:VAL:O	1:A:230:GLN:NE2	2.49	0.45
1:A:8:ASN:ND2	2:A:2013:HOH:O	2.49	0.45
1:A:229:LYS:O	1:A:230:GLN:O	2.36	0.42
1:A:162:GLN:NE2	1:A:196:ALA:HA	2.24	0.42
1:A:213:ARG:HH11	1:A:213:ARG:HD3	1.66	0.42
1:A:228:VAL:O	1:A:229:LYS:O	2.39	0.41
1:A:229:LYS:HB3	1:A:230:GLN:HG3	2.02	0.41
1:A:160:LYS:NZ	2:A:2127:HOH:O	2.49	0.41
1:A:228:VAL:C	1:A:229:LYS:O	2.63	0.41
1:A:69:ARG:HA	1:A:69:ARG:HD3	1.87	0.40
1:A:82:ARG:CZ	1:A:143:HIS:CE1	3.04	0.40
1:A:82:ARG:O	1:A:88:GLY:HA3	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	250/252 (99%)	243 (97%)	5 (2%)	2 (1%)	16 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	229	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	209/209 (100%)	198 (95%)	11 (5%)	20 4

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	6	VAL
1	A	31	LYS
1	A	55	ILE
1	A	59	GLN
1	A	85	LYS
1	A	95	GLN
1	A	146	HIS
1	A	191	MET
1	A	229	LYS
1	A	230	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	162	GLN
1	A	194	HIS
1	A	236	GLN
1	A	240	ASN
1	A	250	HIS

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 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	199:PRO	C	200:VAL	N	1.19

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, 95th 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 ²)	Q<0.9
1	A	252/252 (100%)	-0.17	7 (2%) 55 62	13, 24, 42, 86	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	HIS	4.5
1	A	231	ALA	3.4
1	A	233	ALA	3.3
1	A	229	LYS	3.2
1	A	230	GLN	2.9
1	A	145	PHE	2.7
1	A	200	VAL	2.5

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 oligosaccharides 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.