



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:02 am BST

PDB ID : 3LZ8  
Title : Structure of a putative chaperone dnaj from klebsiella pneumoniae subsp. pneumoniae mgh 78578 at 2.9 a resolution.  
Authors : Filippova, E.V.; Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Bearden, J.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-03-01  
Resolution : 2.90 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.

---

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	:	2.11
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)	:	2.11

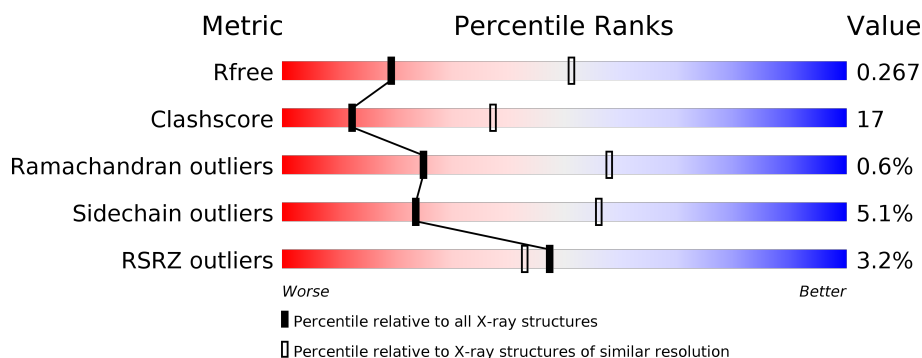
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	329	<div> <div>2%</div> <div> <div></div> <div>38%</div> <div>18%</div> <div>•</div> <div>43%</div> </div> </div>
1	B	329	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>15%</div> <div>•</div> <div>43%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2833 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 Putative chaperone DnaJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1405	908	240	256	1			
1	B	187	Total	C	N	O	S	0	0	0
			1421	916	242	261	2			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP A6TH30
A	-22	HIS	-	expression tag	UNP A6TH30
A	-21	HIS	-	expression tag	UNP A6TH30
A	-20	HIS	-	expression tag	UNP A6TH30
A	-19	HIS	-	expression tag	UNP A6TH30
A	-18	HIS	-	expression tag	UNP A6TH30
A	-17	HIS	-	expression tag	UNP A6TH30
A	-16	SER	-	expression tag	UNP A6TH30
A	-15	SER	-	expression tag	UNP A6TH30
A	-14	GLY	-	expression tag	UNP A6TH30
A	-13	VAL	-	expression tag	UNP A6TH30
A	-12	ASP	-	expression tag	UNP A6TH30
A	-11	LEU	-	expression tag	UNP A6TH30
A	-10	GLY	-	expression tag	UNP A6TH30
A	-9	THR	-	expression tag	UNP A6TH30
A	-8	GLU	-	expression tag	UNP A6TH30
A	-7	ASN	-	expression tag	UNP A6TH30
A	-6	LEU	-	expression tag	UNP A6TH30
A	-5	TYR	-	expression tag	UNP A6TH30
A	-4	PHE	-	expression tag	UNP A6TH30
A	-3	GLN	-	expression tag	UNP A6TH30
A	-2	SER	-	expression tag	UNP A6TH30
A	-1	ASN	-	expression tag	UNP A6TH30
A	0	ALA	-	expression tag	UNP A6TH30
B	-23	MET	-	expression tag	UNP A6TH30

*Continued on next page...*

*Continued from previous page...*

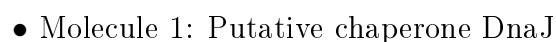
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP A6TH30
B	-21	HIS	-	expression tag	UNP A6TH30
B	-20	HIS	-	expression tag	UNP A6TH30
B	-19	HIS	-	expression tag	UNP A6TH30
B	-18	HIS	-	expression tag	UNP A6TH30
B	-17	HIS	-	expression tag	UNP A6TH30
B	-16	SER	-	expression tag	UNP A6TH30
B	-15	SER	-	expression tag	UNP A6TH30
B	-14	GLY	-	expression tag	UNP A6TH30
B	-13	VAL	-	expression tag	UNP A6TH30
B	-12	ASP	-	expression tag	UNP A6TH30
B	-11	LEU	-	expression tag	UNP A6TH30
B	-10	GLY	-	expression tag	UNP A6TH30
B	-9	THR	-	expression tag	UNP A6TH30
B	-8	GLU	-	expression tag	UNP A6TH30
B	-7	ASN	-	expression tag	UNP A6TH30
B	-6	LEU	-	expression tag	UNP A6TH30
B	-5	TYR	-	expression tag	UNP A6TH30
B	-4	PHE	-	expression tag	UNP A6TH30
B	-3	GLN	-	expression tag	UNP A6TH30
B	-2	SER	-	expression tag	UNP A6TH30
B	-1	ASN	-	expression tag	UNP A6TH30
B	0	ALA	-	expression tag	UNP A6TH30

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0

**i**

- Molecule 1: Putative chaperone DnaJ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.89 Å 67.40 Å 136.82 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.36 – 2.90 34.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.36-2.90) 99.9 (34.20-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.5.0051	Depositor
R, $R_{free}$	0.226 , 0.268 0.231 , 0.267	Depositor DCC
$R_{free}$ test set	654 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.4	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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	0.67	0/1437	0.86	0/1963
1	B	0.63	0/1453	0.85	1/1982 (0.1%)
All	All	0.65	0/2890	0.86	1/3945 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASN	CB-CA-C	-5.09	100.22	110.40

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	1405	0	1418	60	0
1	B	1421	0	1424	42	0
2	A	7	0	0	1	0
All	All	2833	0	2842	96	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 17.

All (96) 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:231:THR:HG22	1:A:233:LYS:H	1.40	0.87
1:B:175:LEU:HD12	1:B:191:LEU:HD23	1.61	0.81
1:B:115:ARG:HG3	1:B:187:PRO:HG2	1.63	0.79
1:A:174:ARG:HB2	1:A:192:TRP:CZ3	2.21	0.76
1:A:180:THR:HG23	1:A:181:PRO:HD2	1.69	0.73
1:B:164:PRO:O	1:B:167:VAL:HG13	1.90	0.71
1:A:180:THR:HG23	1:A:181:PRO:CD	2.24	0.67
1:A:213:VAL:HG12	1:A:215:PRO:HD3	1.78	0.65
1:A:196:HIS:CE1	1:A:198:ALA:HB2	2.33	0.64
1:A:289:LEU:HD12	1:B:289:LEU:HD21	1.81	0.63
1:B:200:HIS:CG	1:B:201:PRO:HD2	2.33	0.63
1:A:174:ARG:HB2	1:A:192:TRP:CH2	2.35	0.62
1:A:146:ASN:C	1:A:148:PHE:H	2.03	0.61
1:B:171:GLN:HE21	1:B:172:ARG:N	1.98	0.61
1:B:286:TRP:HA	1:B:289:LEU:HD13	1.82	0.60
1:B:238:LEU:HD13	1:B:252:ILE:HG12	1.84	0.60
1:A:215:PRO:O	1:A:216:LEU:HD23	2.03	0.59
1:B:137:THR:OG1	1:B:160:ASN:ND2	2.36	0.59
1:B:245:GLN:O	1:B:248:GLN:HB2	2.04	0.58
1:B:133:GLU:OE1	1:B:133:GLU:C	2.43	0.57
1:B:198:ALA:HB1	1:B:199:PRO:HD2	1.87	0.56
1:A:231:THR:HG22	1:A:232:LEU:N	2.22	0.55
1:A:173:ILE:N	1:A:173:ILE:HD12	2.22	0.55
1:A:172:ARG:HG2	1:A:194:VAL:HG12	1.88	0.54
1:B:209:ASN:HD22	1:B:267:PHE:HE2	1.53	0.54
1:B:229:VAL:O	1:B:236:ILE:HD13	2.07	0.54
1:A:175:LEU:HB2	1:A:191:LEU:HB3	1.90	0.54
1:A:175:LEU:HD12	1:A:191:LEU:HD23	1.90	0.53
1:A:205:ILE:HD12	1:A:205:ILE:H	1.74	0.53
1:A:124:ALA:O	1:A:136:ARG:NH2	2.41	0.53
1:B:197:ILE:HG21	1:B:205:ILE:HD11	1.91	0.52
1:A:117:HIS:O	1:A:189:GLY:HA3	2.09	0.51
1:A:180:THR:CG2	1:A:181:PRO:CD	2.89	0.51
1:B:202:LEU:HB3	1:B:212:ILE:CD1	2.41	0.51
1:B:168:VAL:HG13	1:B:171:GLN:HB3	1.91	0.51
1:A:159:LEU:CD1	1:A:175:LEU:HD11	2.41	0.51
1:A:174:ARG:O	1:A:175:LEU:HD23	2.11	0.51
1:A:147:VAL:O	1:A:147:VAL:HG12	2.11	0.51
1:A:274:MET:CG	1:B:272:ILE:CD1	2.90	0.50
1:A:236:ILE:HD13	1:A:236:ILE:H	1.76	0.50
1:A:258:VAL:O	1:A:258:VAL:HG12	2.10	0.50
1:A:140:TYR:HE2	1:A:159:LEU:HD22	1.76	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HA	1:A:156:PRO:HA	1.94	0.49
1:A:196:HIS:CG	1:A:196:HIS:O	2.65	0.49
1:A:274:MET:CG	1:B:272:ILE:HD13	2.42	0.49
1:B:210:LEU:HG	1:B:257:LEU:HD12	1.95	0.49
1:B:208:HIS:HA	1:B:257:LEU:HD22	1.94	0.49
1:A:279:ASP:O	1:A:280:GLU:C	2.51	0.49
1:B:146:ASN:HB3	1:B:148:PHE:H	1.76	0.48
1:B:215:PRO:O	1:B:216:LEU:HD23	2.13	0.48
1:A:205:ILE:N	1:A:205:ILE:HD12	2.29	0.48
1:A:231:THR:HB	1:A:234:GLU:O	2.14	0.48
1:A:231:THR:CG2	1:A:232:LEU:N	2.77	0.48
1:A:125:VAL:HG12	1:A:126:PHE:N	2.28	0.48
1:A:231:THR:HG22	1:A:233:LYS:N	2.20	0.48
1:A:149:GLY:HA2	2:A:311:HOH:O	2.14	0.47
1:A:274:MET:HG2	1:B:272:ILE:CD1	2.43	0.47
1:B:168:VAL:CG1	1:B:171:GLN:HB3	2.43	0.47
1:A:210:LEU:HD13	1:A:257:LEU:HG	1.97	0.47
1:A:130:THR:HG22	1:A:130:THR:O	2.16	0.46
1:B:289:LEU:HD12	1:B:289:LEU:H	1.81	0.46
1:B:213:VAL:O	1:B:215:PRO:HD3	2.16	0.46
1:B:126:PHE:HA	1:B:198:ALA:HB3	1.98	0.45
1:A:138:ILE:N	1:A:138:ILE:HD12	2.31	0.45
1:A:195:ILE:CG2	1:A:196:HIS:N	2.79	0.45
1:A:127:LEU:HD23	1:A:232:LEU:HD21	1.98	0.45
1:B:194:VAL:HG23	1:B:196:HIS:NE2	2.32	0.44
1:B:208:HIS:O	1:B:257:LEU:HB2	2.17	0.44
1:A:159:LEU:HD13	1:A:175:LEU:CD1	2.47	0.44
1:A:196:HIS:ND1	1:A:196:HIS:O	2.51	0.44
1:A:276:THR:O	1:A:277:LYS:C	2.56	0.44
1:A:200:HIS:HD2	1:A:202:LEU:N	2.16	0.43
1:A:117:HIS:H	1:A:180:THR:HB	1.82	0.43
1:A:236:ILE:HD11	1:A:252:ILE:HD13	1.99	0.43
1:B:171:GLN:C	1:B:171:GLN:HE21	2.22	0.43
1:A:145:TYR:CE1	1:A:151:ILE:HD11	2.54	0.43
1:A:201:PRO:O	1:A:202:LEU:HD23	2.19	0.43
1:B:141:ASN:HB3	1:B:154:GLU:HB3	2.01	0.43
1:B:134:GLN:HG3	1:B:163:ILE:HB	2.01	0.42
1:B:115:ARG:HA	1:B:187:PRO:HD2	2.01	0.42
1:B:259:SER:N	1:B:262:HIS:O	2.53	0.42
1:A:289:LEU:CD1	1:B:289:LEU:HD21	2.47	0.42
1:A:125:VAL:CG1	1:A:126:PHE:N	2.82	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:O	1:B:137:THR:HG22	2.18	0.42
1:A:168:VAL:O	1:A:169:ASP:C	2.57	0.42
1:A:194:VAL:HG23	1:A:194:VAL:O	2.20	0.42
1:A:130:THR:O	1:A:130:THR:CG2	2.67	0.41
1:A:140:TYR:CE2	1:A:159:LEU:HD22	2.56	0.41
1:B:285:LEU:O	1:B:289:LEU:HD12	2.21	0.41
1:A:218:PRO:HD3	1:A:273:VAL:O	2.21	0.41
1:B:195:ILE:HG22	1:B:196:HIS:N	2.36	0.41
1:A:146:ASN:O	1:A:148:PHE:N	2.46	0.40
1:A:274:MET:HG3	1:B:272:ILE:CD1	2.51	0.40
1:A:180:THR:CG2	1:A:181:PRO:HD2	2.45	0.40
1:B:164:PRO:O	1:B:167:VAL:CG1	2.65	0.40
1:B:194:VAL:CG2	1:B:196:HIS:NE2	2.85	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	180/329 (55%)	156 (87%)	22 (12%)	2 (1%)	14	42
1	B	181/329 (55%)	172 (95%)	9 (5%)	0	100	100
All	All	361/658 (55%)	328 (91%)	31 (9%)	2 (1%)	25	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	THR
1	A	147	VAL

### 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	146/277 (53%)	139 (95%)	7 (5%)	25	58
1	B	147/277 (53%)	139 (95%)	8 (5%)	22	54
All	All	293/554 (53%)	278 (95%)	15 (5%)	24	56

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

Mol	Chain	Res	Type
1	A	136	ARG
1	A	158	THR
1	A	160	ASN
1	A	161	VAL
1	A	188	ASN
1	A	210	LEU
1	A	236	ILE
1	B	122	GLU
1	B	133	GLU
1	B	137	THR
1	B	155	THR
1	B	171	GLN
1	B	234	GLU
1	B	236	ILE
1	B	284	GLU

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

Mol	Chain	Res	Type
1	A	160	ASN
1	A	200	HIS
1	B	146	ASN
1	B	160	ASN
1	B	171	GLN
1	B	245	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 [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	186/329 (56%)	0.03	6 (3%) 47 43	53, 74, 131, 148	0
1	B	187/329 (56%)	-0.02	6 (3%) 47 43	57, 79, 108, 118	0
All	All	373/658 (56%)	0.01	12 (3%) 47 43	53, 78, 124, 148	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	3.9
1	B	263	THR	3.5
1	A	181	PRO	3.2
1	B	233	LYS	2.8
1	B	253	LYS	2.8
1	B	236	ILE	2.7
1	A	144	VAL	2.6
1	A	114	ALA	2.6
1	A	148	PHE	2.5
1	B	250	LEU	2.5
1	B	240	VAL	2.1
1	A	151	ILE	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.