



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:22 PM UTC

PDB ID : 4KRD / pdb_00004krd
Title : Crystal Structure of Pho85-Pcl10 Complex
Authors : Quioco, F.A.; Zheng, F.
Deposited on : 2013-05-16
Resolution : 1.95 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

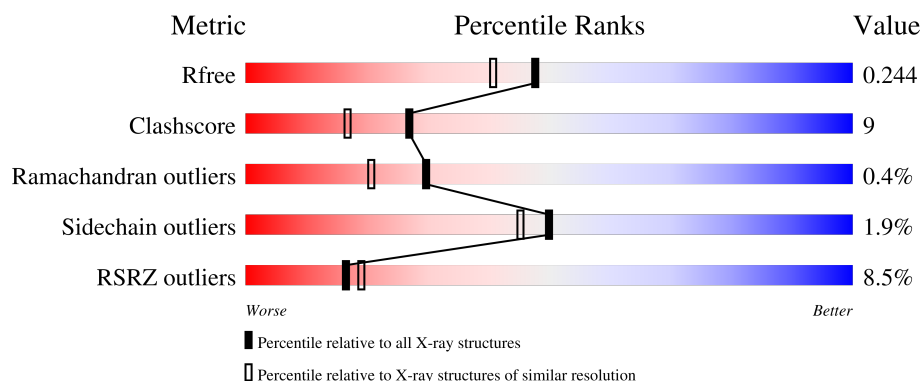
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	317	8% 74% 16% • 7%
2	B	207	8% 73% 18% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4005 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 Cyclin-dependent protein kinase PHO85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	1	0
			2360	1514	401	434	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	MET	-	expression tag	UNP P17157
A	307	GLY	-	expression tag	UNP P17157
A	308	GLY	-	expression tag	UNP P17157
A	309	SER	-	expression tag	UNP P17157
A	310	ARG	-	expression tag	UNP P17157
A	311	SER	-	expression tag	UNP P17157
A	312	HIS	-	expression tag	UNP P17157
A	313	HIS	-	expression tag	UNP P17157
A	314	HIS	-	expression tag	UNP P17157
A	315	HIS	-	expression tag	UNP P17157
A	316	HIS	-	expression tag	UNP P17157
A	317	HIS	-	expression tag	UNP P17157

- Molecule 2 is a protein called PHO85 cyclin-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	1	0
			1497	962	252	274	9			

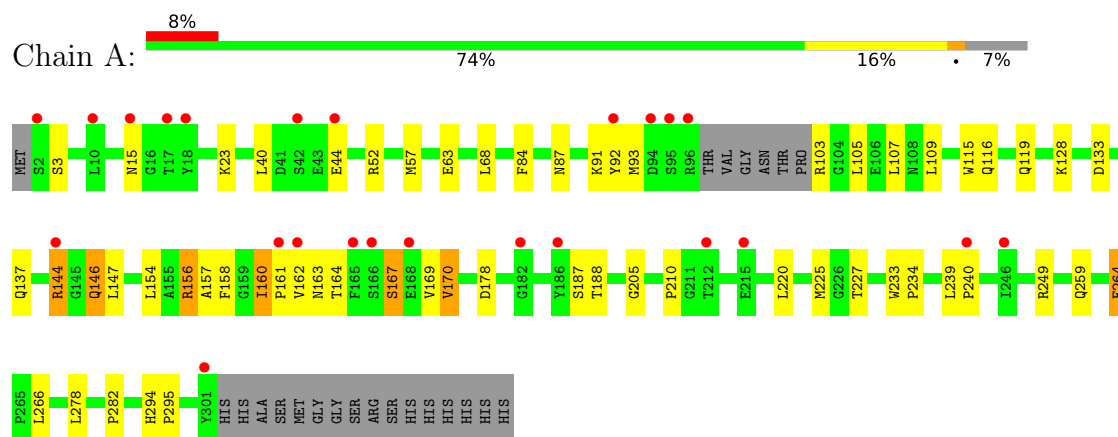
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	49	Total	O	0	0
			49	49		

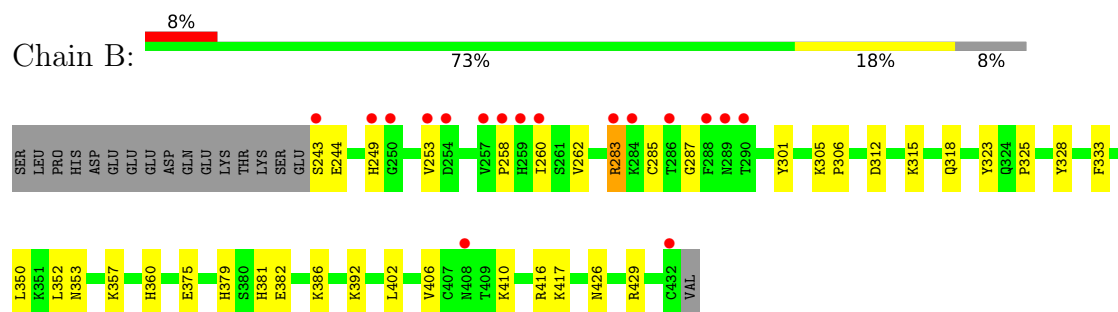
3 Residue-property plots [i](#)

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: Cyclin-dependent protein kinase PHO85



- Molecule 2: PHO85 cyclin-10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.58Å 66.36Å 78.89Å 90.00° 99.21° 90.00°	Depositor
Resolution (Å)	49.92 – 1.95 49.92 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.92-1.95) 99.0 (49.92-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.194 , 0.241 (Not available) , 0.244	Depositor DCC
R_{free} test set	1860 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.7	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	4005	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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	0.52	1/2414 (0.0%)	0.78	3/3270 (0.1%)
2	B	0.50	0/1519	0.74	0/2051
All	All	0.51	1/3933 (0.0%)	0.77	3/5321 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	GLN	C-O	-5.39	1.17	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ILE	CA-C-N	5.22	126.37	119.84
1	A	160	ILE	C-N-CA	5.22	126.37	119.84
1	A	167	SER	N-CA-C	-5.20	106.91	113.20

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	2360	0	2356	47	0
2	B	1497	0	1538	26	0
3	A	99	0	0	1	0
3	B	49	0	0	2	0
All	All	4005	0	3894	71	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 (71) 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:52:ARG:HH12	1:A:156:ARG:NH2	1.74	0.84
1:A:103:ARG:HD3	1:A:205:GLY:O	1.83	0.78
1:A:107:LEU:HG	1:A:264:GLU:HG2	1.71	0.73
1:A:162:VAL:HG13	2:B:375:GLU:OE1	1.92	0.70
1:A:52:ARG:HH12	1:A:156:ARG:HH21	1.38	0.69
2:B:244:GLU:OE2	2:B:249:HIS:HD2	1.76	0.68
1:A:162:VAL:HG12	1:A:164:THR:H	1.59	0.67
1:A:52:ARG:NH1	1:A:156:ARG:HH21	1.97	0.62
1:A:169:VAL:HG23	1:A:170:VAL:HG23	1.84	0.60
2:B:285:CYS:H	2:B:353:ASN:HD21	1.49	0.59
1:A:93:MET:HG2	1:A:105:LEU:HD21	1.84	0.58
2:B:258:PRO:HB2	2:B:260:ILE:HG13	1.85	0.58
1:A:116:GLN:NE2	1:A:147:LEU:H	2.01	0.58
2:B:283:ARG:NH2	2:B:350:LEU:H	2.02	0.57
1:A:259:GLN:HE22	1:A:266:LEU:H	1.52	0.57
1:A:63:GLU:HG3	3:A:446:HOH:O	2.04	0.57
2:B:323:TYR:OH	2:B:379:HIS:HD2	1.87	0.56
1:A:162:VAL:HG12	1:A:163:ASN:N	2.22	0.55
1:A:294:HIS:CG	1:A:295:PRO:HD2	2.43	0.54
2:B:360:HIS:HD2	3:B:540:HOH:O	1.90	0.54
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.23	0.53
1:A:133:ASP:HB2	1:A:154:LEU:HD12	1.91	0.53
1:A:160:ILE:O	1:A:162:VAL:HG23	2.09	0.52
1:A:115:TRP:CZ2	1:A:119:GLN:NE2	2.78	0.51
1:A:178:ASP:CG	1:A:282:PRO:HG3	2.36	0.50
2:B:312:ASP:HA	2:B:315:LYS:HD2	1.93	0.50
1:A:210:PRO:HD2	1:A:220:LEU:HD13	1.94	0.50
1:A:227:THR:HG23	1:A:249:ARG:HG3	1.94	0.50
2:B:253:VAL:HA	2:B:416:ARG:HD2	1.93	0.50
1:A:52:ARG:HH22	1:A:156:ARG:NH2	2.10	0.49
2:B:381:HIS:HE1	2:B:392:LYS:O	1.95	0.49
1:A:107:LEU:CG	1:A:264:GLU:HG2	2.39	0.49
1:A:156:ARG:HD3	1:A:157:ALA:O	2.11	0.49
1:A:187:SER:OG	1:A:188:THR:N	2.46	0.49
1:A:23:LYS:HE3	1:A:84:PHE:CZ	2.48	0.49
1:A:116:GLN:HE22	1:A:146:GLN:HA	1.78	0.49
2:B:382[B]:GLU:HG3	2:B:386:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HG12	1:A:164:THR:N	2.26	0.48
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.78	0.48
1:A:162:VAL:CG1	2:B:375:GLU:OE1	2.61	0.47
2:B:287:GLY:HA2	2:B:352:LEU:HD23	1.96	0.47
2:B:333:PHE:CE2	2:B:417:LYS:HD3	2.50	0.47
1:A:57:MET:HB3	1:A:68:LEU:HD23	1.96	0.47
1:A:116:GLN:HE22	1:A:147:LEU:H	1.63	0.46
1:A:239:LEU:HA	1:A:240:PRO:HD3	1.83	0.45
1:A:162:VAL:CG1	1:A:163:ASN:N	2.78	0.45
2:B:283:ARG:HH22	2:B:350:LEU:H	1.63	0.45
1:A:128:LYS:HA	1:A:158:PHE:CE2	2.52	0.45
2:B:318:GLN:NE2	2:B:328:TYR:OH	2.48	0.45
1:A:57:MET:HE3	1:A:68:LEU:HG	2.00	0.44
1:A:233:TRP:N	1:A:234:PRO:HD3	2.33	0.44
2:B:426:ASN:OD1	2:B:429:ARG:NH2	2.50	0.43
2:B:382[B]:GLU:OE2	2:B:386:LYS:HE3	2.19	0.43
2:B:262:VAL:HG23	2:B:325:PRO:HG3	2.00	0.43
2:B:402:LEU:O	2:B:406:VAL:HG22	2.18	0.43
1:A:147:LEU:C	1:A:147:LEU:HD23	2.43	0.43
1:A:52:ARG:HH22	1:A:156:ARG:HH21	1.66	0.42
2:B:258:PRO:CB	2:B:260:ILE:HG13	2.47	0.42
1:A:44[A]:GLU:O	1:A:44[A]:GLU:HG2	2.19	0.42
2:B:301:TYR:OH	2:B:357:LYS:HD2	2.19	0.42
2:B:318:GLN:NE2	2:B:318:GLN:HA	2.35	0.41
1:A:52:ARG:NH2	1:A:156:ARG:HH21	2.17	0.41
1:A:52:ARG:NH1	1:A:156:ARG:NH2	2.51	0.41
1:A:107:LEU:CD1	1:A:264:GLU:HG2	2.50	0.41
1:A:92:TYR:OH	1:A:109:LEU:HD21	2.21	0.41
1:A:87:ASN:OD1	1:A:91:LYS:HB2	2.21	0.41
2:B:243:SER:O	2:B:410:LYS:CE	2.69	0.41
1:A:137:GLN:HE21	1:A:137:GLN:HB2	1.61	0.40
1:A:225:MET:HE2	1:A:278:LEU:O	2.22	0.40
2:B:305:LYS:HA	2:B:306:PRO:HD3	1.94	0.40
2:B:357:LYS:HG3	3:B:527:HOH:O	2.22	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	291/317 (92%)	281 (97%)	8 (3%)	2 (1%)	18	10
2	B	189/207 (91%)	189 (100%)	0	0	100	100
All	All	480/524 (92%)	470 (98%)	8 (2%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	VAL
1	A	161	PRO

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	260/284 (92%)	253 (97%)	7 (3%)	39	32
2	B	169/194 (87%)	168 (99%)	1 (1%)	78	79
All	All	429/478 (90%)	421 (98%)	8 (2%)	50	45

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	15	ASN
1	A	40	LEU
1	A	144	ARG

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Mol	Chain	Res	Type
1	A	156	ARG
1	A	167	SER
1	A	264	GLU
2	B	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	137	GLN
1	A	146	GLN
1	A	259	GLN
1	A	261	HIS
1	A	275	HIS
1	A	293	HIS
2	B	318	GLN
2	B	353	ASN
2	B	360	HIS
2	B	379	HIS
2	B	381	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](#)

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, 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	294/317 (92%)	0.53	24 (8%)	17 20	24, 41, 62, 78	1 (0%)
2	B	190/207 (91%)	0.57	17 (8%)	15 17	24, 44, 70, 94	1 (0%)
All	All	484/524 (92%)	0.54	41 (8%)	16 19	24, 42, 65, 94	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	VAL	5.4
2	B	289	ASN	4.5
2	B	257	VAL	4.2
2	B	259	HIS	4.1
1	A	144	ARG	3.6
1	A	44[A]	GLU	3.6
2	B	286	THR	3.6
1	A	165	PHE	3.4
1	A	92	TYR	3.1
2	B	260	ILE	3.0
1	A	186	TYR	3.0
1	A	301	TYR	3.0
1	A	2	SER	2.9
1	A	15	ASN	2.8
2	B	408	ASN	2.8
1	A	168	GLU	2.8
2	B	254	ASP	2.8
1	A	17	THR	2.7
1	A	215	GLU	2.7
1	A	95	SER	2.7
1	A	246	ILE	2.7
1	A	96	ARG	2.6
2	B	288	PHE	2.6
1	A	240	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	250	GLY	2.5
1	A	94	ASP	2.5
1	A	182	GLY	2.4
2	B	249	HIS	2.4
2	B	258	PRO	2.4
2	B	243	SER	2.4
1	A	212	THR	2.4
2	B	283	ARG	2.4
1	A	18	TYR	2.3
1	A	161	PRO	2.3
2	B	432	CYS	2.3
2	B	253	VAL	2.2
2	B	290	THR	2.2
1	A	42	SER	2.2
1	A	10	LEU	2.1
2	B	284	LYS	2.1
1	A	166	SER	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 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.