



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:28 AM UTC

PDB ID : 6FDO / pdb_00006fdo
Title : Rio2 structure
Authors : Fribourg, S.
Deposited on : 2017-12-26
Resolution : 2.60 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

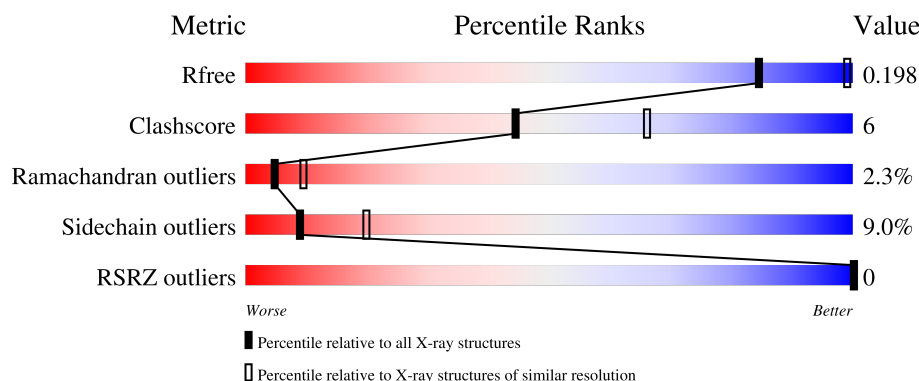
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	353	 61% 16% •• 19%
1	B	353	 63% 14% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4675 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 Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2318	1476	397	430	15			
1	B	284	Total	C	N	O	S	0	0	0
			2296	1464	390	427	15			

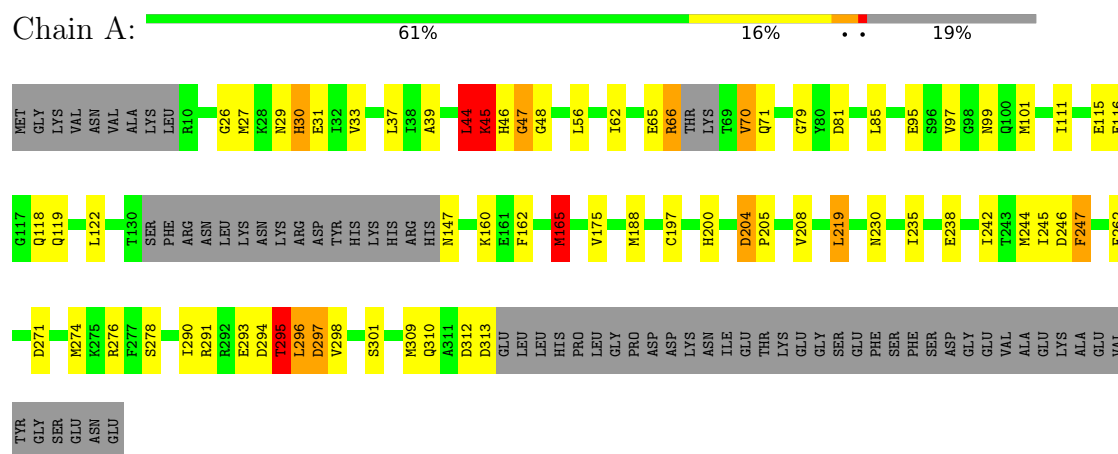
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	28	Total	O	0	0
			28	28		

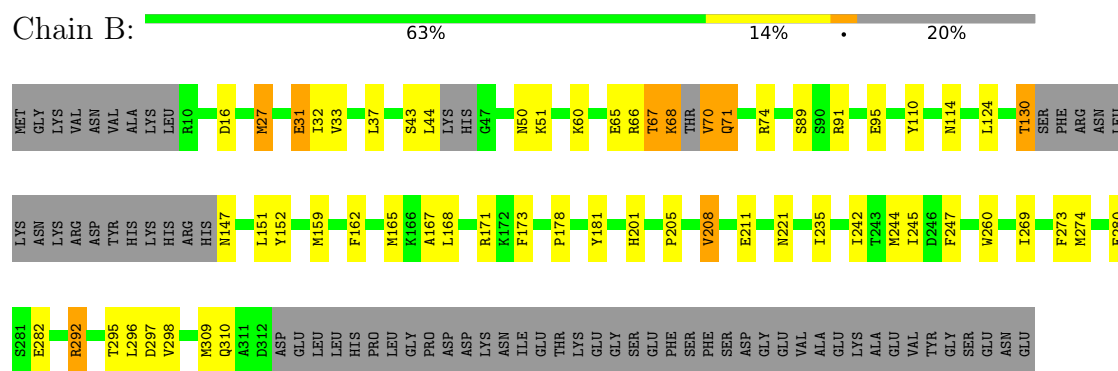
3 Residue-property plots

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: Serine/threonine-protein kinase RIO2



• Molecule 1: Serine/threonine-protein kinase RIO2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	67.56Å 67.56Å 312.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.69 – 2.60 42.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.69-2.60) 100.0 (42.69-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.195 , 0.250 0.162 , 0.198	Depositor DCC
R_{free} test set	1194 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.324 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4675	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

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	0.89	1/2369 (0.0%)	1.49	16/3195 (0.5%)
1	B	0.88	1/2345 (0.0%)	1.48	9/3162 (0.3%)
All	All	0.89	2/4714 (0.0%)	1.49	25/6357 (0.4%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	MET	SD-CE	-6.00	1.64	1.79
1	B	269	ILE	CG1-CD1	5.02	1.71	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	VAL	CA-C-N	9.30	138.45	121.70
1	A	70	VAL	C-N-CA	9.30	138.45	121.70
1	A	44	LEU	CA-C-N	7.37	135.61	121.54
1	A	44	LEU	C-N-CA	7.37	135.61	121.54
1	A	45	LYS	CA-C-N	7.06	134.41	121.70
1	A	45	LYS	C-N-CA	7.06	134.41	121.70
1	B	16	ASP	CA-C-N	6.96	129.92	120.38
1	B	16	ASP	C-N-CA	6.96	129.92	120.38
1	B	296	LEU	N-CA-C	6.93	120.96	112.23
1	B	147	ASN	CA-C-N	6.73	129.04	120.56
1	B	147	ASN	C-N-CA	6.73	129.04	120.56
1	B	51	LYS	N-CA-C	-6.07	103.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	204	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	147	ASN	CA-CB-CG	5.74	118.33	112.60
1	A	81	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	39	ALA	CA-C-N	5.43	128.02	120.63
1	A	39	ALA	C-N-CA	5.43	128.02	120.63
1	A	246	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	79	GLY	CA-C-N	5.25	127.26	120.44
1	A	79	GLY	C-N-CA	5.25	127.26	120.44
1	B	114	ASN	CA-C-N	5.12	127.09	120.44
1	B	114	ASN	C-N-CA	5.12	127.09	120.44
1	A	219	LEU	CA-C-N	5.07	127.07	120.28
1	A	219	LEU	C-N-CA	5.07	127.07	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	THR	Peptide

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	2318	0	2275	31	2
1	B	2296	0	2257	26	0
2	A	33	0	0	1	0
2	B	28	0	0	0	0
All	All	4675	0	4532	55	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.

All (55) 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:159:MET:HE1	1:B:310:GLN:HG3	1.62	0.81
1:A:296:LEU:O	1:A:298:VAL:N	2.16	0.76
1:B:167:ALA:HB1	1:B:298:VAL:HG23	1.71	0.70
1:A:219:LEU:HD21	1:A:244:MET:HE1	1.78	0.65
1:A:111:ILE:HD11	1:A:119:GLN:HB3	1.80	0.64
1:A:296:LEU:N	1:A:296:LEU:HD23	2.13	0.63
1:A:165:MET:HE1	1:A:188:MET:HB2	1.84	0.58
1:A:208:VAL:HG23	1:A:242:ILE:HD11	1.85	0.58
1:B:67:THR:HG1	1:B:70:VAL:N	2.02	0.58
1:A:310:GLN:OE1	1:B:130:THR:HG21	2.04	0.57
1:A:165:MET:HE1	1:A:188:MET:CB	2.35	0.57
1:A:293:GLU:HG3	1:A:294:ASP:H	1.70	0.56
1:B:65:GLU:O	1:B:71:GLN:HA	2.07	0.55
1:B:33:VAL:HG23	1:B:37:LEU:HD23	1.88	0.54
1:B:32:ILE:HD11	1:B:70:VAL:HG23	1.91	0.51
1:A:235:ILE:HG13	1:A:245:ILE:HG13	1.95	0.49
1:A:45:LYS:H	1:A:47:GLY:H	1.61	0.49
1:A:230:ASN:HB3	1:B:260:TRP:CZ2	2.48	0.48
1:A:262:PHE:CE1	1:A:290:ILE:HD11	2.48	0.48
1:B:165:MET:HE3	1:B:178:PRO:HB3	1.94	0.48
1:B:208:VAL:HG23	1:B:242:ILE:HD11	1.96	0.48
1:A:33:VAL:HG23	1:A:37:LEU:HD23	1.96	0.47
1:B:162:PHE:HB3	1:B:309:MET:HE1	1.94	0.47
1:A:26:GLY:O	1:A:29:ASN:O	2.33	0.47
1:B:244:MET:HG2	1:B:247:PHE:HD2	1.79	0.47
1:A:56:LEU:HB3	1:A:62:ILE:HG12	1.96	0.46
1:B:235:ILE:O	1:B:242:ILE:HA	2.16	0.46
1:B:168:LEU:O	1:B:173:PHE:HB2	2.15	0.46
1:B:167:ALA:CB	1:B:298:VAL:HG23	2.41	0.46
1:B:68:LYS:HB2	1:B:70:VAL:N	2.31	0.45
1:B:208:VAL:HG22	1:B:273:PHE:CZ	2.51	0.45
1:B:27:MET:HE1	1:B:74:ARG:HA	1.97	0.45
1:B:167:ALA:O	1:B:171:ARG:HD2	2.16	0.45
1:B:221:ASN:O	1:B:292:ARG:HA	2.17	0.45
1:A:44:LEU:HB3	1:A:47:GLY:HA2	2.00	0.43
1:A:85:LEU:HD13	1:A:97:VAL:HG21	2.00	0.43
1:A:197:CYS:C	1:A:276:ARG:HH12	2.27	0.43
1:B:274:MET:SD	1:B:280:GLU:HB2	2.59	0.43
1:B:110:TYR:CE1	1:B:124:LEU:HD12	2.54	0.43
1:A:293:GLU:H	1:A:295:THR:HG23	1.84	0.42
1:B:159:MET:HG3	1:B:181:TYR:CZ	2.55	0.42
1:A:31:GLU:HG2	2:A:413:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HB3	1:A:45:LYS:H	1.50	0.42
1:A:175:VAL:HG12	1:A:244:MET:HB3	2.01	0.42
1:A:200:HIS:HA	1:A:276:ARG:HD2	2.02	0.42
1:B:31:GLU:OE2	1:B:130:THR:HG23	2.19	0.42
1:A:274:MET:O	1:A:278:SER:HA	2.20	0.41
1:B:205:PRO:HA	1:B:208:VAL:HG13	2.03	0.41
1:A:205:PRO:HA	1:A:208:VAL:CG1	2.51	0.41
1:A:27:MET:CE	1:A:147:ASN:HB3	2.51	0.41
1:B:27:MET:HB3	1:B:151:LEU:HD22	2.02	0.41
1:A:296:LEU:C	1:A:298:VAL:N	2.79	0.41
1:A:162:PHE:HB3	1:A:309:MET:HE1	2.02	0.40
1:A:244:MET:HG2	1:A:247:PHE:HD2	1.85	0.40
1:A:296:LEU:N	1:A:296:LEU:CD2	2.84	0.40

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:66:ARG:CZ	1:A:294:ASP:OD1[5_665]	2.14	0.06
1:A:66:ARG:NE	1:A:294:ASP:OD1[5_665]	2.15	0.05

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	282/353 (80%)	261 (93%)	13 (5%)	8 (3%)	4	6
1	B	278/353 (79%)	252 (91%)	21 (8%)	5 (2%)	6	14
All	All	560/706 (79%)	513 (92%)	34 (6%)	13 (2%)	5	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	71	GLN
1	A	297	ASP
1	B	71	GLN
1	B	292	ARG
1	A	30	HIS
1	A	44	LEU
1	A	295	THR
1	A	48	GLY
1	B	67	THR
1	B	50	ASN
1	B	43	SER
1	A	47	GLY

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	252/312 (81%)	226 (90%)	26 (10%)	7	15
1	B	250/312 (80%)	231 (92%)	19 (8%)	12	27
All	All	502/624 (80%)	457 (91%)	45 (9%)	9	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	44	LEU
1	A	45	LYS
1	A	46	HIS
1	A	65	GLU
1	A	66	ARG
1	A	70	VAL
1	A	95	GLU
1	A	99	ASN
1	A	101	MET
1	A	115	GLU

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Mol	Chain	Res	Type
1	A	116	GLU
1	A	118	GLN
1	A	122	LEU
1	A	160	LYS
1	A	165	MET
1	A	204	ASP
1	A	238	GLU
1	A	247	PHE
1	A	291	ARG
1	A	295	THR
1	A	296	LEU
1	A	297	ASP
1	A	301	SER
1	A	312	ASP
1	A	313	ASP
1	B	27	MET
1	B	31	GLU
1	B	44	LEU
1	B	60	LYS
1	B	66	ARG
1	B	68	LYS
1	B	70	VAL
1	B	89	SER
1	B	91	ARG
1	B	95	GLU
1	B	130	THR
1	B	152	TYR
1	B	201	HIS
1	B	208	VAL
1	B	211	GLU
1	B	245	ILE
1	B	282	GLU
1	B	295	THR
1	B	297	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	92	GLN
1	A	222	HIS
1	A	233	ASN

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Mol	Chain	Res	Type
1	B	77	ASN
1	B	147	ASN
1	B	200	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 [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	286/353 (81%)	-1.28	0 100 100	51, 75, 114, 135	0
1	B	284/353 (80%)	-1.16	0 100 100	51, 79, 122, 150	0
All	All	570/706 (80%)	-1.22	0 100 100	51, 77, 120, 150	0

There are no RSRZ outliers to report.

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.