



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:23 PM UTC

PDB ID : 6B9X / pdb_00006b9x
Title : Crystal structure of Ragulator
Authors : SU, M.-Y.; Hurley, J.H.
Deposited on : 2017-10-11
Resolution : 1.42 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

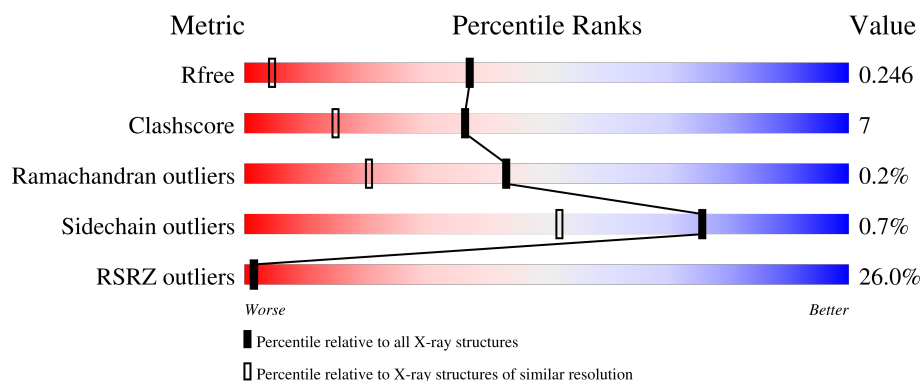
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	161	17% 35% 63%
2	B	126	25% 94% 6%
3	C	124	25% 84% 12% ...
4	D	99	21% 82% 8% 9%
5	E	173	9% 48% 5% 47%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3997 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 Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	0	0	0
			469	302	79	88			

- Molecule 2 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			949	596	163	183	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q9Y2Q5

- Molecule 3 is a protein called Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	121	Total	C	N	O	S	0	0	0
			939	604	158	176	1			

- Molecule 4 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	90	Total	C	N	O	S	0	0	0
			684	427	125	130	2			

- Molecule 5 is a protein called Hepatitis B virus x interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	91	Total	C	N	O	S	0	0	0
			666	406	115	138	7			

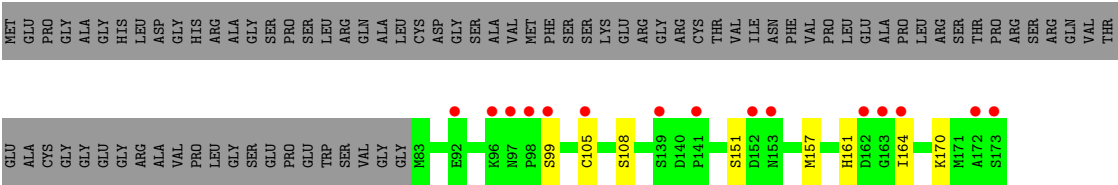
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total 39	O 39	0	0
6	B	66	Total 66	O 66	0	0
6	C	62	Total 62	O 62	0	0
6	D	57	Total 57	O 57	0	0
6	E	66	Total 66	O 66	0	0

i

- Molecule 1: Ragulator complex protein LAMTOR1





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	168.71Å 168.71Å 52.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	146.10 – 1.42 146.10 – 1.43	Depositor EDS
% Data completeness (in resolution range)	86.8 (146.10-1.42) 86.8 (146.10-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	41.29 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.212 , 0.237 0.218 , 0.246	Depositor DCC
R_{free} test set	1860 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3997	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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	0.28	0/481	0.41	0/658
2	B	0.38	1/960 (0.1%)	0.51	0/1300
3	C	0.43	1/956 (0.1%)	0.64	4/1297 (0.3%)
4	D	0.42	1/692 (0.1%)	0.59	0/934
5	E	0.34	0/672	0.53	0/911
All	All	0.38	3/3761 (0.1%)	0.55	4/5100 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	87	PRO	C-O	-6.10	1.16	1.24
4	D	34	GLU	C-O	-5.83	1.17	1.24
2	B	36	GLY	C-O	-5.59	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	87	PRO	CA-C-N	6.86	131.31	121.50
3	C	87	PRO	C-N-CA	6.86	131.31	121.50
3	C	86	LEU	CA-CB-CG	6.46	138.90	116.30
3	C	86	LEU	CB-CG-CD2	5.07	125.90	110.70

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	469	0	478	4	0
2	B	949	0	960	4	0
3	C	939	0	963	35	0
4	D	684	0	694	8	0
5	E	666	0	663	8	0
6	A	39	0	0	0	0
6	B	66	0	0	3	0
6	C	62	0	0	1	0
6	D	57	0	0	0	0
6	E	66	0	0	1	0
All	All	3997	0	3758	54	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 7.

All (54) 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)
3:C:86:LEU:CD2	3:C:118:ARG:CD	1.86	1.52
3:C:86:LEU:HG	3:C:87:PRO:CD	1.41	1.49
3:C:86:LEU:CD2	3:C:118:ARG:HD2	1.07	1.48
3:C:86:LEU:HD21	3:C:118:ARG:CG	1.57	1.34
3:C:86:LEU:CG	3:C:87:PRO:HD3	1.62	1.27
3:C:86:LEU:CG	3:C:87:PRO:CD	2.19	1.18
3:C:86:LEU:HD21	3:C:118:ARG:CD	1.56	1.18
3:C:86:LEU:HD21	3:C:118:ARG:HG3	1.37	1.04
3:C:86:LEU:CB	3:C:87:PRO:HD3	1.91	0.99
3:C:86:LEU:HG	3:C:87:PRO:HD2	1.01	0.99
3:C:86:LEU:CB	3:C:87:PRO:CD	2.48	0.89
3:C:5:LEU:HD11	3:C:113:LEU:HD21	1.58	0.86
3:C:86:LEU:HD23	3:C:118:ARG:CD	2.00	0.86
3:C:86:LEU:HD22	3:C:118:ARG:HD2	0.87	0.84
3:C:86:LEU:O	6:C:201:HOH:O	1.95	0.83
3:C:86:LEU:CD1	3:C:87:PRO:HD3	2.09	0.82
2:B:27:ASN:ND2	6:B:201:HOH:O	2.21	0.73
3:C:86:LEU:CD2	3:C:118:ARG:HG3	2.08	0.72
3:C:86:LEU:CD2	3:C:118:ARG:CG	2.37	0.71
3:C:5:LEU:HD11	3:C:113:LEU:CD2	2.25	0.67
5:E:105:CYS:SG	5:E:164:ILE:HD11	2.34	0.67
3:C:86:LEU:HB2	3:C:87:PRO:HD3	1.78	0.66
3:C:86:LEU:HD21	3:C:118:ARG:HD2	1.16	0.65
4:D:5:LEU:H	4:D:5:LEU:CD1	2.10	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:LYS:HG2	3:C:35:VAL:HG22	1.80	0.64
3:C:86:LEU:HD22	3:C:118:ARG:CD	1.82	0.64
5:E:161:HIS:O	5:E:164:ILE:HG22	1.99	0.63
1:A:129:LEU:HD23	5:E:157:MET:HE3	1.79	0.62
1:A:143:LEU:HD11	5:E:164:ILE:HD12	1.81	0.62
3:C:86:LEU:HD12	3:C:87:PRO:HD3	1.80	0.62
4:D:3:SER:O	4:D:7:GLN:HG2	2.01	0.60
4:D:5:LEU:H	4:D:5:LEU:HD12	1.66	0.60
1:A:116:HIS:HD2	4:D:8:GLY:C	2.16	0.54
3:C:115:GLU:OE1	3:C:118:ARG:NE	2.39	0.54
4:D:3:SER:O	4:D:3:SER:OG	2.24	0.52
3:C:2:ALA:O	3:C:4:ASP:N	2.44	0.51
3:C:5:LEU:HD22	3:C:113:LEU:HD11	1.94	0.49
2:B:61:ASN:ND2	6:B:209:HOH:O	2.45	0.49
5:E:99:SER:OG	5:E:170:LYS:HE3	2.13	0.48
4:D:4:ALA:HA	4:D:7:GLN:CD	2.39	0.48
3:C:80:VAL:HG13	3:C:93:ILE:HD13	1.97	0.47
4:D:63:PHE:HA	5:E:151:SER:HB3	1.97	0.46
3:C:5:LEU:CD2	3:C:113:LEU:HD11	2.47	0.45
3:C:42:GLU:O	3:C:42:GLU:OE2	2.35	0.45
3:C:24:VAL:HG11	3:C:117:LEU:HD23	2.00	0.44
2:B:97:GLU:OE2	6:B:202:HOH:O	2.21	0.44
4:D:13:PRO:O	4:D:14:ASP:OD1	2.36	0.43
3:C:5:LEU:CD1	3:C:113:LEU:HD11	2.50	0.42
2:B:2:LEU:HD21	2:B:7:LEU:HB2	2.02	0.42
1:A:129:LEU:HD23	5:E:157:MET:CE	2.49	0.41
3:C:5:LEU:HD13	3:C:113:LEU:HD11	2.01	0.41
3:C:42:GLU:OE2	3:C:45:LEU:HB2	2.20	0.41
3:C:115:GLU:O	3:C:118:ARG:HB3	2.21	0.41
5:E:108:SER:HA	6:E:205:HOH:O	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	58/161 (36%)	57 (98%)	1 (2%)	0	100	100
2	B	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
3	C	119/124 (96%)	115 (97%)	3 (2%)	1 (1%)	16	3
4	D	88/99 (89%)	87 (99%)	1 (1%)	0	100	100
5	E	89/173 (51%)	88 (99%)	1 (1%)	0	100	100
All	All	478/683 (70%)	470 (98%)	7 (2%)	1 (0%)	43	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	86	LEU

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	54/141 (38%)	54 (100%)	0	100	100
2	B	98/98 (100%)	97 (99%)	1 (1%)	68	39
3	C	105/108 (97%)	104 (99%)	1 (1%)	68	39
4	D	75/83 (90%)	74 (99%)	1 (1%)	61	29
5	E	77/140 (55%)	77 (100%)	0	100	100
All	All	409/570 (72%)	406 (99%)	3 (1%)	76	52

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	25	LEU
3	C	122	GLU
4	D	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	116	HIS
1	A	130	GLN
2	B	51	ASN
2	B	109	GLN
3	C	59	GLN
3	C	68	ASN
4	D	38	GLN
4	D	60	ASN
5	E	112	ASN
5	E	161	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	60/161 (37%)	1.83	28 (46%)	0 0	22, 33, 56, 60	0
2	B	126/126 (100%)	1.39	32 (25%)	1 1	22, 31, 52, 60	0
3	C	121/124 (97%)	1.40	31 (25%)	1 1	21, 32, 51, 63	0
4	D	90/99 (90%)	1.39	21 (23%)	2 2	21, 29, 50, 59	0
5	E	91/173 (52%)	0.80	15 (16%)	4 5	21, 27, 43, 51	0
All	All	488/683 (71%)	1.34	127 (26%)	1 1	21, 30, 52, 63	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	86	LEU	10.4
2	B	37	TYR	9.7
4	D	5	LEU	8.6
1	A	156	VAL	7.5
4	D	4	ALA	7.2
2	B	123	ALA	7.2
3	C	2	ALA	6.6
2	B	124	ALA	6.5
5	E	173	SER	6.0
3	C	120	VAL	5.7
2	B	125	SER	5.4
3	C	121	VAL	5.3
1	A	97	SER	5.2
2	B	66	GLU	5.2
2	B	0	ALA	5.1
1	A	100	THR	5.0
3	C	113	LEU	5.0
4	D	56	HIS	4.9
4	D	7	GLN	4.8
1	A	153	GLU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	92	ARG	4.7
2	B	2	LEU	4.5
3	C	87	PRO	4.5
2	B	1	MET	4.4
5	E	98	PRO	4.4
4	D	13	PRO	4.2
5	E	164	ILE	4.1
5	E	172	ALA	4.1
3	C	43	HIS	4.1
3	C	3	ASP	4.1
4	D	14	ASP	4.0
3	C	38	ASP	4.0
1	A	102	TRP	4.0
3	C	122	GLU	3.9
1	A	150	ALA	3.9
2	B	3	ARG	3.9
2	B	64	PHE	3.9
4	D	58	GLY	3.9
3	C	5	LEU	3.9
3	C	42	GLU	3.8
1	A	105	LEU	3.7
1	A	101	HIS	3.7
4	D	59	MET	3.7
5	E	152	ASP	3.7
2	B	65	ASN	3.7
4	D	3	SER	3.7
2	B	63	ALA	3.6
3	C	35	VAL	3.5
4	D	6	THR	3.5
4	D	8	GLY	3.5
3	C	32	VAL	3.5
1	A	116	HIS	3.5
3	C	33	ILE	3.5
1	A	155	VAL	3.5
5	E	97	ASN	3.4
2	B	38	GLY	3.4
3	C	40	ALA	3.4
3	C	6	LYS	3.3
1	A	151	LYS	3.3
2	B	118	PRO	3.3
2	B	121	GLN	3.2
2	B	4	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	TYR	3.1
1	A	99	LEU	3.1
2	B	122	VAL	3.0
5	E	139	SER	3.0
1	A	104	LYS	3.0
2	B	36	GLY	3.0
5	E	163	GLY	3.0
5	E	153	ASN	3.0
4	D	35	ASN	3.0
4	D	60	ASN	3.0
1	A	141	SER	2.9
1	A	154	LEU	2.9
3	C	4	ASP	2.8
4	D	34	GLU	2.8
3	C	117	LEU	2.8
2	B	62	GLN	2.8
2	B	120	THR	2.8
3	C	37	ASN	2.8
4	D	61	VAL	2.7
1	A	149	ASP	2.6
2	B	117	GLU	2.6
3	C	78	TYR	2.6
1	A	133	SER	2.6
3	C	45	LEU	2.5
3	C	119	GLN	2.5
1	A	152	GLU	2.5
5	E	105	CYS	2.5
3	C	48	GLY	2.5
4	D	55	LEU	2.5
3	C	76	ASN	2.5
3	C	118	ARG	2.4
3	C	31	PRO	2.4
2	B	40	THR	2.4
2	B	34	TYR	2.4
1	A	124	ILE	2.3
2	B	119	LEU	2.3
4	D	82	GLN	2.3
4	D	54	ARG	2.3
1	A	148	VAL	2.3
4	D	12	ILE	2.3
5	E	141	PRO	2.3
5	E	96	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	88	ASN	2.2
1	A	126	PHE	2.2
2	B	8	THR	2.2
3	C	30	VAL	2.2
5	E	162	ASP	2.2
3	C	39	ASN	2.2
3	C	46	ARG	2.2
2	B	116	GLU	2.2
2	B	114	TYR	2.2
3	C	41	PRO	2.2
5	E	99	SER	2.2
5	E	92	GLU	2.1
1	A	98	SER	2.1
2	B	32	LEU	2.1
1	A	130	GLN	2.1
1	A	106	PRO	2.1
2	B	39	ASP	2.1
2	B	87	ALA	2.1
1	A	103	LYS	2.1
2	B	70	LYS	2.1
1	A	107	PRO	2.1
1	A	134	ARG	2.0
4	D	38	GLN	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.