



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 8, 2025 – 02:07 PM EDT

PDB ID : 9CLB / pdb\_00009clb  
Title : Crystal structure of Bak bound to the inhibitory aBAK  
Authors : Birkinshaw, R.W.; Berger, S.A.; Lee, E.F.; Harris, T.J.; Tran, S.; Bera, A.K.; Arguinchona, L.; Kang, A.; Sankaran, B.; Kasapgil, S.; Miller, M.S.; Smyth, S.; Uren, R.; Kluck, R.; Colman, P.M.; Fairlie, W.D.; Czabotar, P.E.; Baker, D.  
Deposited on : 2024-07-10  
Resolution : 2.86 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

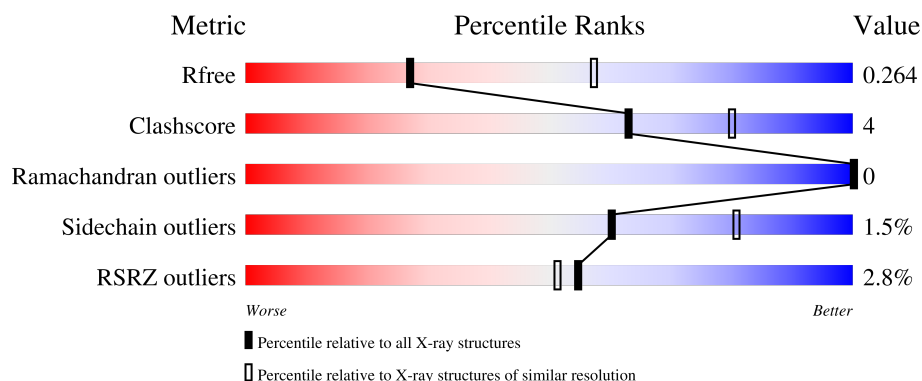
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 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))
$R_{free}$	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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  $\geq 3$ , 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	101	<div> <div>4%</div> <div>67% 12% 21%</div> </div>
1	C	101	<div> <div>3%</div> <div>71% 7% 21%</div> </div>
1	E	101	<div> <div>3%</div> <div>72% 6% 21%</div> </div>
1	G	101	<div> <div>3%</div> <div>68% 12% 20%</div> </div>
2	B	119	<div> <div>3%</div> <div>86% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	119	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>82%</div><div>13%</div><div>5%</div></div></div>
2	F	119	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>87%</div><div>10%</div><div></div></div></div>
2	H	119	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>82%</div><div>15%</div><div></div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6403 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 Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	1	0
			669	437	115	115	2			
1	C	80	Total	C	N	O	S	0	1	0
			664	434	113	115	2			
1	E	80	Total	C	N	O	S	0	0	0
			657	428	114	113	2			
1	G	81	Total	C	N	O	S	0	0	0
			657	428	113	114	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	engineered mutation	UNP Q16611
C	166	SER	CYS	engineered mutation	UNP Q16611
E	166	SER	CYS	engineered mutation	UNP Q16611
G	166	SER	CYS	engineered mutation	UNP Q16611

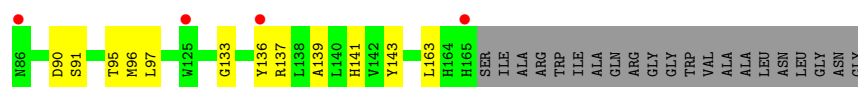
- Molecule 2 is a protein called aBAK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			940	584	172	183	1			
2	D	113	Total	C	N	O	S	0	0	0
			928	575	170	182	1			
2	F	115	Total	C	N	O	S	0	0	0
			949	589	173	186	1			
2	H	115	Total	C	N	O	S	0	0	0
			939	582	172	184	1			

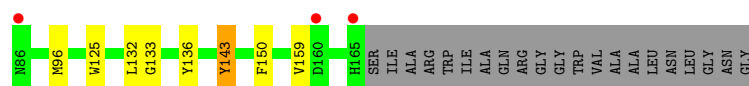
### 3 Residue-property plots

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.

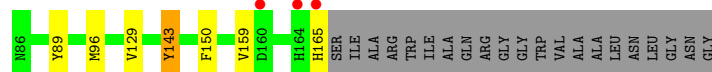
- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 1: Bcl-2 homologous antagonist/killer



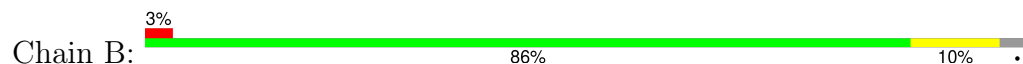
- Molecule 1: Bcl-2 homologous antagonist/killer



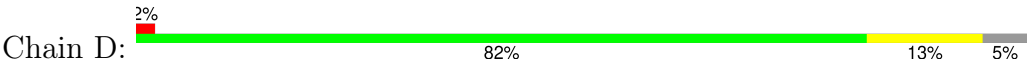
- Molecule 1: Bcl-2 homologous antagonist/killer



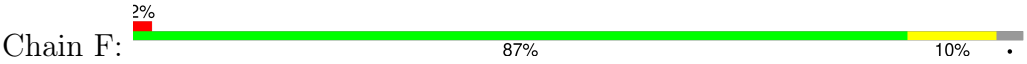
- Molecule 2: aBAK



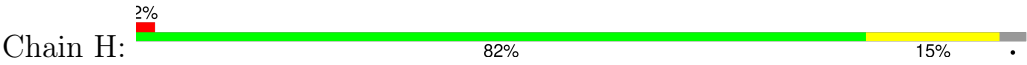
- Molecule 2: aBAK



• Molecule 2: aBAK



• Molecule 2: aBAK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.50Å 74.49Å 76.31Å 113.13° 90.15° 105.51°	Depositor
Resolution (Å)	40.56 – 2.86 40.56 – 2.86	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.56-2.86) 97.2 (40.56-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.86Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, $R_{free}$	0.221 , 0.270 0.222 , 0.264	Depositor DCC
$R_{free}$ test set	1114 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.17% 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	0.18	0/689	0.34	0/933
1	C	0.16	0/683	0.29	0/925
1	E	0.18	0/676	0.34	0/915
1	G	0.20	0/675	0.32	0/914
2	B	0.16	0/947	0.32	0/1261
2	D	0.13	0/935	0.29	0/1246
2	F	0.17	0/956	0.31	0/1273
2	H	0.20	0/946	0.39	0/1261
All	All	0.17	0/6507	0.33	0/8728

There are no bond length outliers.

There are no bond angle outliers.

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	669	0	637	8	0
1	C	664	0	632	8	0
1	E	657	0	630	6	0
1	G	657	0	627	9	0
2	B	940	0	963	7	0
2	D	928	0	941	8	0
2	F	949	0	969	7	0
2	H	939	0	947	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6403	0	6346	50	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 4.

All (50) 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)
2:D:15:MET:HE2	2:D:61:ILE:HG23	1.70	0.73
2:B:50:TYR:OH	2:B:112:ARG:NH1	2.29	0.66
1:E:96:MET:HE3	2:F:51:ILE:HG23	1.78	0.65
1:G:88:ARG:NH1	2:H:94:GLU:OE2	2.32	0.63
1:A:96:MET:HE3	2:B:51:ILE:HG23	1.83	0.60
2:H:75:LEU:HD22	2:H:80:LEU:HD23	1.86	0.57
2:H:94:GLU:HG3	2:H:98:LYS:HE3	1.86	0.57
1:G:96:MET:HE3	2:H:51:ILE:HG23	1.87	0.56
2:D:94:GLU:HG3	2:D:98:LYS:HE3	1.88	0.55
2:H:15:MET:HE1	2:H:96:LEU:HB3	1.88	0.55
2:H:88:GLU:OE1	2:H:91:ARG:NH1	2.37	0.55
2:D:88:GLU:OE1	2:D:91:ARG:NH1	2.38	0.54
2:F:94:GLU:HG3	2:F:98:LYS:HE3	1.89	0.54
1:C:133:GLY:HA2	1:C:136[A]:TYR:CE2	2.46	0.51
2:F:99:GLU:O	2:F:103:LYS:HG2	2.11	0.50
1:C:136[B]:TYR:CD1	1:G:151:LEU:HD22	2.46	0.50
1:C:96:MET:HE3	2:D:51:ILE:HG23	1.94	0.49
1:A:90:ASP:OD1	1:A:137:ARG:NH1	2.46	0.49
1:G:158:VAL:HG12	1:G:162:MET:HE2	1.95	0.49
1:A:143:TYR:HB3	1:E:143:TYR:CD2	2.49	0.47
2:B:23:LYS:HE2	2:B:107:TYR:OH	2.14	0.47
2:H:23:LYS:HE2	2:H:107:TYR:CE2	2.49	0.46
1:A:97:LEU:HD13	1:A:141:HIS:HB2	1.98	0.46
1:A:139:ALA:HB2	1:E:150:PHE:CD1	2.51	0.46
2:F:114:LYS:HD3	2:F:114:LYS:HA	1.80	0.46
2:H:39:THR:HG22	2:H:41:SER:H	1.80	0.46
2:H:23:LYS:HE2	2:H:107:TYR:CZ	2.50	0.46
1:A:133:GLY:HA2	1:A:136[B]:TYR:CE2	2.50	0.46
2:D:18:VAL:HG11	2:D:61:ILE:HG13	1.98	0.45
1:C:132:LEU:O	1:C:136[B]:TYR:HD2	2.00	0.45
2:B:99:GLU:O	2:B:103:LYS:HG3	2.17	0.45
2:D:3:ASP:N	2:D:4:PRO:HD2	2.31	0.45
2:D:16:GLU:HA	2:D:19:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:CD2	1:G:143:TYR:HB3	2.52	0.45
2:H:36:LEU:HD12	2:H:36:LEU:HA	1.86	0.43
1:C:159:VAL:HG21	1:E:129:VAL:HG22	2.01	0.43
2:B:101:ASP:CG	2:B:104:ARG:HH22	2.27	0.43
1:E:89:TYR:OH	2:F:62:GLU:OE2	2.30	0.42
2:D:76:LYS:HD2	2:D:86:PHE:CG	2.55	0.42
2:F:6:LYS:HE3	2:F:6:LYS:HB3	1.86	0.42
2:F:3:ASP:N	2:F:4:PRO:HD2	2.35	0.41
2:H:4:PRO:HB3	2:H:89:PHE:HD1	1.85	0.41
1:G:133:GLY:HA2	1:G:136:TYR:CE2	2.55	0.41
1:G:155:THR:O	1:G:159:VAL:HG22	2.20	0.41
2:B:3:ASP:N	2:B:4:PRO:HD2	2.36	0.41
1:C:125:TRP:HE1	1:E:159:VAL:HG23	1.85	0.41
1:C:150:PHE:CD1	1:G:139:ALA:HB2	2.56	0.41
1:A:136[A]:TYR:HD2	1:G:151:LEU:HB3	1.86	0.41
1:A:163:LEU:HD21	2:H:66:ARG:NH1	2.37	0.40
2:B:6:LYS:HE3	2:B:6:LYS:HB3	1.89	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	79/101 (78%)	79 (100%)	0	0	100	100
1	C	79/101 (78%)	79 (100%)	0	0	100	100
1	E	78/101 (77%)	78 (100%)	0	0	100	100
1	G	79/101 (78%)	78 (99%)	1 (1%)	0	100	100
2	B	112/119 (94%)	112 (100%)	0	0	100	100
2	D	111/119 (93%)	111 (100%)	0	0	100	100
2	F	113/119 (95%)	113 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	113/119 (95%)	113 (100%)	0	0	100	100
All	All	764/880 (87%)	763 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	68/81 (84%)	66 (97%)	2 (3%)	37	63
1	C	67/81 (83%)	66 (98%)	1 (2%)	60	81
1	E	67/81 (83%)	65 (97%)	2 (3%)	36	62
1	G	66/81 (82%)	65 (98%)	1 (2%)	60	81
2	B	98/100 (98%)	98 (100%)	0	100	100
2	D	96/100 (96%)	95 (99%)	1 (1%)	73	87
2	F	99/100 (99%)	97 (98%)	2 (2%)	50	73
2	H	96/100 (96%)	95 (99%)	1 (1%)	73	87
All	All	657/724 (91%)	647 (98%)	10 (2%)	60	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	95	THR
1	C	143	TYR
2	D	39	THR
1	E	143	TYR
1	E	165	HIS
2	F	43	LYS
2	F	116	GLU
1	G	142	VAL
2	H	19	VAL

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

Mol	Chain	Res	Type
2	B	14	GLN
2	D	14	GLN
2	D	84	GLN
1	E	99	HIS
2	F	14	GLN
2	F	84	GLN
2	H	10	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 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, 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	80/101 (79%)	0.08	4 (5%)	35	30	19, 43, 77, 131	1 (1%)
1	C	80/101 (79%)	0.16	3 (3%)	44	39	20, 47, 75, 103	1 (1%)
1	E	80/101 (79%)	0.03	3 (3%)	44	39	29, 42, 77, 138	0
1	G	81/101 (80%)	0.10	3 (3%)	45	39	33, 44, 74, 112	0
2	B	114/119 (95%)	0.22	3 (2%)	57	54	27, 57, 82, 96	0
2	D	113/119 (94%)	0.30	2 (1%)	67	64	37, 69, 108, 118	0
2	F	115/119 (96%)	0.15	2 (1%)	69	65	24, 54, 88, 112	0
2	H	115/119 (96%)	0.11	2 (1%)	69	65	32, 61, 87, 100	0
All	All	778/880 (88%)	0.15	22 (2%)	55	51	19, 52, 88, 138	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	3	ASP	3.5
1	C	86	ASN	3.4
1	E	160	ASP	3.4
1	G	166	SER	3.0
2	D	16	GLU	3.0
1	C	165	HIS	2.9
1	G	86	ASN	2.9
2	B	2	ALA	2.8
2	F	3	ASP	2.7
1	C	160	ASP	2.7
2	B	80	LEU	2.7
1	A	86	ASN	2.6
1	A	165	HIS	2.6
1	E	164	HIS	2.5
2	H	2	ALA	2.4
1	A	125	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	62	GLU	2.3
1	A	136[A]	TYR	2.3
2	D	3	ASP	2.3
1	G	161	PHE	2.1
1	E	165	HIS	2.1
2	F	36	LEU	2.1

## 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.