



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:34 AM GMT

PDB ID : 1B6D  
Title : BENICE JONES PROTEIN DEL: AN ENTIRE IMMUNOGLOBULIN  
KAPPA LIGHT-CHAIN DIMER  
Authors : Roussel, A.; Spinelli, S.; Deret, S.; Aucouturier, P.; Cambillau, C.  
Deposited on : 1999-01-13  
Resolution : 2.74 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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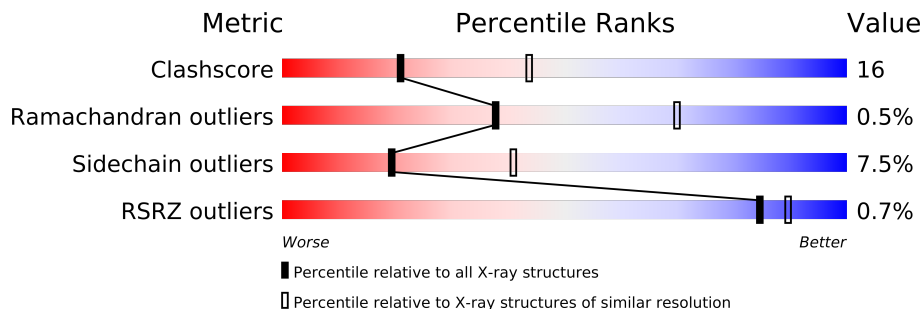
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.74 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))
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4305 atoms, of which 964 are hydrogens and 0 are deuterium.

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 IMMUNOGLOBULIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	H	N	O	S	8	0	0
			1995	1010	377	269	334	5			
1	B	212	Total	C	H	N	O	S	28	0	0
			1995	1010	377	269	334	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	ASN	CONFLICT	GB 4768677
A	31	SER	ASN	CONFLICT	GB 4768677
A	43	ALA	THR	CONFLICT	GB 4768677
A	49	HIS	TYR	CONFLICT	GB 4768677
A	50	ALA	GLY	CONFLICT	GB 4768677
A	53	SER	ASN	CONFLICT	GB 4768677
A	72	SER	ILE	CONFLICT	GB 4768677
A	83	LEU	ILE	CONFLICT	GB 4768677
A	93	SER	ASN	CONFLICT	GB 4768677
A	177	SER	ASN	CONFLICT	GB 4768677
B	30	SER	ASN	CONFLICT	GB 4768677
B	31	SER	ASN	CONFLICT	GB 4768677
B	43	ALA	THR	CONFLICT	GB 4768677
B	49	HIS	TYR	CONFLICT	GB 4768677
B	50	ALA	GLY	CONFLICT	GB 4768677
B	53	SER	ASN	CONFLICT	GB 4768677
B	72	SER	ILE	CONFLICT	GB 4768677
B	83	LEU	ILE	CONFLICT	GB 4768677
B	93	SER	ASN	CONFLICT	GB 4768677
B	177	SER	ASN	CONFLICT	GB 4768677

- Molecule 2 is water.

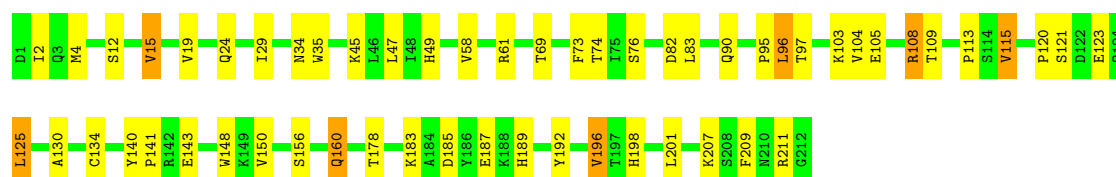
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	57	Total 171	H 114	O 57	0	0
2	B	48	Total 144	H 96	O 48	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

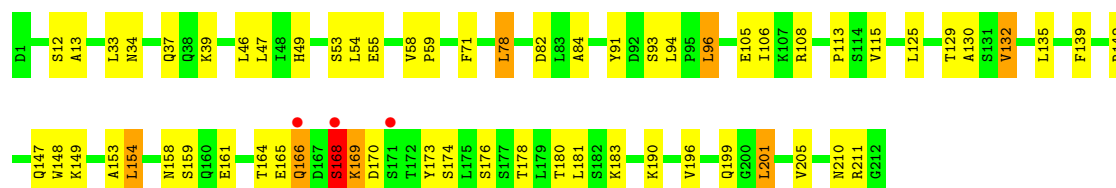
#### • Molecule 1: IMMUNOGLOBULIN

Chain A: 



#### • Molecule 1: IMMUNOGLOBULIN

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.60Å 129.20Å 86.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.74 19.57 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.4 (6.00-2.74) 94.3 (19.57-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.70 (at 2.75Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.207 , 0.265 0.181 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 17.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 13394 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.44	0/1652	0.69	0/2242
1	B	0.50	1/1652 (0.1%)	0.76	2/2242 (0.1%)
All	All	0.47	1/3304 (0.0%)	0.73	2/4484 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	GLU	C-N	-7.62	1.16	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	SER	O-C-N	5.32	131.22	122.70
1	B	170	ASP	O-C-N	5.21	131.03	122.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1618	377	1192	46	0
1	B	1618	377	1190	53	0
2	A	57	114	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	96	0	2	0
All	All	3341	964	2382	98	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:ASN:ND2	1:A:49:HIS:HA	1.73	1.02
1:A:34:ASN:HD22	1:A:49:HIS:HA	1.36	0.90
1:B:34:ASN:ND2	1:B:49:HIS:HD2	1.75	0.84
1:B:54:LEU:HG	1:B:58:VAL:CG2	2.07	0.83
1:B:34:ASN:HD21	1:B:49:HIS:HD2	1.28	0.81
1:B:199:GLN:OE1	2:B:260:HOH:O	1.97	0.81
1:B:54:LEU:HG	1:B:58:VAL:HG23	1.62	0.79
1:A:34:ASN:HD21	1:A:49:HIS:CD2	2.01	0.79
1:A:105:GLU:HG2	2:A:217:HOH:H2	1.46	0.77
1:B:166:GLN:NE2	1:B:173:TYR:CZ	2.54	0.74
1:B:166:GLN:NE2	1:B:173:TYR:CE2	2.54	0.74
1:A:115:VAL:HG11	1:A:196:VAL:HG11	1.70	0.73
1:B:34:ASN:ND2	1:B:49:HIS:CD2	2.56	0.73
1:B:34:ASN:HD21	1:B:49:HIS:CD2	2.07	0.72
1:A:183:LYS:O	1:A:187:GLU:HG2	1.94	0.67
1:B:142:ARG:HB2	1:B:173:TYR:CZ	2.31	0.66
1:B:164:THR:HG22	1:B:174:SER:H	1.64	0.62
1:B:147:GLN:CG	1:B:154:LEU:HD21	2.31	0.61
1:B:201:LEU:HG	1:B:205:VAL:HG23	1.83	0.61
1:B:78:LEU:HD23	1:B:82:ASP:HB2	1.85	0.59
1:B:149:LYS:HA	1:B:153:ALA:O	2.04	0.57
1:A:15:VAL:HG13	2:A:255:HOH:O	2.04	0.57
1:B:132:VAL:HG22	1:B:148:TRP:CH2	2.40	0.57
1:A:15:VAL:O	2:A:264:HOH:O	2.22	0.56
1:A:143:GLU:HB2	2:A:229:HOH:H1	1.70	0.56
1:A:49:HIS:HE1	2:A:233:HOH:O	1.88	0.56
1:A:61:ARG:HB2	1:A:76:SER:OG	2.04	0.56
1:B:190:LYS:NZ	1:B:211:ARG:NH2	2.54	0.55
1:A:95:PRO:O	1:A:97:THR:HG23	2.06	0.55
1:A:189:HIS:O	1:A:211:ARG:HD3	2.09	0.53
1:B:159:SER:HA	1:B:178:THR:O	2.09	0.52
1:A:24:GLN:HA	1:A:69:THR:O	2.11	0.51
1:A:34:ASN:HD21	1:A:49:HIS:HA	1.65	0.51
1:B:142:ARG:HB2	1:B:173:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:LEU:HD22	1:B:71:PHE:CG	2.45	0.51
1:B:78:LEU:CD2	1:B:82:ASP:HB2	2.40	0.51
1:A:120:PRO:HG2	1:A:130:ALA:HB1	1.93	0.50
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.46	0.50
1:A:45:LYS:HE2	2:A:248:HOH:O	2.11	0.50
1:B:108:ARG:H	2:B:256:HOH:H2	1.60	0.50
1:B:12:SER:HA	1:B:105:GLU:O	2.12	0.50
1:A:96:LEU:HD22	1:A:96:LEU:H	1.78	0.49
1:B:166:GLN:NE2	1:B:173:TYR:CD2	2.80	0.48
1:A:115:VAL:HG11	1:A:196:VAL:CG1	2.39	0.48
1:B:34:ASN:HB3	1:B:46:LEU:HD11	1.95	0.48
1:A:35:TRP:CE2	1:A:73:PHE:HB2	2.49	0.48
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.47	0.47
1:B:142:ARG:O	1:B:142:ARG:HG2	2.15	0.47
1:A:192:TYR:HB2	1:A:209:PHE:CE1	2.50	0.47
1:B:94:LEU:HD23	1:B:96:LEU:HD13	1.97	0.47
1:A:12:SER:HA	1:A:105:GLU:O	2.16	0.46
1:B:161:GLU:HA	1:B:176:SER:O	2.14	0.46
1:B:166:GLN:NE2	1:B:173:TYR:CE1	2.83	0.46
1:A:49:HIS:CE1	2:A:233:HOH:H1	2.34	0.46
1:B:13:ALA:O	1:B:106:ILE:HD12	2.16	0.46
1:B:34:ASN:OD1	1:B:91:TYR:CD2	2.69	0.46
1:B:13:ALA:O	1:B:106:ILE:HA	2.16	0.46
1:B:49:HIS:O	1:B:53:SER:HB2	2.15	0.45
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.97	0.45
1:A:160:GLN:HG2	1:A:178:THR:HB	1.97	0.45
1:A:125:LEU:HD11	1:A:130:ALA:HB2	1.99	0.45
1:B:129:THR:HG22	1:B:130:ALA:N	2.31	0.44
1:A:4:MET:SD	1:A:90:GLN:HB3	2.57	0.44
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.52	0.44
1:B:190:LYS:HZ2	1:B:211:ARG:NH2	2.16	0.44
1:B:39:LYS:HD3	1:B:84:ALA:HB2	2.00	0.43
1:A:34:ASN:HD21	1:A:49:HIS:CG	2.34	0.43
1:A:108:ARG:HD3	1:A:109:THR:O	2.18	0.43
1:B:164:THR:HG23	1:B:164:THR:O	2.18	0.43
1:B:190:LYS:HZ3	1:B:211:ARG:NH2	2.16	0.43
1:B:115:VAL:HA	1:B:135:LEU:O	2.19	0.43
1:B:34:ASN:HB3	1:B:46:LEU:CD1	2.49	0.43
1:B:113:PRO:HB3	1:B:139:PHE:HB3	2.00	0.43
1:A:143:GLU:HB2	2:A:229:HOH:O	2.17	0.43
1:A:108:ARG:HD2	1:A:140:TYR:CG	2.54	0.43
1:A:45:LYS:HA	2:A:221:HOH:H2	1.81	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:VAL:HG22	1:A:207:LYS:HG3	2.01	0.42
1:A:34:ASN:HD21	1:A:49:HIS:HD2	1.57	0.42
1:B:164:THR:HG22	1:B:174:SER:N	2.30	0.42
1:A:15:VAL:CG1	2:A:255:HOH:O	2.66	0.42
2:A:260:HOH:O	1:B:94:LEU:HD12	2.20	0.42
1:B:132:VAL:HG22	1:B:148:TRP:CZ3	2.54	0.41
1:B:58:VAL:HA	1:B:59:PRO:HD3	1.87	0.41
1:B:125:LEU:O	1:B:183:LYS:HD2	2.20	0.41
1:B:55:GLU:O	1:B:58:VAL:HG22	2.20	0.41
1:A:187:GLU:O	1:A:211:ARG:NH1	2.53	0.41
1:B:147:GLN:HG2	1:B:154:LEU:HD21	2.01	0.41
1:A:19:VAL:O	1:A:74:THR:HA	2.20	0.41
1:A:47:LEU:HA	1:A:58:VAL:HG21	2.02	0.41
1:A:105:GLU:HG2	2:A:217:HOH:O	2.15	0.41
1:A:49:HIS:CE1	2:A:233:HOH:O	2.69	0.41
2:A:260:HOH:O	1:B:94:LEU:CD1	2.68	0.41
1:A:96:LEU:HD22	1:B:46:LEU:HD22	2.03	0.41
1:B:201:LEU:HG	1:B:205:VAL:CG2	2.49	0.40
1:A:125:LEU:CD1	1:A:130:ALA:HB2	2.51	0.40
1:A:2:ILE:HD13	1:A:29:ILE:HG22	2.04	0.40
1:B:180:THR:O	1:B:181:LEU:HD23	2.22	0.40
1:A:141:PRO:O	1:A:198:HIS:HE1	2.05	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	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
1	B	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	22	50
All	All	420/424 (99%)	396 (94%)	22 (5%)	2 (0%)	38	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	LYS
1	B	168	SER

### 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	186/186 (100%)	170 (91%)	16 (9%)	15	32
1	B	186/186 (100%)	174 (94%)	12 (6%)	24	49
All	All	372/372 (100%)	344 (92%)	28 (8%)	19	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	83	LEU
1	A	96	LEU
1	A	103	LYS
1	A	104	VAL
1	A	108	ARG
1	A	115	VAL
1	A	121	SER
1	A	123	GLU
1	A	125	LEU
1	A	150	VAL
1	A	156	SER
1	A	160	GLN
1	A	185	ASP
1	A	196	VAL
1	A	201	LEU
1	B	78	LEU
1	B	93	SER
1	B	96	LEU
1	B	132	VAL
1	B	154	LEU
1	B	158	ASN
1	B	166	GLN
1	B	168	SER

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Mol	Chain	Res	Type
1	B	169	LYS
1	B	196	VAL
1	B	201	LEU
1	B	210	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	34	ASN
1	A	49	HIS
1	A	89	GLN
1	A	137	ASN
1	A	189	HIS
1	A	198	HIS
1	B	34	ASN
1	B	49	HIS
1	B	89	GLN
1	B	155	GLN
1	B	158	ASN
1	B	210	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	211/212 (99%)	-0.41	0 100 100	3, 18, 47, 57	4 (1%)
1	B	211/212 (99%)	-0.29	3 (1%) 72 78	3, 26, 49, 67	5 (2%)
All	All	422/424 (99%)	-0.35	3 (0%) 84 89	3, 22, 49, 67	9 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	GLN	3.3
1	B	171	SER	2.9
1	B	168	SER	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.