



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:49 AM GMT

PDB ID : 2YIK  
Title : Catalytic domain of Clostridium thermocellum CelT  
Authors : Tsai, J.-Y.; Kesavulu, M.M.; Hsiao, C.-D.  
Deposited on : 2011-05-16  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

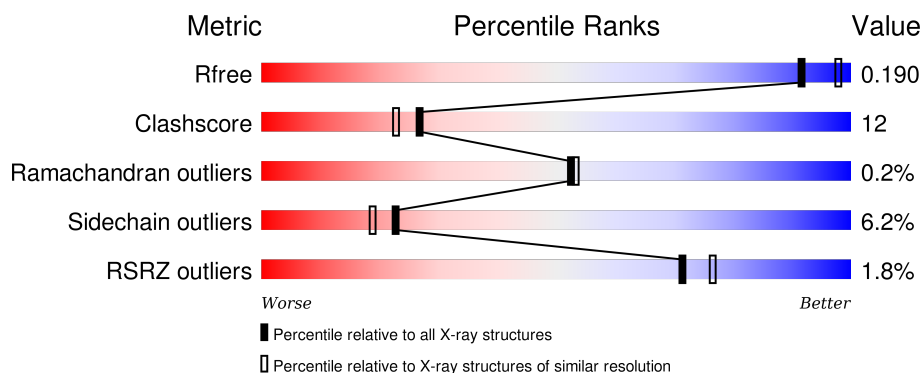
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	611	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4281 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 ENDOGLUCANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	1
			3934	2501	661	754	18			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

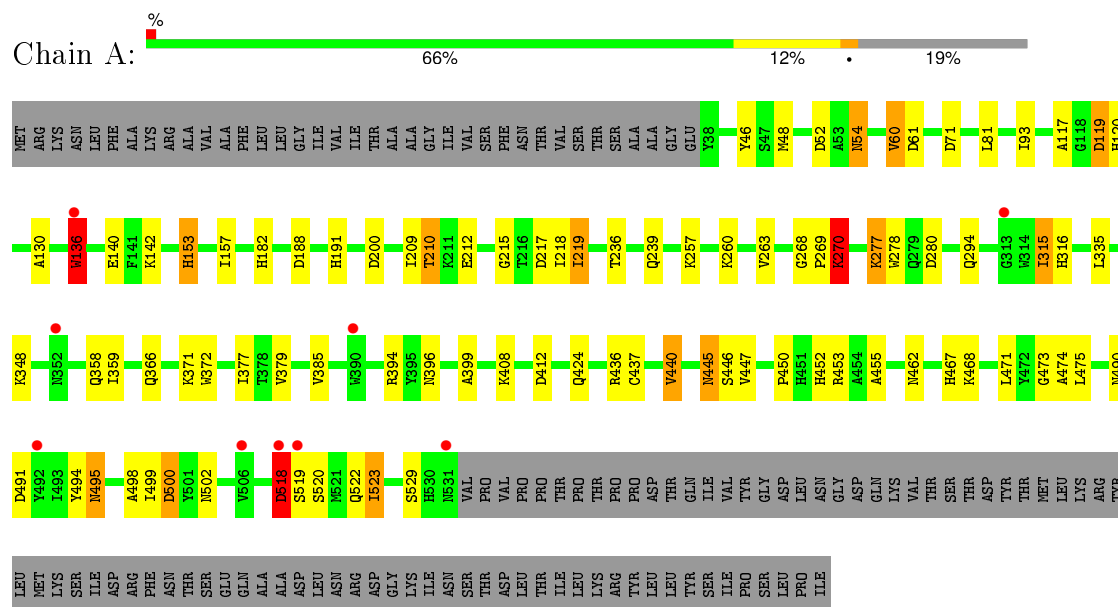
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total	O	0	0
			343	343		

### 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: ENDOGLUCANASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.86 Å 96.86 Å 159.92 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.38 – 2.10 29.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.9 (29.38-2.10) 90.6 (29.38-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.42 (at 2.10 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.182 , 0.199 0.179 , 0.190	Depositor DCC
$R_{free}$ test set	2136 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42491 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.45	0/4059	0.70	5/5521 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	TRP	CA-CB-CG	7.81	128.54	113.70
1	A	270	LYS	CA-C-N	5.57	127.35	116.20
1	A	119	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	518	ASP	CB-CA-C	-5.34	99.72	110.40
1	A	268	GLY	C-N-CD	5.12	139.16	128.40

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	3934	0	3595	91	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	343	0	0	10	1
All	All	4281	0	3595	91	1

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 12.

All (91) 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:210:THR:HG22	1:A:212:GLU:H	1.29	0.96
1:A:445:ASN:HD22	1:A:445:ASN:H	1.13	0.91
1:A:54:ASN:HD21	1:A:452:HIS:HE1	1.20	0.89
1:A:396:ASN:HD21	1:A:424:GLN:HE21	1.23	0.86
1:A:60:VAL:HG13	1:A:71:ASP:HA	1.58	0.86
1:A:436:ARG:HH11	1:A:436:ARG:HG3	1.37	0.86
1:A:462:ASN:HD22	1:A:490:ASN:HD22	1.20	0.86
1:A:523:ILE:HD12	4:A:2340:HOH:O	1.76	0.85
1:A:372:TRP:HA	1:A:377:ILE:HD13	1.59	0.84
1:A:136:TRP:HZ3	1:A:140:GLU:OE2	1.61	0.84
1:A:475:LEU:H	1:A:502:ASN:HD21	1.27	0.82
1:A:452:HIS:HD2	1:A:455:ALA:H	1.26	0.80
1:A:315:ILE:HD11	1:A:399:ALA:HA	1.65	0.78
1:A:269:PRO:HG2	4:A:2196:HOH:O	1.83	0.77
1:A:215:GLY:O	1:A:219:ILE:HD13	1.84	0.77
1:A:153:HIS:O	1:A:157:ILE:HD13	1.85	0.76
1:A:499:ILE:HD12	1:A:500:ASP:N	2.04	0.72
1:A:54:ASN:ND2	1:A:452:HIS:HE1	1.87	0.71
1:A:210:THR:CG2	1:A:212:GLU:H	2.03	0.71
1:A:81:LEU:HD11	1:A:93:ILE:HD12	1.72	0.71
1:A:358:GLN:C	1:A:359:ILE:HD12	2.11	0.70
1:A:377:ILE:N	1:A:377:ILE:HD12	2.07	0.69
1:A:385:VAL:H	1:A:424:GLN:HE22	1.39	0.69
1:A:348:LYS:HE2	1:A:359:ILE:HD13	1.75	0.68
1:A:385:VAL:H	1:A:424:GLN:NE2	1.92	0.67
1:A:371:LYS:HG2	1:A:377:ILE:CD1	2.25	0.67
1:A:518:ASP:HB2	1:A:520:SER:H	1.59	0.66
1:A:119:ASP:OD2	1:A:191:HIS:HE1	1.80	0.65
1:A:48:MET:HE3	4:A:2006:HOH:O	1.97	0.64
1:A:436:ARG:NH1	1:A:436:ARG:HG3	2.11	0.64
1:A:315:ILE:HG13	1:A:316:HIS:H	1.65	0.62
1:A:136:TRP:CZ3	1:A:140:GLU:OE2	2.47	0.62
1:A:315:ILE:HD13	1:A:399:ALA:HB2	1.82	0.61
1:A:239:GLN:NE2	4:A:2179:HOH:O	2.33	0.60
1:A:452:HIS:CD2	1:A:455:ALA:H	2.16	0.60
1:A:54:ASN:HD21	1:A:452:HIS:CE1	2.10	0.59
1:A:210:THR:HG22	1:A:212:GLU:N	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ILE:H	1:A:523:ILE:CD1	2.17	0.58
1:A:277:LYS:HD3	1:A:277:LYS:N	2.18	0.58
1:A:371:LYS:HG2	1:A:377:ILE:HD11	1.85	0.57
1:A:366:GLN:NE2	4:A:2273:HOH:O	2.38	0.56
1:A:519:SER:O	1:A:522:GLN:NE2	2.38	0.55
1:A:372:TRP:CA	1:A:377:ILE:HD13	2.34	0.55
1:A:371:LYS:HG2	1:A:377:ILE:HD12	1.88	0.54
1:A:130:ALA:HB2	1:A:499:ILE:HD13	1.89	0.54
1:A:209:ILE:HG21	1:A:219:ILE:HD11	1.89	0.54
1:A:217:ASP:CG	1:A:218:ILE:HD12	2.29	0.52
1:A:440:VAL:HG13	1:A:474:ALA:HB3	1.92	0.52
1:A:120:HIS:HE1	4:A:2084:HOH:O	1.91	0.52
1:A:445:ASN:ND2	1:A:445:ASN:H	1.93	0.52
1:A:523:ILE:N	1:A:523:ILE:HD13	2.25	0.52
1:A:218:ILE:HD13	1:A:263:VAL:CG2	2.41	0.51
1:A:437:CYS:HB3	1:A:446:SER:HA	1.92	0.51
1:A:359:ILE:N	1:A:359:ILE:HD12	2.26	0.51
1:A:445:ASN:HD22	1:A:445:ASN:N	1.90	0.51
1:A:117:ALA:HA	1:A:498:ALA:HA	1.93	0.51
1:A:396:ASN:ND2	1:A:424:GLN:HE21	2.00	0.50
1:A:52:ASP:OD1	1:A:153:HIS:HE1	1.94	0.50
1:A:523:ILE:N	1:A:523:ILE:CD1	2.75	0.49
1:A:188:ASP:OD2	1:A:270:LYS:HE3	2.12	0.49
1:A:436:ARG:HD3	1:A:447:VAL:HG12	1.95	0.48
1:A:348:LYS:CE	1:A:359:ILE:HD13	2.42	0.48
1:A:462:ASN:ND2	1:A:490:ASN:HD22	1.99	0.48
1:A:182:HIS:HE1	4:A:2051:HOH:O	1.97	0.47
1:A:153:HIS:CE1	1:A:157:ILE:HD11	2.49	0.47
1:A:182:HIS:HD2	4:A:2087:HOH:O	1.98	0.47
1:A:450:PRO:O	1:A:467:HIS:HE1	1.97	0.47
1:A:81:LEU:CD1	1:A:93:ILE:HD12	2.44	0.47
1:A:436:ARG:HD3	1:A:447:VAL:CG1	2.47	0.45
1:A:436:ARG:NH1	4:A:2315:HOH:O	2.49	0.45
1:A:377:ILE:CD1	1:A:377:ILE:N	2.77	0.43
1:A:491:ASP:OD2	1:A:494:TYR:HB2	2.19	0.43
1:A:315:ILE:HG13	1:A:316:HIS:N	2.31	0.43
1:A:130:ALA:CB	1:A:499:ILE:HD13	2.48	0.43
1:A:523:ILE:HD13	4:A:2341:HOH:O	2.17	0.42
1:A:209:ILE:HD13	1:A:219:ILE:CD1	2.49	0.42
1:A:219:ILE:CD1	1:A:219:ILE:N	2.82	0.42
1:A:157:ILE:N	1:A:157:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:HE3	1:A:280:ASP:OD1	2.19	0.42
1:A:495:ASN:HD22	1:A:495:ASN:HA	1.54	0.42
1:A:260:LYS:HB3	1:A:278:TRP:CE2	2.55	0.41
1:A:453:ARG:HH11	1:A:453:ARG:HG3	1.86	0.41
1:A:52:ASP:OD1	1:A:153:HIS:CE1	2.73	0.41
1:A:218:ILE:N	1:A:218:ILE:HD12	2.36	0.41
1:A:440:VAL:HG22	1:A:471:LEU:O	2.20	0.41
1:A:46:TYR:O	1:A:473:GLY:HA3	2.21	0.41
1:A:120:HIS:CD2	1:A:200:ASP:OD2	2.74	0.41
1:A:371:LYS:C	1:A:377:ILE:HD13	2.41	0.40
1:A:371:LYS:C	1:A:377:ILE:CD1	2.89	0.40
1:A:475:LEU:H	1:A:502:ASN:ND2	2.08	0.40
1:A:408:LYS:HA	1:A:412:ASP:HA	2.03	0.40

All (1) 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)
4:A:2172:HOH:O	4:A:2172:HOH:O[7_555]	1.91	0.29

## 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	492/611 (80%)	477 (97%)	14 (3%)	1 (0%)	52 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LYS

### 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	402/505 (80%)	377 (94%)	25 (6%)	23	19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	60	VAL
1	A	61	ASP
1	A	136	TRP
1	A	142	LYS
1	A	153	HIS
1	A	210	THR
1	A	219	ILE
1	A	236	THR
1	A	257	LYS
1	A	270	LYS
1	A	277	LYS
1	A	294	GLN
1	A	315	ILE
1	A	335	LEU
1	A	379	VAL
1	A	394	ARG
1	A	440	VAL
1	A	445	ASN
1	A	468	LYS
1	A	495	ASN
1	A	500	ASP
1	A	518	ASP
1	A	523	ILE
1	A	529	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	120	HIS
1	A	153	HIS
1	A	162	ASN
1	A	182	HIS
1	A	191	HIS
1	A	229	ASN
1	A	232	ASN
1	A	341	GLN
1	A	352	ASN
1	A	354	ASN
1	A	366	GLN
1	A	424	GLN
1	A	445	ASN
1	A	451	HIS
1	A	452	HIS
1	A	462	ASN
1	A	495	ASN
1	A	502	ASN
1	A	530	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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, 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	494/611 (80%)	-0.34	9 (1%) 71 76	20, 28, 42, 54	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	TYR	3.3
1	A	519	SER	3.1
1	A	313	GLY	3.0
1	A	136	TRP	2.6
1	A	390	TRP	2.5
1	A	531	ASN	2.5
1	A	352	ASN	2.4
1	A	518	ASP	2.4
1	A	506	VAL	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1333	1/1	0.98	0.10	-0.07	30,30,30,30	0
2	CA	A	1332	1/1	0.98	0.08	-0.28	29,29,29,29	0
2	CA	A	1531	1/1	0.93	0.06	-0.95	32,32,32,32	0
3	ZN	A	1533	1/1	1.00	0.05	-2.06	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.