



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:27 AM GMT

PDB ID : 3II1
Title : Structural characterization of difunctional glucanase-xylanse CelM2
Authors : Hwang, K.Y.; Nam, K.H.
Deposited on : 2009-07-31
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

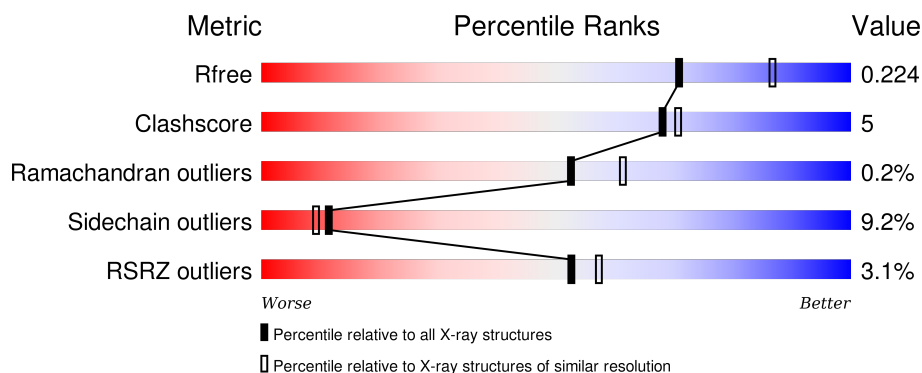
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 ≥ 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	535	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	A	561	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4332 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.

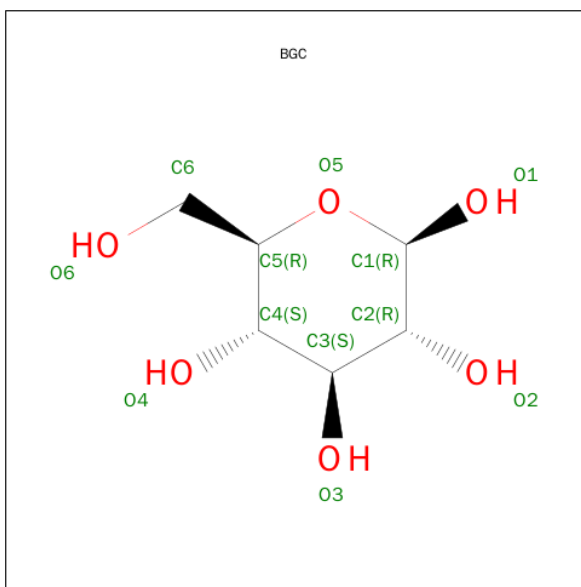
- Molecule 1 is a protein called Cellulase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4025	2526	707	783	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	INITIATING METHIONINE	UNP A1E9A6
A	17	ALA	-	EXPRESSION TAG	UNP A1E9A6
A	18	SER	-	EXPRESSION TAG	UNP A1E9A6
A	19	MET	-	EXPRESSION TAG	UNP A1E9A6
A	20	THR	-	EXPRESSION TAG	UNP A1E9A6
A	21	GLY	-	EXPRESSION TAG	UNP A1E9A6
A	22	GLY	-	EXPRESSION TAG	UNP A1E9A6
A	23	GLN	-	EXPRESSION TAG	UNP A1E9A6
A	24	GLN	-	EXPRESSION TAG	UNP A1E9A6
A	25	MET	-	EXPRESSION TAG	UNP A1E9A6
A	26	GLY	-	EXPRESSION TAG	UNP A1E9A6
A	27	ARG	-	EXPRESSION TAG	UNP A1E9A6
A	28	GLY	-	EXPRESSION TAG	UNP A1E9A6
A	29	SER	-	EXPRESSION TAG	UNP A1E9A6
A	30	MET	-	EXPRESSION TAG	UNP A1E9A6

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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

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

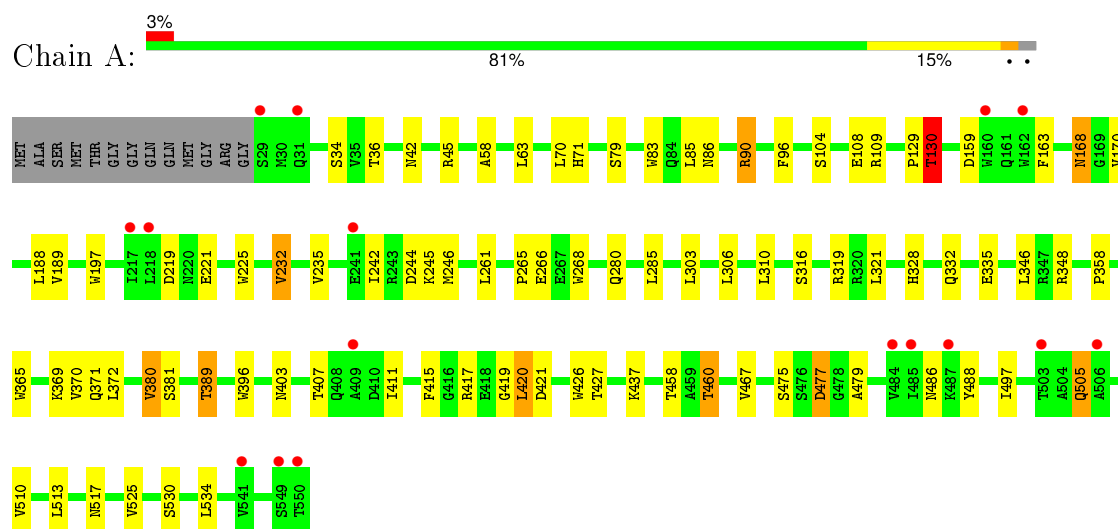
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total	O	0	0
			292	292		

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: Cellulase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.59Å 87.43Å 110.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 2.25 29.64 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.64-2.25) 91.8 (29.64-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.170 , 0.221 0.174 , 0.224	Depositor DCC
R_{free} test set	1888 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.1	EDS
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 37174 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4332	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.04	3/4133 (0.1%)	0.97	8/5655 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	VAL	CB-CG2	-5.41	1.41	1.52
1	A	96	PHE	CE2-CZ	5.37	1.47	1.37
1	A	415	PHE	CE1-CZ	5.09	1.47	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	417	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	A	159	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	232	VAL	CG1-CB-CG2	5.68	119.99	110.90
1	A	244	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	45	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	130	THR	N-CA-CB	-5.30	100.23	110.30
1	A	45	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4025	0	3818	37	0
2	A	12	0	12	1	0
3	A	3	0	0	0	0
4	A	292	0	0	2	0
All	All	4332	0	3830	37	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 5.

All (37) 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:268:TRP:HE1	1:A:280:GLN:HE22	1.16	0.92
1:A:389:THR:HG23	1:A:420:LEU:HD23	1.49	0.91
1:A:332:GLN:HE21	1:A:365:TRP:HE1	1.27	0.83
1:A:58:ALA:H	1:A:71:HIS:HE1	1.33	0.77
1:A:130:THR:HG23	1:A:245:LYS:HD3	1.69	0.74
1:A:58:ALA:H	1:A:71:HIS:CE1	2.06	0.73
1:A:130:THR:HB	1:A:219:ASP:HB2	1.74	0.70
1:A:389:THR:HG23	1:A:420:LEU:CD2	2.25	0.67
1:A:221:GLU:OE2	2:A:561:BGC:H1	1.94	0.67
1:A:477:ASP:HB3	1:A:479:ALA:H	1.62	0.64
1:A:458:THR:HG22	1:A:460:THR:HG22	1.81	0.61
1:A:90:ARG:HD2	1:A:90:ARG:N	2.18	0.59
1:A:389:THR:CG2	1:A:420:LEU:HD23	2.32	0.53
1:A:319:ARG:HD2	4:A:922:HOH:O	2.09	0.52
1:A:268:TRP:HE1	1:A:280:GLN:NE2	1.95	0.52
1:A:86:ASN:HD21	1:A:109:ARG:H	1.59	0.49
1:A:265:PRO:O	1:A:266:GLU:HB2	2.11	0.49
1:A:419:GLY:HA2	4:A:927:HOH:O	2.12	0.49
1:A:266:GLU:OE2	1:A:328:HIS:HE1	1.96	0.49
1:A:348:ARG:HD2	1:A:403:ASN:OD1	2.12	0.49
1:A:79:SER:O	1:A:129:PRO:HB3	2.12	0.49
1:A:63:LEU:HD11	1:A:71:HIS:CD2	2.48	0.48
1:A:221:GLU:OE2	1:A:328:HIS:HD2	1.98	0.47
1:A:437:LYS:HE2	1:A:517:ASN:O	2.17	0.45
1:A:130:THR:HG23	1:A:245:LYS:CD	2.44	0.44
1:A:486:ASN:OD1	1:A:488:TYR:HD1	1.99	0.44
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.66	0.42
1:A:358:PRO:O	1:A:369:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:THR:HG22	1:A:225:TRP:CZ2	2.55	0.41
1:A:335:GLU:OE1	1:A:335:GLU:N	2.51	0.41
1:A:242:ILE:O	1:A:246:MET:HG3	2.21	0.41
1:A:389:THR:HG22	1:A:421:ASP:H	1.85	0.41
1:A:83:TRP:CD1	1:A:197:TRP:HB2	2.56	0.41
1:A:168:ASN:ND2	1:A:170:VAL:H	2.19	0.40
1:A:407:THR:O	1:A:411:ILE:HG13	2.22	0.40
1:A:510:VAL:CG2	1:A:525:VAL:HG12	2.52	0.40
1:A:426:TRP:HA	1:A:427:THR:HA	1.74	0.40

There are no symmetry-related clashes.

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	520/535 (97%)	501 (96%)	18 (4%)	1 (0%)	52 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	GLN

5.3.2 Protein sidechains [i](#)

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	422/430 (98%)	383 (91%)	39 (9%)	11 9

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	36	THR
1	A	42	ASN
1	A	70	LEU
1	A	85	LEU
1	A	90	ARG
1	A	104	SER
1	A	108	GLU
1	A	130	THR
1	A	163	PHE
1	A	168	ASN
1	A	188	LEU
1	A	189	VAL
1	A	232	VAL
1	A	235	VAL
1	A	261	LEU
1	A	285	LEU
1	A	306	LEU
1	A	310	LEU
1	A	316	SER
1	A	321	LEU
1	A	346	LEU
1	A	370	VAL
1	A	371	GLN
1	A	372	LEU
1	A	380	VAL
1	A	381	SER
1	A	389	THR
1	A	396	TRP
1	A	420	LEU
1	A	460	THR
1	A	467	VAL
1	A	475	SER
1	A	477	ASP
1	A	497	ILE
1	A	505	GLN
1	A	513	LEU
1	A	530	SER

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Mol	Chain	Res	Type
1	A	534	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	42	ASN
1	A	71	HIS
1	A	86	ASN
1	A	168	ASN
1	A	176	ASN
1	A	180	ASN
1	A	199	GLN
1	A	280	GLN
1	A	328	HIS
1	A	332	GLN
1	A	371	GLN
1	A	505	GLN
1	A	520	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	A	561	-	12,12,12	1.04	1 (8%)	17,17,17	2.47	10 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	561	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	561	BGC	C1-C2	2.11	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	561	BGC	C4-C3-C2	-4.49	102.42	110.79
2	A	561	BGC	C3-C4-C5	-4.22	102.84	110.20
2	A	561	BGC	O4-C4-C3	2.33	115.58	110.34
2	A	561	BGC	O4-C4-C5	2.36	115.49	109.24
2	A	561	BGC	O1-C1-C2	2.57	116.10	109.21
2	A	561	BGC	O3-C3-C4	2.70	116.42	110.34
2	A	561	BGC	O5-C5-C6	2.74	113.28	106.36
2	A	561	BGC	O5-C1-C2	2.88	114.40	109.80
2	A	561	BGC	C1-O5-C5	2.90	118.84	113.47
2	A	561	BGC	C1-C2-C3	2.93	114.79	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	BGC	1	0

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, 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	522/535 (97%)	-0.18	16 (3%) 52 57	7, 24, 44, 60	7 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	LYS	17.0
1	A	550	THR	7.2
1	A	241	GLU	6.0
1	A	218	LEU	3.6
1	A	506	ALA	3.5
1	A	162	TRP	3.5
1	A	29	SER	3.2
1	A	541	VAL	2.8
1	A	485	ILE	2.7
1	A	549	SER	2.6
1	A	409	ALA	2.4
1	A	503	THR	2.4
1	A	217	ILE	2.4
1	A	160	TRP	2.3
1	A	31	GLN	2.0
1	A	484	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, 95th 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(Å ²)	Q<0.9
2	BGC	A	561	12/12	0.81	0.22	2.29	45,53,63,65	0
3	ZN	A	573	1/1	0.99	0.11	-	35,35,35,35	0
3	ZN	A	572	1/1	0.99	0.10	-	29,29,29,29	0
3	ZN	A	571	1/1	0.99	0.08	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.