



# Full wwPDB X-ray Structure Validation Report

Aug 9, 2020 – 10:10 PM BST

PDB ID : 4CSI  
Title : Crystal structure of the thermostable Cellobiohydrolase Cel7A from the fungus *Humicola grisea* var. *thermoidea*.  
Authors : Haddad-Momeni, M.; Goedegebuur, F.; Hansson, H.; Karkehabadi, S.; Askarieh, G.; Mitchinson, C.; Larenas, E.; Stahlberg, J.; Sandgren, M.  
Deposited on : 2014-03-07  
Resolution : 1.80 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

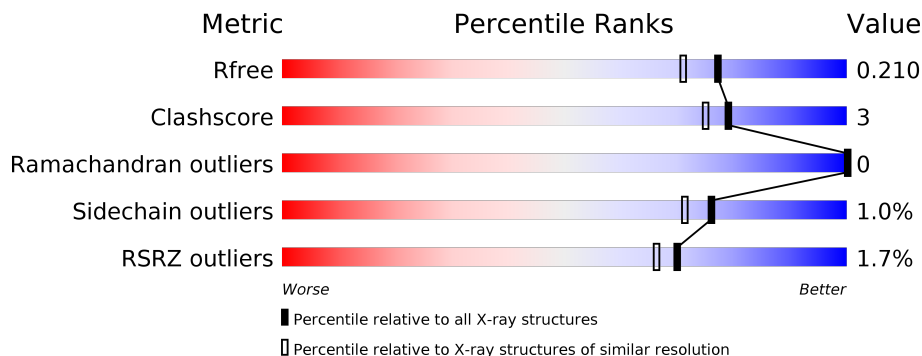
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	439	 2% 91% 8%
1	B	439	 % 93% 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7388 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.

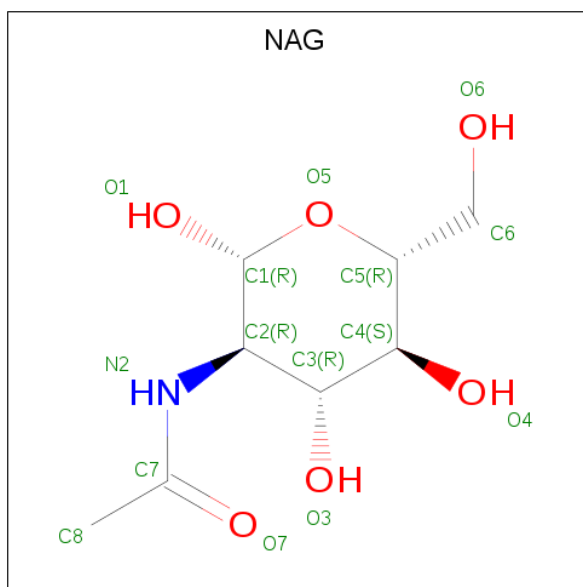
- Molecule 1 is a protein called CELLULASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	Total 3343	C 2063	N 568	O 682	S 30	0	13	0
1	B	431	Total 3285	C 2024	N 563	O 667	S 31	0	10	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	HIS	TYR	conflict	UNP Q12621
B	101	HIS	TYR	conflict	UNP Q12621

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
3	B	1	7	4	3	0	0

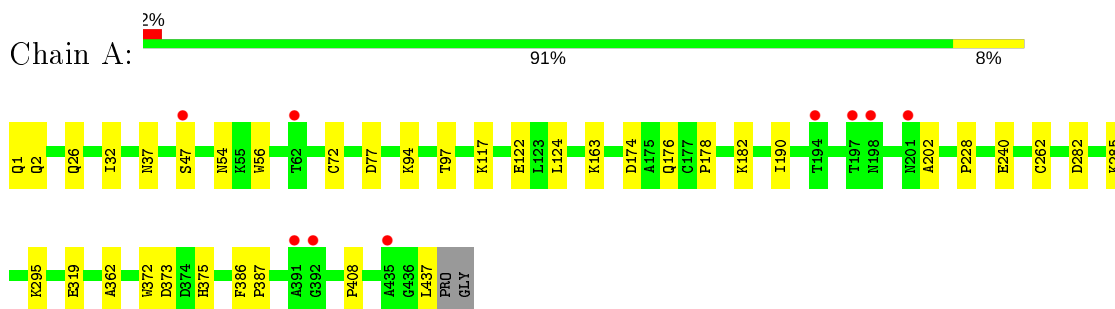
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	388	389	389	0	1
4	B	329	329	329	0	0

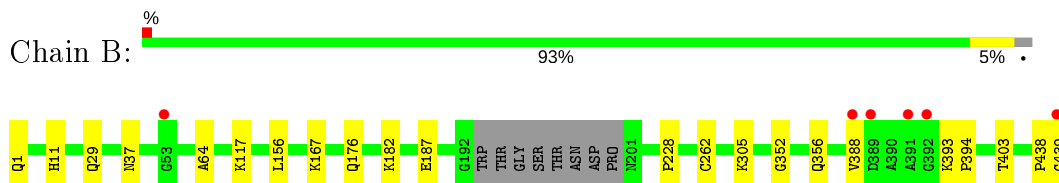
### 3 Residue-property plots [i](#)

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: CELLULASE



- Molecule 1: CELLULASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.93Å 85.27Å 135.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.32 – 1.80 33.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.32-1.80) 99.8 (33.96-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.164 , 0.210 0.165 , 0.210	Depositor DCC
$R_{free}$ test set	3297 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PCA, NAG

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	0.49	0/3444	0.67	1/4668 (0.0%)
1	B	0.49	0/3365	0.65	0/4556
All	All	0.49	0/6809	0.66	1/9224 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	SER	N-CA-C	-5.06	97.34	111.00

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	3343	0	3152	24	0
1	B	3285	0	3088	14	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
3	A	7	0	10	3	0
3	B	7	0	10	0	0
4	A	389	0	0	4	0
4	B	329	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7388	0	6286	36	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 3.

All (36) 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:77[A]:ASP:OD1	4:A:2077:HOH:O	1.72	1.06
1:A:176:GLN:HG2	3:A:1439:PEG:C1	2.15	0.77
1:A:176:GLN:HG2	3:A:1439:PEG:H11	1.69	0.75
1:A:176:GLN:CG	3:A:1439:PEG:H11	2.17	0.75
1:A:319:GLU:HB2	2:A:1438:NAG:H81	1.75	0.67
1:A:2[A]:GLN:HE22	1:A:163:LYS:NZ	1.96	0.64
1:B:388:VAL:HG13	1:B:403:THR:HB	1.88	0.55
1:A:2[B]:GLN:HB3	1:A:72:CYS:HB3	1.89	0.54
1:A:228:PRO:HD2	1:A:262:CYS:O	2.09	0.52
1:B:228:PRO:HD2	1:B:262:CYS:O	2.11	0.51
1:B:64:ALA:HB1	1:B:187:GLU:HB3	1.92	0.51
1:A:2[A]:GLN:NE2	1:A:163:LYS:HE2	2.27	0.50
1:A:2[B]:GLN:OE1	1:A:163:LYS:HE2	2.11	0.50
1:A:2[B]:GLN:HG3	4:A:2003:HOH:O	2.11	0.50
1:A:375:HIS:CD2	1:A:408:PRO:HG2	2.47	0.49
1:A:124:LEU:HD23	1:B:29:GLN:OE1	2.13	0.49
1:B:352:GLY:HA3	1:B:356:GLN:HB2	1.96	0.47
1:B:156:LEU:O	4:B:2158:HOH:O	2.20	0.47
1:B:11:HIS:HE1	1:B:167:LYS:O	1.98	0.47
1:A:372:TRP:HE3	1:A:373:ASP:O	1.99	0.46
1:B:176[B]:GLN:NE2	4:B:2169:HOH:O	2.48	0.46
1:B:393:LYS:HG3	1:B:394:PRO:HD2	1.99	0.45
1:A:94:LYS:HE3	1:A:97:THR:OG1	2.18	0.44
1:B:305:LYS:HE2	4:B:2268:HOH:O	2.17	0.44
1:A:122:GLU:HG3	1:A:362:ALA:O	2.18	0.44
1:A:56:TRP:CD2	1:A:190:ILE:HG22	2.53	0.43
1:A:117:LYS:NZ	4:A:2140:HOH:O	2.39	0.43
1:A:54:ASN:HB2	1:A:202:ALA:O	2.19	0.43
1:A:295:LYS:HE2	1:B:29:GLN:OE1	2.20	0.42
1:A:182:LYS:HE3	4:A:2043:HOH:O	2.20	0.41
1:B:182[A]:LYS:HD3	1:B:182[A]:LYS:HA	1.88	0.41
1:A:386:PHE:HA	1:A:387:PRO:C	2.41	0.41
1:A:282:ASP:HB3	1:A:285[B]:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:HIS:HD2	4:B:2038:HOH:O	2.03	0.41
1:A:174:ASP:OD1	1:A:178:PRO:HD3	2.22	0.40
1:B:438:PRO:O	1:B:439:GLY:C	2.60	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	449/439 (102%)	441 (98%)	8 (2%)	0	100	100
1	B	437/439 (100%)	433 (99%)	4 (1%)	0	100	100
All	All	886/878 (101%)	874 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	367/354 (104%)	361 (98%)	6 (2%)	62	54
1	B	357/354 (101%)	355 (99%)	2 (1%)	86	84
All	All	724/708 (102%)	716 (99%)	8 (1%)	76	68

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	32[A]	ILE
1	A	32[B]	ILE
1	A	37	ASN
1	A	240	GLU
1	A	437	LEU
1	B	37	ASN
1	B	117	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	375	HIS
1	B	11	HIS
1	B	54	ASN
1	B	136	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	PCA	A	1	1	7,8,9	0.46	0	9,10,12	1.67	1 (11%)
1	PCA	B	1	1	7,8,9	0.70	0	9,10,12	1.53	1 (11%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1	PCA	CB-CA-C	-4.45	106.57	112.70
1	B	1	PCA	CB-CA-C	-3.77	107.51	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	NAG	B	1440	1	14,14,15	0.61	0	17,19,21	1.12	1 (5%)
3	PEG	B	1441	-	6,6,6	0.41	0	5,5,5	0.43	0
3	PEG	A	1439	-	6,6,6	0.55	0	5,5,5	0.36	0
2	NAG	A	1438	1	14,14,15	0.85	1 (7%)	17,19,21	1.11	2 (11%)

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	NAG	B	1440	1	-	2/6/23/26	0/1/1/1
3	PEG	B	1441	-	-	2/4/4/4	-
3	PEG	A	1439	-	-	1/4/4/4	-
2	NAG	A	1438	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1438	NAG	O5-C1	-2.28	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1438	NAG	O5-C1-C2	-3.07	106.44	111.29
2	B	1440	NAG	C1-O5-C5	2.40	115.44	112.19
2	A	1438	NAG	C2-N2-C7	-2.30	119.63	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1441	PEG	O2-C3-C4-O4
2	B	1440	NAG	C4-C5-C6-O6
2	B	1440	NAG	O5-C5-C6-O6
3	A	1439	PEG	C4-C3-O2-C2
3	B	1441	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1439	PEG	3	0
2	A	1438	NAG	1	0

## 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 [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	436/439 (99%)	-0.28	9 (2%) 63 59	8, 15, 32, 44	2 (0%)
1	B	430/439 (97%)	-0.32	6 (1%) 75 72	8, 16, 30, 48	3 (0%)
All	All	866/878 (98%)	-0.30	15 (1%) 70 66	8, 16, 31, 48	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	GLY	4.8
1	A	197	THR	3.8
1	B	389	ASP	3.2
1	B	391	ALA	3.0
1	B	388	VAL	2.9
1	A	201	ASN	2.9
1	A	391	ALA	2.6
1	A	47	SER	2.5
1	A	435	ALA	2.4
1	B	392	GLY	2.4
1	B	439	GLY	2.2
1	B	53	GLY	2.2
1	A	62	THR	2.2
1	A	194	THR	2.1
1	A	198	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PCA	A	1	8/9	0.96	0.08	14,14,14,14	0
1	PCA	B	1	8/9	0.97	0.07	13,14,14,14	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	B	1441	7/7	0.66	0.27	34,37,41,41	0
3	PEG	A	1439	7/7	0.76	0.25	26,31,33,35	0
2	NAG	B	1440	14/15	0.92	0.11	18,21,23,23	0
2	NAG	A	1438	14/15	0.94	0.10	18,19,20,21	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.