wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:39 PM GMT

PDB ID	:	1Q2E
Title	:	CELLOBIOHYDROLASE CEL7A WITH LOOP DELETION 245-252 AND BOUND NON-HYDROLYSABLE CELLOTETRAOSE
Authors	:	Stahlberg, J.; Harris, M.; Jones, T.A.
Deposited on	:	2003-07-24
Resolution	:	1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

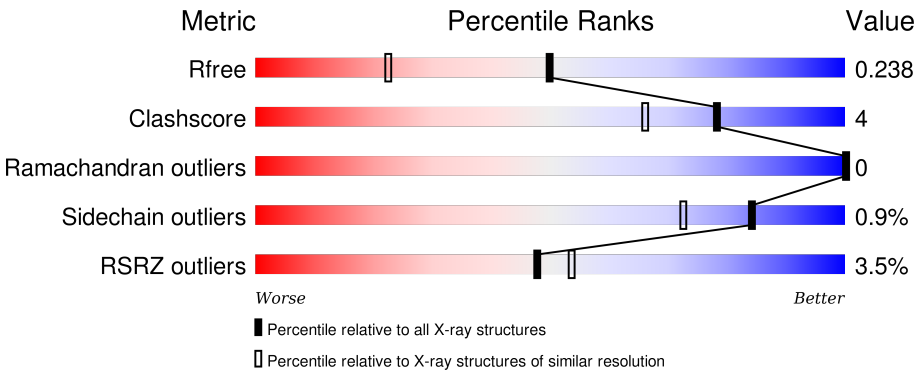
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 <=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	426	4% 92% 8%
1	B	426	3% 92% 8%

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
3	GLC	A	903	X	-	-	-
3	GLC	A	904	X	-	-	-
3	GLC	B	903	X	-	-	-
3	GLC	B	904	X	-	-	-
5	CA	B	499	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7037 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 EXOCELLOBIOHYDROLASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3156	1936	521	673	26	0	0	0
1	B	426	3156	1936	521	673	26	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	MODIFIED RESIDUE	UNP P00725
A	94	ASP	GLY	CLONING ARTIFACT	UNP P00725
A	?	-	GLY	DELETION	UNP P00725
A	?	-	THR	DELETION	UNP P00725
A	?	-	TYR	DELETION	UNP P00725
A	?	-	SER	DELETION	UNP P00725
A	?	-	ASP	DELETION	UNP P00725
A	?	-	ASN	DELETION	UNP P00725
A	?	-	ARG	DELETION	UNP P00725
A	?	-	TYR	DELETION	UNP P00725
B	1	PCA	GLN	MODIFIED RESIDUE	UNP P00725
B	94	ASP	GLY	CLONING ARTIFACT	UNP P00725
B	?	-	GLY	DELETION	UNP P00725
B	?	-	THR	DELETION	UNP P00725
B	?	-	TYR	DELETION	UNP P00725
B	?	-	SER	DELETION	UNP P00725
B	?	-	ASP	DELETION	UNP P00725
B	?	-	ASN	DELETION	UNP P00725
B	?	-	ARG	DELETION	UNP P00725
B	?	-	TYR	DELETION	UNP P00725

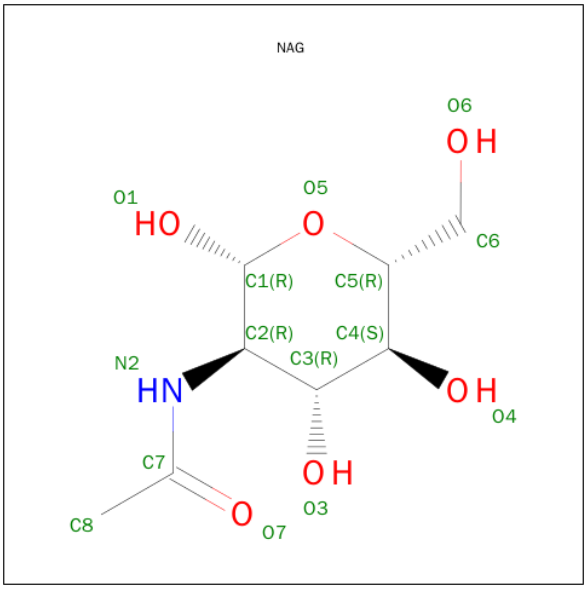
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	O	S	0	0
			24	13	10	1		
2	B	2	Total	C	O	S	0	0
			24	13	10	1		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			22	12	10		
3	B	2	Total	C	O	0	0
			22	12	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

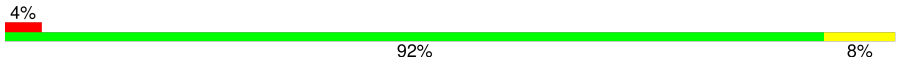
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	271	271	271	0	0
			Total	O		
6	B	333	333	333	0	0

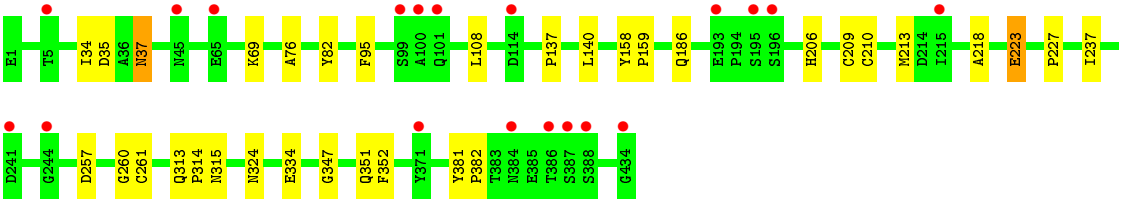
3 Residue-property plots (i)

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: EXOCELLOBIOHYDROLASE I

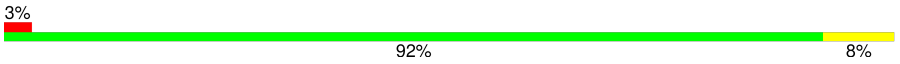
Chain A:

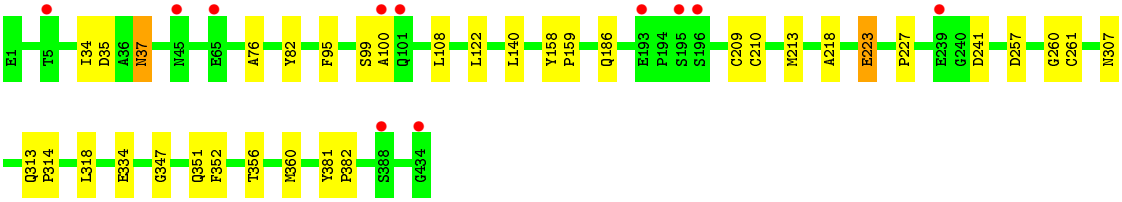




- Molecule 1: EXOCELLOBIOHYDROLASE I

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.34Å 84.31Å 110.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 31.25 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.75) 100.0 (31.25-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.82 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.239 0.228 , 0.238	Depositor DCC
R_{free} test set	2320 reflections (2.94%)	DCC
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.3	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 78983 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7037	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.05 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0487e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, CA, GLC, MGL, SGC, PCA

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	0.31	0/3222	0.67	0/4393
1	B	0.32	0/3222	0.68	0/4393
All	All	0.32	0/6444	0.67	0/8786

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	0
3	B	2	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	903	GLC	C1
3	A	904	GLC	C1
3	B	903	GLC	C1
3	B	904	GLC	C1

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	3156	0	2867	22	0
1	B	3156	0	2867	22	0
2	A	24	0	22	0	0
2	B	24	0	22	0	0
3	A	22	0	19	0	0
3	B	22	0	19	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	B	1	0	0	0	0
6	A	271	0	0	4	0
6	B	333	0	0	3	0
All	All	7037	0	5842	44	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.

The worst 5 of 44 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:B:122:LEU:HD12	1:B:360:MET:HE1	1.60	0.84
1:B:356:THR:HA	1:B:360:MET:HE2	1.61	0.80
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.62	0.79
1:A:313:GLN:HE21	1:A:314:PRO:HD2	1.49	0.77
1:A:314:PRO:HG2	6:A:1150:HOH:O	1.86	0.75

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	424/426 (100%)	414 (98%)	10 (2%)	0	100	100
1	B	424/426 (100%)	418 (99%)	6 (1%)	0	100	100
All	All	848/852 (100%)	832 (98%)	16 (2%)	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	349/349 (100%)	347 (99%)	2 (1%)	90	83
1	B	349/349 (100%)	345 (99%)	4 (1%)	80	66
All	All	698/698 (100%)	692 (99%)	6 (1%)	84	72

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	ASN
1	B	307	ASN
1	B	223	GLU
1	A	223	GLU
1	B	241	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	ASN
1	A	413	ASN
1	B	307	ASN
1	A	315	ASN
1	B	186	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)

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	1.90	1 (14%)	9,10,12	1.41	2 (22%)
1	PCA	B	1	1	7,8,9	1.92	1 (14%)	9,10,12	1.38	2 (22%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	4.51	1.48	1.33
1	B	1	PCA	CD-N	4.55	1.48	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	CA-N-CD	-2.51	105.41	113.81
1	A	1	PCA	CB-CA-C	-2.43	109.44	112.76
1	B	1	PCA	CB-CA-C	-2.42	109.46	112.76
1	B	1	PCA	CA-N-CD	-2.38	105.85	113.81

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)

8 carbohydrates 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	MGL	A	901	2	13,13,13	0.92	1 (7%)	18,18,18	0.79	1 (5%)
2	SGC	A	902	3,2	9,11,12	0.58	0	10,15,17	0.96	1 (10%)
3	GLC	A	903	3,2	11,11,12	0.51	0	14,15,17	0.53	0
3	GLC	A	904	3	11,11,12	0.56	0	14,15,17	0.48	0
2	MGL	B	901	2	13,13,13	0.91	1 (7%)	18,18,18	0.74	1 (5%)
2	SGC	B	902	3,2	9,11,12	0.53	0	10,15,17	1.11	1 (10%)
3	GLC	B	903	3,2	11,11,12	0.52	0	14,15,17	0.55	0
3	GLC	B	904	3	11,11,12	0.64	0	14,15,17	0.48	0

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	MGL	A	901	2	-	0/4/24/24	0/1/1/1
2	SGC	A	902	3,2	-	0/2/19/22	0/1/1/1
3	GLC	A	903	3,2	1/1/4/5	0/2/19/22	0/1/1/1
3	GLC	A	904	3	1/1/4/5	0/2/19/22	0/1/1/1
2	MGL	B	901	2	-	0/4/24/24	0/1/1/1
2	SGC	B	902	3,2	-	0/2/19/22	0/1/1/1
3	GLC	B	903	3,2	1/1/4/5	0/2/19/22	0/1/1/1
3	GLC	B	904	3	1/1/4/5	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	MGL	O1-C1	2.70	1.44	1.40
2	A	901	MGL	O1-C1	2.72	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	902	SGC	C1-O5-C5	2.03	114.82	112.25
2	B	902	SGC	C1-C2-C3	2.08	112.00	109.54
2	B	901	MGL	O1-C1-C2	2.53	111.19	108.21
2	A	901	MGL	O1-C1-C2	2.76	111.46	108.21

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	904	GLC	C1
3	B	903	GLC	C1
3	A	903	GLC	C1
3	A	904	GLC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	NAG	A	435	1	14,14,15	0.45	0	15,19,21	0.87	1 (6%)
4	NAG	B	436	1	14,14,15	0.58	0	15,19,21	0.99	1 (6%)

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
4	NAG	A	435	1	-	0/6/23/26	0/1/1/1
4	NAG	B	436	1	-	0/6/23/26	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(^{o})	Ideal(^{o})
4	B	436	NAG	C2-N2-C7	-2.85	119.38	123.04
4	A	435	NAG	C2-N2-C7	-2.33	120.05	123.04

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 (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, 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	425/426 (99%)	0.56	19 (4%)	37	43	7, 11, 18, 26	0
1	B	425/426 (99%)	0.45	11 (2%)	59	65	5, 8, 16, 21	0
All	All	850/852 (99%)	0.51	30 (3%)	48	53	5, 10, 17, 26	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	ALA	6.5
1	A	101	GLN	5.0
1	A	387	SER	4.7
1	A	100	ALA	4.6
1	A	388	SER	4.0

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. 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
1	PCA	A	1	8/9	0.94	0.11	-	12,13,13,13	0
1	PCA	B	1	8/9	0.97	0.08	-	9,9,9,9	0

6.3 Carbohydrates (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	SGC	B	902	11/12	0.93	0.13	1.17	8,11,12,13	0
3	GLC	B	903	11/12	0.94	0.11	0.06	9,10,11,11	0
3	GLC	A	904	11/12	0.93	0.12	-0.12	8,10,11,11	0
2	SGC	A	902	11/12	0.95	0.12	-0.27	8,12,13,13	0
3	GLC	A	903	11/12	0.93	0.11	-0.31	9,10,12,12	0
3	GLC	B	904	11/12	0.93	0.11	-0.31	7,8,9,10	0
2	MGL	B	901	13/13	0.79	0.24	-	13,15,15,16	0
2	MGL	A	901	13/13	0.86	0.22	-	12,14,14,14	0

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
5	CA	B	499	1/1	0.35	1.74	135.04	54,54,54,54	0
4	NAG	B	436	14/15	-	-	-	10,10,10,10	14
4	NAG	A	435	14/15	-	-	-	11,11,11,11	14

6.5 Other polymers (i)

There are no such residues in this entry.