Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 01:58 AM EDT

PDB ID	:	1RQ5
Title	:	Structural Basis for the Exocellulase Activity of the Cellobiohydrolase CbhA from C. thermocellum
Authors	:	Schubot, F.D.; Kataeva, I.A.; Chang, J.; Shah, A.K.; Ljungdahl, L.G.; Rose, J.P.; Wang, B.C.
Deposited on	:	2003-12-04
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

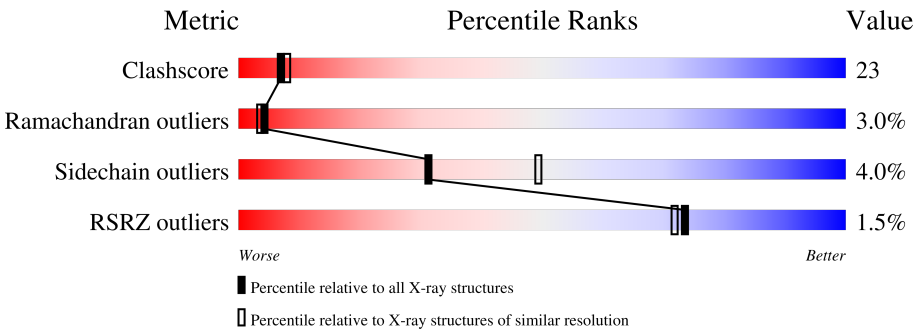
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	610	% 61% 32% 5% •
2	B	4	50% 50%

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	B	1	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5223 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 Cellobiohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4789	3059	799	911	20	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	795	GLN	GLU	engineered mutation	UNP Q59325
A	814	GLN	-	SEE REMARK 999	UNP Q59325
A	815	TYR	-	SEE REMARK 999	UNP Q59325
A	816	THR	-	SEE REMARK 999	UNP Q59325
A	817	ASP	-	SEE REMARK 999	UNP Q59325

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	B	4	45	24	21	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

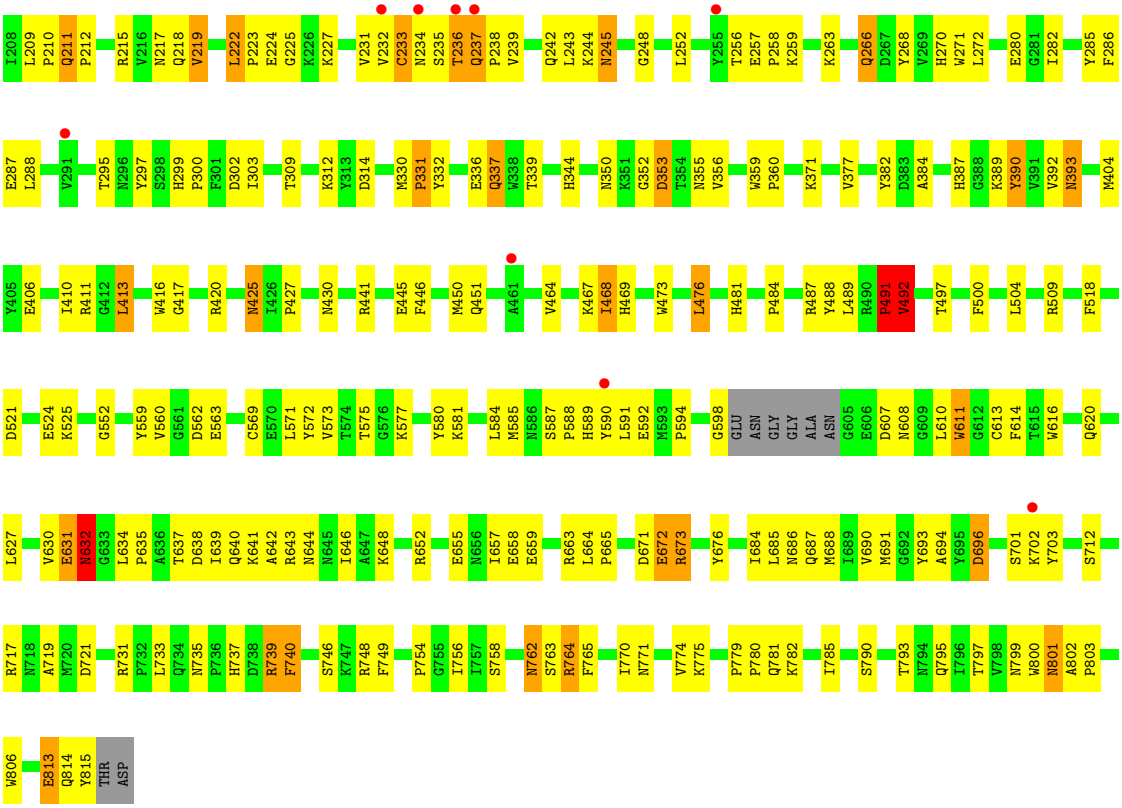
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	387	387	387	0	0

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: Cellobiohydrolase

Chain A:



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	108.60Å 108.60Å 119.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 50.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	72.0 (20.00-2.40) 80.0 (50.34-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	7.18 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.270 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5223	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BGC, 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	0.48	3/4943 (0.1%)	0.80	11/6742 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	VAL	C-N	-9.89	1.15	1.33
1	A	813	GLU	CD-OE2	6.98	1.33	1.25
1	A	218	GLN	C-N	-5.50	1.21	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	MET	C-N-CD	-19.74	77.17	120.60
1	A	219	VAL	O-C-N	-13.84	99.67	123.20
1	A	330	MET	C-N-CA	13.73	179.67	122.00
1	A	219	VAL	CA-C-N	9.51	135.23	116.20
1	A	673	ARG	N-CA-C	-6.60	93.18	111.00
1	A	331	PRO	CA-N-CD	-6.34	102.62	111.50
1	A	352	GLY	N-CA-C	6.08	128.30	113.10
1	A	222	LEU	C-N-CD	-5.35	108.83	120.60
1	A	491	PRO	N-CA-C	5.28	125.84	112.10
1	A	218	GLN	O-C-N	-5.17	114.42	122.70
1	A	413	LEU	CA-CB-CG	5.03	126.87	115.30

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	4789	0	4493	214	0
2	B	45	0	39	5	0
3	A	2	0	0	0	0
4	A	387	0	0	16	0
All	All	5223	0	4532	215	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 23.

All (215) 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:719:ALA:H	1:A:781:GLN:HE21	1.13	0.94
1:A:337:GLN:H	1:A:337:GLN:HE21	0.99	0.92
1:A:350:ASN:HD21	1:A:481:HIS:HA	1.33	0.90
1:A:685:LEU:HA	1:A:688:MET:HE3	1.52	0.88
1:A:491:PRO:O	1:A:492:VAL:HB	1.74	0.88
1:A:584:LEU:HD11	1:A:627:LEU:HD11	1.56	0.87
1:A:591:LEU:HD22	1:A:642:ALA:HB2	1.54	0.87
1:A:210:PRO:O	1:A:211:GLN:HB2	1.75	0.87
1:A:632:ASN:HD22	1:A:634:LEU:H	1.23	0.86
1:A:790:SER:OG	1:A:793:THR:HG22	1.75	0.86
1:A:337:GLN:H	1:A:337:GLN:NE2	1.72	0.86
1:A:610:LEU:O	1:A:611:TRP:HB2	1.76	0.85
1:A:209:LEU:HB3	1:A:731:ARG:HH12	1.42	0.85
1:A:300:PRO:HG3	4:A:898:HOH:O	1.79	0.81
1:A:684:ILE:HG22	1:A:688:MET:HE2	1.64	0.80
1:A:225:GLY:O	1:A:227:LYS:NZ	2.15	0.79
1:A:209:LEU:HB3	1:A:731:ARG:NH1	1.99	0.78
1:A:719:ALA:H	1:A:781:GLN:NE2	1.82	0.78
1:A:764:ARG:HH11	1:A:764:ARG:HG2	1.52	0.75
1:A:337:GLN:HE21	1:A:337:GLN:N	1.80	0.74
1:A:572:TYR:CE2	1:A:632:ASN:HB2	2.22	0.74
1:A:344:HIS:CD2	1:A:487:ARG:HD2	2.24	0.72
1:A:350:ASN:ND2	1:A:481:HIS:HA	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ILE:HG23	1:A:690:VAL:HG13	1.73	0.70
1:A:632:ASN:ND2	1:A:634:LEU:H	1.88	0.70
1:A:295:THR:HA	1:A:297:TYR:CE2	2.27	0.69
1:A:500:PHE:CE1	1:A:504:LEU:HD22	2.27	0.68
1:A:770:ILE:HD13	1:A:785:ILE:HG22	1.76	0.68
1:A:404:MET:HB3	1:A:806:TRP:CD1	2.30	0.67
1:A:353:ASP:H	1:A:356:VAL:HG22	1.60	0.67
1:A:491:PRO:O	1:A:492:VAL:CB	2.44	0.66
1:A:607:ASP:HA	1:A:610:LEU:CD1	2.26	0.64
1:A:764:ARG:HG2	1:A:764:ARG:NH1	2.13	0.64
1:A:581:LYS:O	1:A:585:MET:HG3	1.98	0.63
1:A:559:TYR:OH	1:A:589:HIS:NE2	2.28	0.63
1:A:756:ILE:HA	1:A:801:ASN:HD21	1.63	0.63
1:A:234:ASN:HA	1:A:268:TYR:CB	2.29	0.62
1:A:775:LYS:HE3	4:A:947:HOH:O	2.00	0.61
1:A:585:MET:HA	1:A:590:TYR:CD1	2.35	0.61
1:A:684:ILE:O	1:A:688:MET:HE2	2.00	0.61
1:A:245:ASN:C	1:A:245:ASN:HD22	2.03	0.61
1:A:209:LEU:HG	4:A:1164:HOH:O	2.00	0.61
1:A:764:ARG:N	1:A:764:ARG:HD2	2.17	0.60
1:A:212:PRO:HG2	1:A:299:HIS:CD2	2.37	0.60
1:A:739:ARG:NH2	2:B:2:BGC:O2	2.34	0.60
1:A:631:GLU:O	1:A:632:ASN:O	2.19	0.60
1:A:693:TYR:O	1:A:696:ASP:HB2	2.01	0.59
1:A:813:GLU:C	1:A:815:TYR:H	2.06	0.59
1:A:393:ASN:HD21	1:A:799:ASN:CG	2.05	0.59
1:A:607:ASP:HA	1:A:610:LEU:HD12	1.85	0.59
1:A:451:GLN:HE22	1:A:525:LYS:HD2	1.68	0.58
1:A:639:ILE:O	1:A:643:ARG:HG3	2.03	0.58
1:A:665:PRO:HG2	1:A:687:GLN:NE2	2.18	0.58
1:A:481:HIS:HB2	4:A:924:HOH:O	2.03	0.58
1:A:353:ASP:H	1:A:356:VAL:CG2	2.17	0.57
1:A:562:ASP:HB2	1:A:620:GLN:H	1.69	0.57
1:A:242:GLN:OE1	1:A:244:LYS:HE3	2.05	0.57
1:A:272:LEU:C	1:A:272:LEU:HD23	2.25	0.57
1:A:684:ILE:HG22	1:A:688:MET:CE	2.33	0.57
1:A:258:PRO:HA	1:A:270:HIS:ND1	2.19	0.57
1:A:813:GLU:C	1:A:815:TYR:N	2.58	0.57
1:A:441:ARG:HG3	1:A:518:PHE:CZ	2.39	0.57
1:A:575:THR:HB	1:A:577:LYS:HG3	1.87	0.57
1:A:236:THR:O	1:A:237:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:O	1:A:339:THR:HG23	2.06	0.56
1:A:721:ASP:OD1	1:A:731:ARG:NH2	2.37	0.56
1:A:665:PRO:HG2	1:A:687:GLN:HE22	1.71	0.56
1:A:222:LEU:HB3	1:A:223:PRO:HD2	1.87	0.55
1:A:441:ARG:O	1:A:445:GLU:HG2	2.07	0.55
1:A:685:LEU:HA	1:A:688:MET:CE	2.31	0.55
1:A:239:VAL:O	1:A:256:THR:HG23	2.06	0.55
1:A:280:GLU:HA	1:A:303:ILE:O	2.05	0.55
1:A:672:GLU:HA	1:A:672:GLU:OE1	2.07	0.55
1:A:476:LEU:HA	1:A:739:ARG:HG3	1.88	0.55
1:A:664:LEU:H	1:A:664:LEU:HD23	1.72	0.54
1:A:569:CYS:SG	1:A:584:LEU:HD13	2.47	0.54
1:A:694:ALA:HB1	1:A:703:TYR:CD1	2.43	0.54
1:A:748:ARG:NH1	4:A:1010:HOH:O	2.40	0.54
1:A:524:GLU:HG2	1:A:524:GLU:O	2.07	0.53
1:A:644:ASN:O	1:A:648:LYS:HG3	2.09	0.53
1:A:469:HIS:CD2	1:A:552:GLY:HA3	2.43	0.53
1:A:245:ASN:C	1:A:245:ASN:ND2	2.62	0.52
1:A:353:ASP:HA	1:A:356:VAL:CG2	2.39	0.52
1:A:663:ARG:HB2	1:A:717:ARG:NH1	2.24	0.52
1:A:509:ARG:HD2	4:A:1087:HOH:O	2.09	0.52
1:A:634:LEU:O	1:A:635:PRO:C	2.48	0.52
1:A:813:GLU:O	1:A:815:TYR:N	2.42	0.52
1:A:234:ASN:HA	1:A:268:TYR:HB3	1.90	0.52
1:A:610:LEU:O	1:A:611:TRP:CB	2.55	0.52
1:A:344:HIS:HD2	1:A:487:ARG:HD2	1.71	0.52
1:A:259:LYS:HE2	1:A:271:TRP:CZ2	2.45	0.51
1:A:233:CYS:HB3	1:A:270:HIS:CD2	2.46	0.51
1:A:389:LYS:HB3	1:A:446:PHE:CZ	2.45	0.51
1:A:285:TYR:O	1:A:285:TYR:CD1	2.64	0.51
1:A:353:ASP:N	1:A:353:ASP:OD1	2.45	0.50
1:A:746:SER:HB3	1:A:749:PHE:CE1	2.46	0.50
1:A:497:THR:O	1:A:500:PHE:HB3	2.12	0.50
1:A:664:LEU:HD11	1:A:676:TYR:OH	2.11	0.49
1:A:217:ASN:OD1	1:A:219:VAL:HG12	2.12	0.49
1:A:657:ILE:HG23	1:A:663:ARG:HB3	1.93	0.49
1:A:280:GLU:HG3	4:A:988:HOH:O	2.13	0.49
1:A:637:THR:O	1:A:640:GLN:HB2	2.12	0.49
1:A:607:ASP:O	1:A:610:LEU:HG	2.11	0.49
1:A:355:ASN:ND2	4:A:1127:HOH:O	2.46	0.49
1:A:390:TYR:N	1:A:390:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:HG12	1:A:488:TYR:O	2.13	0.49
1:A:719:ALA:HB1	1:A:782:LYS:HE3	1.93	0.49
1:A:652:ARG:O	1:A:655:GLU:HB3	2.13	0.49
1:A:282:ILE:HA	1:A:302:ASP:OD1	2.13	0.48
1:A:231:VAL:HG12	1:A:232:VAL:N	2.28	0.48
1:A:719:ALA:N	1:A:781:GLN:HE21	1.95	0.48
1:A:571:LEU:HB3	1:A:580:TYR:CD1	2.48	0.48
1:A:802:ALA:N	1:A:803:PRO:HD2	2.29	0.48
1:A:560:VAL:HA	1:A:563:GLU:OE1	2.13	0.48
1:A:685:LEU:HD23	1:A:688:MET:HE3	1.95	0.48
1:A:390:TYR:CD2	1:A:467:LYS:HD2	2.49	0.48
1:A:212:PRO:CD	1:A:299:HIS:NE2	2.77	0.48
1:A:243:LEU:HD13	1:A:286:PHE:CE1	2.49	0.48
1:A:632:ASN:ND2	1:A:632:ASN:C	2.67	0.47
1:A:737:HIS:HE1	2:B:2:BGC:O2	1.96	0.47
1:A:217:ASN:OD1	1:A:219:VAL:CG1	2.62	0.47
1:A:591:LEU:HD13	1:A:641:LYS:HB3	1.97	0.47
1:A:272:LEU:C	1:A:272:LEU:CD2	2.83	0.47
1:A:382:TYR:CD1	1:A:387:HIS:HA	2.50	0.46
1:A:795:GLN:NE2	2:B:2:BGC:O3	2.42	0.46
1:A:764:ARG:N	1:A:764:ARG:CD	2.78	0.46
1:A:233:CYS:HB3	1:A:270:HIS:NE2	2.31	0.46
1:A:611:TRP:N	4:A:1137:HOH:O	2.28	0.46
1:A:655:GLU:O	1:A:659:GLU:HG2	2.16	0.46
1:A:740:PHE:O	1:A:749:PHE:HB3	2.16	0.46
1:A:473:TRP:CZ3	2:B:2:BGC:H2	2.51	0.46
1:A:525:LYS:HE3	4:A:1146:HOH:O	2.15	0.46
1:A:332:TYR:CD2	1:A:427:PRO:HG3	2.51	0.46
1:A:591:LEU:HD11	1:A:638:ASP:HB3	1.98	0.46
1:A:223:PRO:HG2	1:A:224:GLU:H	1.81	0.45
1:A:735:ASN:HA	4:A:872:HOH:O	2.16	0.45
1:A:212:PRO:HD2	1:A:299:HIS:NE2	2.31	0.45
1:A:212:PRO:HD3	4:A:1164:HOH:O	2.16	0.45
1:A:655:GLU:HG2	1:A:659:GLU:OE2	2.16	0.45
1:A:594:PRO:HG2	1:A:620:GLN:HE21	1.81	0.45
1:A:731:ARG:HH11	1:A:731:ARG:HG3	1.81	0.45
1:A:687:GLN:O	1:A:691:MET:HG3	2.17	0.45
1:A:746:SER:HB3	1:A:749:PHE:HE1	1.82	0.45
1:A:572:TYR:HE2	1:A:632:ASN:HB2	1.78	0.45
1:A:655:GLU:CG	1:A:659:GLU:OE2	2.64	0.45
1:A:245:ASN:ND2	1:A:248:GLY:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLY:O	1:A:420:ARG:NH1	2.50	0.45
1:A:356:VAL:HG11	1:A:468:ILE:HG13	1.99	0.45
1:A:573:VAL:HG21	1:A:630:VAL:CG1	2.46	0.45
1:A:332:TYR:CE2	1:A:427:PRO:HG3	2.51	0.45
1:A:630:VAL:CG1	1:A:631:GLU:HG3	2.47	0.45
1:A:223:PRO:HG2	1:A:224:GLU:N	2.32	0.45
1:A:242:GLN:OE1	1:A:244:LYS:CE	2.64	0.45
1:A:762:ASN:HD22	1:A:762:ASN:C	2.20	0.45
1:A:309:THR:O	1:A:312:LYS:HG2	2.17	0.45
1:A:406:GLU:OE1	1:A:509:ARG:NH2	2.29	0.45
1:A:630:VAL:HG12	1:A:631:GLU:HG3	1.99	0.45
1:A:263:LYS:O	1:A:266:GLN:OE1	2.34	0.44
1:A:733:LEU:CD2	1:A:758:SER:HB2	2.47	0.44
1:A:371:LYS:HB3	4:A:1153:HOH:O	2.16	0.44
1:A:770:ILE:HD13	1:A:785:ILE:CG2	2.46	0.44
1:A:314:ASP:HB3	1:A:754:PRO:O	2.17	0.44
1:A:762:ASN:ND2	1:A:764:ARG:HD3	2.32	0.44
1:A:413:LEU:O	1:A:416:TRP:HB3	2.17	0.44
1:A:665:PRO:CG	1:A:687:GLN:NE2	2.81	0.44
1:A:243:LEU:HB3	1:A:252:LEU:HB3	1.98	0.44
1:A:430:ASN:HB3	4:A:1130:HOH:O	2.18	0.44
1:A:257:GLU:O	1:A:270:HIS:HA	2.18	0.43
1:A:464:VAL:HG21	1:A:500:PHE:CG	2.53	0.43
1:A:598:GLY:HA3	1:A:608:ASN:HA	1.98	0.43
1:A:287:GLU:HG2	1:A:288:LEU:N	2.34	0.43
2:B:1:BGC:H6C1	2:B:2:BGC:HB	1.82	0.43
1:A:271:TRP:HH2	1:A:658:GLU:O	2.00	0.43
1:A:468:ILE:HB	1:A:489:LEU:HD23	2.00	0.43
1:A:359:TRP:HA	1:A:360:PRO:HD3	1.94	0.43
1:A:684:ILE:C	1:A:688:MET:HE2	2.38	0.43
1:A:215:ARG:HB3	1:A:717:ARG:HA	2.00	0.43
1:A:215:ARG:HH11	1:A:215:ARG:HG3	1.84	0.43
1:A:790:SER:CB	1:A:793:THR:HG22	2.48	0.43
1:A:212:PRO:O	1:A:215:ARG:NE	2.47	0.43
1:A:411:ARG:NH1	1:A:411:ARG:HG2	2.34	0.43
1:A:225:GLY:O	1:A:227:LYS:HG3	2.19	0.42
1:A:775:LYS:CE	4:A:947:HOH:O	2.63	0.42
1:A:377:VAL:HG11	1:A:450:MET:SD	2.59	0.42
1:A:392:VAL:O	1:A:393:ASN:CB	2.67	0.42
1:A:790:SER:OG	1:A:793:THR:CG2	2.56	0.42
1:A:764:ARG:O	1:A:765:PHE:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:C	1:A:236:THR:H	2.23	0.42
1:A:763:SER:HB3	1:A:780:PRO:HA	2.01	0.42
1:A:393:ASN:HD22	1:A:616:TRP:HB3	1.84	0.42
1:A:702:LYS:HE3	1:A:703:TYR:CE2	2.55	0.42
1:A:746:SER:C	1:A:748:ARG:H	2.24	0.42
1:A:665:PRO:CG	1:A:684:ILE:HG23	2.49	0.41
1:A:765:PHE:HB3	1:A:771:ASN:OD1	2.20	0.41
1:A:589:HIS:O	1:A:592:GLU:HB2	2.21	0.41
1:A:763:SER:C	1:A:764:ARG:HD2	2.41	0.41
1:A:770:ILE:O	1:A:774:VAL:HG22	2.20	0.41
1:A:209:LEU:HA	1:A:210:PRO:HD3	1.75	0.41
1:A:210:PRO:O	1:A:211:GLN:CB	2.56	0.41
1:A:271:TRP:CH2	1:A:658:GLU:O	2.73	0.41
1:A:337:GLN:NE2	1:A:337:GLN:N	2.54	0.41
1:A:587:SER:HA	1:A:588:PRO:HD3	1.93	0.41
1:A:464:VAL:HG21	1:A:500:PHE:CD2	2.55	0.41
1:A:521:ASP:O	1:A:525:LYS:HG2	2.20	0.41
1:A:779:PRO:HA	1:A:780:PRO:HD3	1.99	0.41
1:A:425:ASN:C	1:A:425:ASN:ND2	2.74	0.41
1:A:411:ARG:HG2	1:A:411:ARG:HH11	1.86	0.40
1:A:614:PHE:HE1	1:A:686:ASN:OD1	2.04	0.40
1:A:632:ASN:HD22	1:A:632:ASN:C	2.24	0.40
1:A:781:GLN:O	1:A:781:GLN:HG2	2.20	0.40
1:A:359:TRP:CE3	1:A:488:TYR:HB2	2.56	0.40
1:A:410:ILE:HA	4:A:875:HOH:O	2.21	0.40
1:A:797:THR:HG23	1:A:800:TRP:CE3	2.56	0.40
1:A:571:LEU:HB3	1:A:580:TYR:CE1	2.56	0.40
1:A:685:LEU:HD23	1:A:688:MET:CE	2.52	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	598/610 (98%)	541 (90%)	39 (6%)	18 (3%)	4 3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	331	PRO
1	A	492	VAL
1	A	631	GLU
1	A	632	ASN
1	A	673	ARG
1	A	235	SER
1	A	671	ASP
1	A	672	GLU
1	A	236	THR
1	A	611	TRP
1	A	701	SER
1	A	211	GLN
1	A	393	ASN
1	A	814	GLN
1	A	384	ALA
1	A	238	PRO
1	A	491	PRO

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	496/503 (99%)	476 (96%)	20 (4%)	31 49

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	CYS
1	A	245	ASN
1	A	266	GLN

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Mol	Chain	Res	Type
1	A	337	GLN
1	A	353	ASP
1	A	390	TYR
1	A	425	ASN
1	A	468	ILE
1	A	476	LEU
1	A	484	PRO
1	A	492	VAL
1	A	613	CYS
1	A	632	ASN
1	A	696	ASP
1	A	712	SER
1	A	739	ARG
1	A	740	PHE
1	A	762	ASN
1	A	764	ARG
1	A	801	ASN

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

Mol	Chain	Res	Type
1	A	211	GLN
1	A	245	ASN
1	A	337	GLN
1	A	350	ASN
1	A	372	ASN
1	A	393	ASN
1	A	425	ASN
1	A	451	GLN
1	A	531	GLN
1	A	632	ASN
1	A	660	GLN
1	A	687	GLN
1	A	722	GLN
1	A	734	GLN
1	A	735	ASN
1	A	737	HIS
1	A	762	ASN
1	A	781	GLN
1	A	795	GLN
1	A	801	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)

4 monosaccharides 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	BGC	B	1	2	12,12,12	1.31	2 (16%)	17,17,17	0.96	1 (5%)
2	BGC	B	2	2	11,11,12	1.25	2 (18%)	15,15,17	0.84	0
2	BGC	B	3	2	11,11,12	1.69	3 (27%)	15,15,17	3.48	5 (33%)
2	BGC	B	4	2	11,11,12	1.05	1 (9%)	15,15,17	0.52	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	BGC	B	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	BGC	B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	B	4	2	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	BGC	O5-C1	3.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	BGC	O5-C5	2.69	1.50	1.44
2	B	2	BGC	O5-C5	2.57	1.48	1.43
2	B	3	BGC	O5-C5	2.31	1.48	1.43
2	B	4	BGC	O5-C1	2.20	1.47	1.43
2	B	3	BGC	O3-C3	-2.18	1.37	1.43
2	B	1	BGC	C1-C2	2.04	1.57	1.52
2	B	2	BGC	C4-C5	2.03	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	BGC	C3-C4-C5	-9.25	93.73	110.24
2	B	3	BGC	C1-O5-C5	7.48	122.32	112.19
2	B	3	BGC	O2-C2-C3	-4.18	101.76	110.14
2	B	3	BGC	O3-C3-C4	-2.97	103.48	110.35
2	B	3	BGC	O5-C1-C2	2.72	114.97	110.77
2	B	1	BGC	C3-C4-C5	-2.04	106.60	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	BGC	C1

All (4) torsion outliers are listed below:

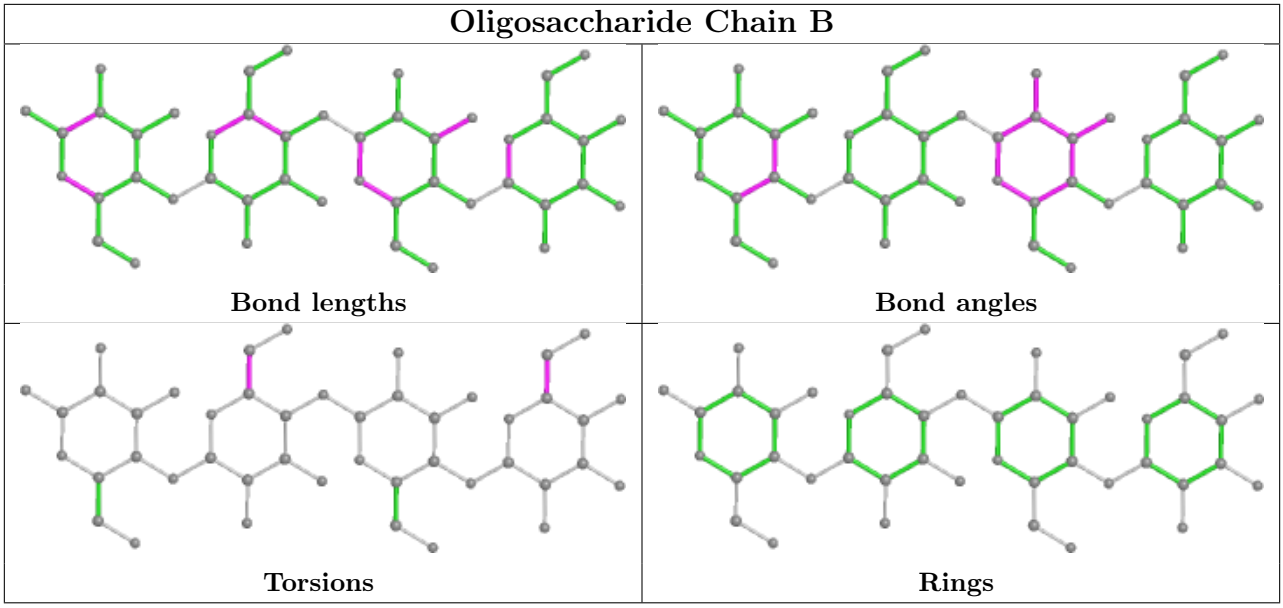
Mol	Chain	Res	Type	Atoms
2	B	4	BGC	O5-C5-C6-O6
2	B	2	BGC	O5-C5-C6-O6
2	B	4	BGC	C4-C5-C6-O6
2	B	2	BGC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	BGC	1	0
2	B	2	BGC	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	219:VAL	C	220:GLY	N	1.15

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	602/610 (98%)	-0.18	9 (1%) 73 72	5, 23, 41, 55	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	GLN	4.9
1	A	255	TYR	3.0
1	A	236	THR	2.9
1	A	590	TYR	2.7
1	A	232	VAL	2.3
1	A	234	ASN	2.3
1	A	291	VAL	2.2
1	A	702	LYS	2.1
1	A	461	ALA	2.1

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)

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, 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	B-factors(Å^2)	Q<0.9
2	BGC	B	3	11/12	0.60	0.29	42,46,51,51	0
2	BGC	B	4	11/12	0.70	0.20	53,53,54,56	0
2	BGC	B	2	11/12	0.80	0.15	30,32,34,40	0

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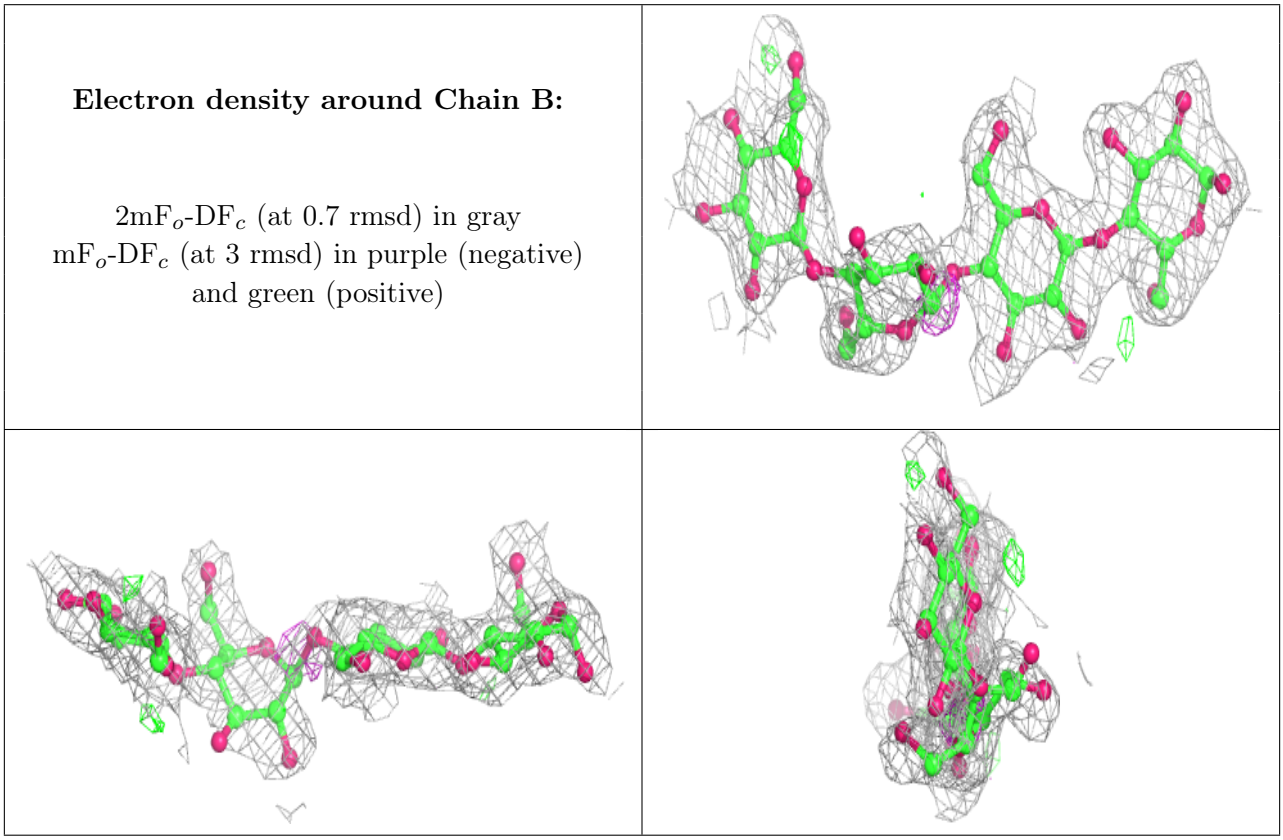
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	B	1	12/12	0.87	0.14	26,28,29,31	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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, 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	B-factors(Å^2)	Q<0.9
3	CA	A	818	1/1	0.99	0.11	19,19,19,19	0
3	CA	A	819	1/1	0.99	0.08	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.