Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 08:05 PM EDT

PDB ID	:	2EAD
Title	:	Crystal structure of 1,2-a-L-fucosidase from Bifidobacterium bifidum in complex with substrate
Authors	:	Nagae, M.; Tsuchiya, A.; Katayama, T.; Yamamoto, K.; Wakatsuki, S.; Kato, R.
Deposited on	:	2007-01-31
Resolution	:	1.89 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:

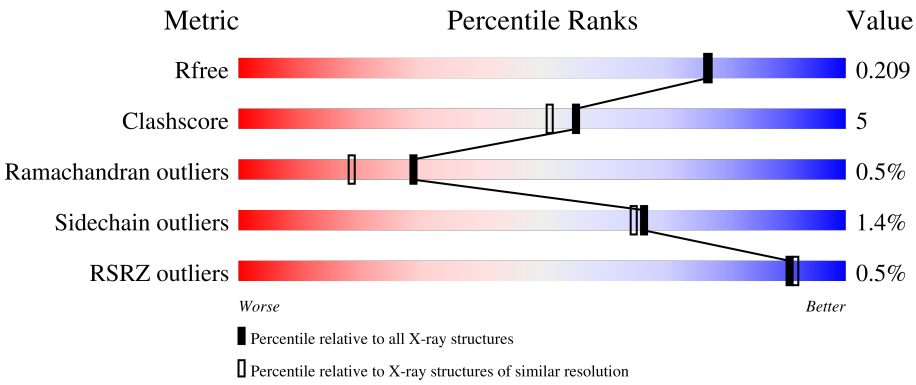
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	899	% 88% 10% ••
1	B	899	89% 8% ••
2	C	3	67% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15308 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.

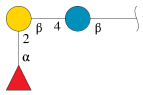
- Molecule 1 is a protein called Alpha-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	886	6744	4197	1166	1366	15	0	0	0
1	B	884	6732	4191	1164	1362	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q6JV24
A	566	ALA	GLU	engineered mutation	UNP Q6JV24
B	0	MET	-	initiating methionine	UNP Q6JV24
B	566	ALA	GLU	engineered mutation	UNP Q6JV24

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

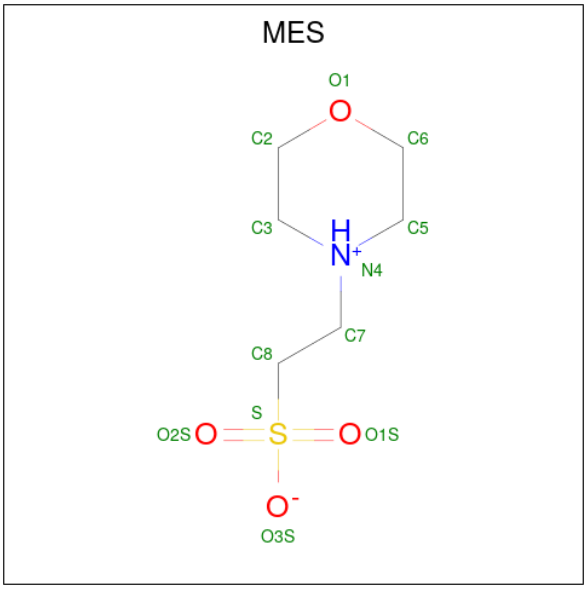


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	3	33	18	15	0	0	0

- 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
3	B	2	2	2	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	12	6	1	4	1	0	0

- Molecule 5 is water.

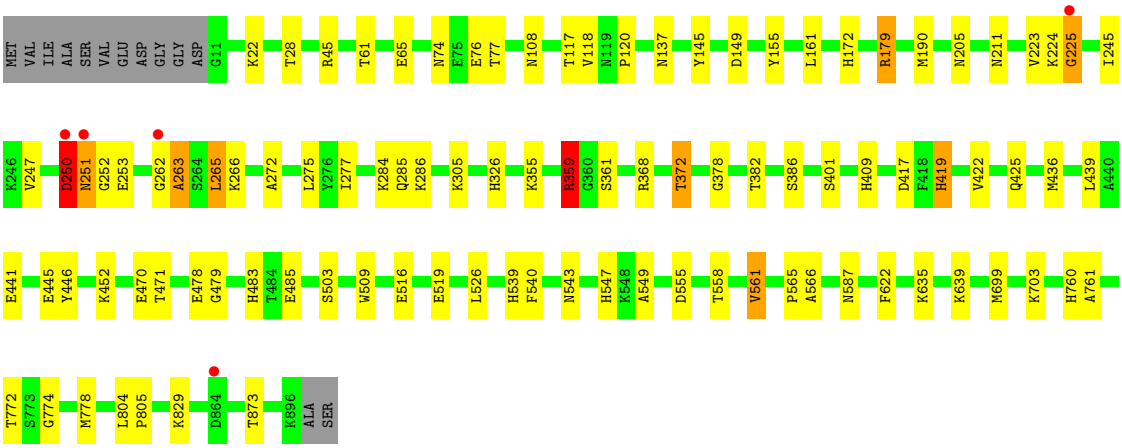
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	831	831	831	0	0
5	B	952	Total 952	O 952	0	0

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.

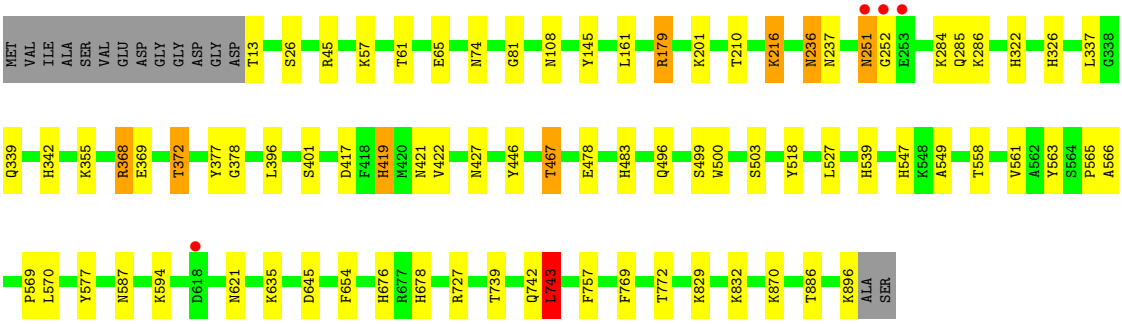
• Molecule 1: Alpha-fucosidase

Chain A:



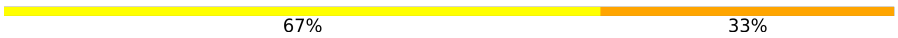
• Molecule 1: Alpha-fucosidase

Chain B:



• Molecule 2: alpha-L-fucopyranose-(1-2)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.45Å 72.74Å 129.21Å 90.00° 96.68° 90.00°	Depositor
Resolution (Å)	37.60 – 1.89 37.60 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.9 (37.60-1.89) 96.9 (37.60-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.159 , 0.210 0.160 , 0.209	Depositor DCC
R_{free} test set	6320 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15308	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 56.89 % 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 2.5631e-05. 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, 0.333 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: MES, BGC, GAL, FUC, 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	0.71	0/6890	0.72	5/9372 (0.1%)
1	B	0.72	0/6878	0.73	6/9356 (0.1%)
All	All	0.71	0/13768	0.72	11/18728 (0.1%)

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	179	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	179	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	A	179	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	743	LEU	CA-CB-CG	-7.69	97.61	115.30
1	B	368	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	179	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	368	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	359	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	252	GLY	N-CA-C	-6.04	98.01	113.10
1	A	225	GLY	N-CA-C	-5.87	98.42	113.10
1	A	265	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ASP	Peptide
1	B	251	ASN	Peptide

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	6744	0	6425	73	0
1	B	6732	0	6418	64	0
2	C	33	0	30	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	B	12	0	12	0	0
5	A	831	0	0	10	0
5	B	952	0	0	18	0
All	All	15308	0	12885	134	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 (134) 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:13:THR:N	5:B:1704:HOH:O	1.88	1.04
1:A:137:ASN:HD22	1:A:211:ASN:HD22	1.14	0.93
1:A:483:HIS:HD2	1:A:503:SER:H	1.12	0.93
1:A:262:GLY:HA3	1:A:263:ALA:HB2	1.51	0.93
1:B:355:LYS:HD3	5:B:1805:HOH:O	1.69	0.91
1:B:566:ALA:H	1:B:676:HIS:HE1	1.17	0.86
1:A:117:THR:HG23	5:A:1604:HOH:O	1.75	0.85
1:B:499:SER:HB3	1:B:570:LEU:HD21	1.58	0.85
1:A:471:THR:HG21	5:A:1287:HOH:O	1.76	0.84
1:B:417:ASP:OD1	1:B:419:HIS:HD2	1.64	0.81
1:B:108:ASN:HD21	1:B:561:VAL:H	1.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLY:HA3	1:A:263:ALA:CB	2.10	0.80
1:B:372:THR:HG23	5:B:926:HOH:O	1.83	0.78
1:A:368:ARG:O	1:A:372:THR:HB	1.84	0.77
1:B:483:HIS:HD2	1:B:503:SER:H	1.30	0.77
1:A:372:THR:HG23	5:A:935:HOH:O	1.85	0.75
1:B:566:ALA:H	1:B:676:HIS:CE1	2.04	0.75
1:A:108:ASN:HD21	1:A:561:VAL:H	1.33	0.74
1:A:74:ASN:HD21	1:A:401:SER:H	1.36	0.74
1:A:417:ASP:OD1	1:A:419:HIS:HD2	1.70	0.73
1:A:483:HIS:CD2	1:A:503:SER:H	2.02	0.73
1:B:74:ASN:HD21	1:B:401:SER:H	1.36	0.72
1:B:285:GLN:HE22	1:B:446:TYR:HA	1.53	0.71
1:B:81:GLY:H	1:B:236:ASN:HD21	1.37	0.71
1:A:452:LYS:HE3	1:A:470:GLU:O	1.91	0.69
1:A:372:THR:CG2	5:A:935:HOH:O	2.41	0.68
1:B:355:LYS:CD	5:B:1805:HOH:O	2.37	0.68
1:B:419:HIS:HE1	2:C:2:GAL:O3	1.77	0.67
1:B:81:GLY:H	1:B:236:ASN:ND2	1.92	0.66
1:A:409:HIS:HE1	1:A:485:GLU:OE2	1.79	0.66
1:B:421:ASN:OD1	1:B:577:TYR:OH	2.10	0.65
1:A:262:GLY:CA	1:A:263:ALA:CB	2.77	0.63
1:A:205:ASN:HD22	1:A:266:LYS:HE2	1.65	0.62
1:A:65:GLU:O	1:A:179:ARG:NH2	2.30	0.61
1:A:445:GLU:OE1	1:B:870:LYS:NZ	2.34	0.61
1:A:355:LYS:HE3	5:A:1372:HOH:O	2.01	0.61
1:A:251:ASN:C	1:A:253:GLU:H	2.05	0.60
1:A:245:ILE:HG12	1:A:277:ILE:HG12	1.81	0.60
1:B:108:ASN:ND2	1:B:561:VAL:H	2.00	0.59
1:B:26:SER:HA	1:B:45:ARG:HD3	1.83	0.59
1:A:161:LEU:O	1:A:326:HIS:HE1	1.84	0.59
1:A:549:ALA:HB2	1:A:558:THR:HG23	1.85	0.59
1:B:161:LEU:O	1:B:326:HIS:HE1	1.86	0.59
1:A:587:ASN:HD22	1:A:635:LYS:NZ	2.00	0.59
1:A:224:LYS:O	1:A:225:GLY:C	2.42	0.58
1:A:539:HIS:HD2	5:A:1434:HOH:O	1.86	0.58
1:B:368:ARG:O	1:B:372:THR:HB	2.03	0.58
1:B:587:ASN:HD22	1:B:635:LYS:NZ	2.02	0.57
1:B:467:THR:HG22	5:B:1018:HOH:O	2.03	0.57
1:A:382:THR:HG22	1:A:439:LEU:HD23	1.86	0.57
1:B:539:HIS:HD2	5:B:1248:HOH:O	1.88	0.57
1:A:108:ASN:ND2	1:A:561:VAL:H	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:SER:O	1:A:439:LEU:HG	2.05	0.56
1:A:478:GLU:OE1	1:A:539:HIS:HE1	1.88	0.56
1:A:587:ASN:HD22	1:A:635:LYS:HZ1	1.52	0.56
1:A:285:GLN:HE22	1:A:446:TYR:HA	1.69	0.56
1:B:467:THR:HG21	5:B:1227:HOH:O	2.05	0.56
1:A:251:ASN:O	1:A:253:GLU:N	2.39	0.56
1:B:563:TYR:CD1	1:B:570:LEU:HD23	2.43	0.54
1:B:108:ASN:ND2	1:B:561:VAL:HG23	2.22	0.54
1:B:478:GLU:OE1	1:B:539:HIS:HE1	1.91	0.54
1:A:359:ARG:NH2	1:A:361:SER:OG	2.41	0.54
1:B:483:HIS:CD2	1:B:503:SER:H	2.18	0.54
1:A:74:ASN:ND2	1:A:401:SER:H	2.05	0.54
1:A:804:LEU:HD12	1:A:805:PRO:HD2	1.90	0.54
1:B:496:GLN:NE2	5:B:1853:HOH:O	2.40	0.53
1:A:137:ASN:ND2	1:A:211:ASN:HD22	1.94	0.53
1:B:74:ASN:ND2	1:B:401:SER:H	2.05	0.52
1:B:417:ASP:OD1	1:B:419:HIS:CD2	2.54	0.52
1:A:284:LYS:HD3	1:A:286:LYS:HD3	1.91	0.52
1:A:479:GLY:HA3	1:A:540:PHE:HB2	1.90	0.51
1:A:419:HIS:HE1	5:A:1445:HOH:O	1.93	0.51
1:B:145:TYR:OH	1:B:179:ARG:HD3	2.10	0.51
1:B:57:LYS:HD2	5:B:1699:HOH:O	2.11	0.50
1:A:483:HIS:HD2	1:A:503:SER:N	1.94	0.50
1:A:108:ASN:ND2	1:A:561:VAL:HG23	2.27	0.49
1:A:409:HIS:HD2	5:A:1189:HOH:O	1.96	0.49
1:B:210:THR:OG1	1:B:216:LYS:HE3	2.13	0.48
1:A:22:LYS:HD3	5:A:1679:HOH:O	2.13	0.48
1:B:594:LYS:NZ	5:B:1777:HOH:O	2.41	0.48
1:B:284:LYS:HE3	1:B:286:LYS:HD3	1.96	0.48
1:A:699:MET:HG3	1:A:703:LYS:HE3	1.95	0.48
1:A:28:THR:O	1:A:45:ARG:NH1	2.47	0.47
1:A:190:MET:HB3	1:A:277:ILE:HB	1.96	0.47
1:B:621:ASN:HA	5:B:1428:HOH:O	2.15	0.47
1:A:565:PRO:HA	1:A:566:ALA:HA	1.70	0.46
1:A:149:ASP:OD1	1:A:172:HIS:HE1	1.99	0.46
1:A:247:VAL:HG22	1:A:275:LEU:HD22	1.97	0.46
1:A:305:LYS:HE3	1:B:886:THR:HA	1.98	0.45
1:B:65:GLU:O	1:B:179:ARG:NH2	2.43	0.45
1:B:739:THR:HA	1:B:742:GLN:HE21	1.82	0.45
1:A:223:VAL:CG1	1:A:265:LEU:HD13	2.46	0.45
1:B:337:LEU:O	1:B:368:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:NH2	5:B:1718:HOH:O	2.50	0.45
1:B:342:HIS:HE1	5:B:1355:HOH:O	1.99	0.44
1:A:117:THR:CG2	5:A:1604:HOH:O	2.46	0.44
1:A:425:GLN:HG2	1:A:509:TRP:CD1	2.53	0.44
1:B:339:GLN:HB2	1:B:369:GLU:HA	1.98	0.44
1:A:543:ASN:HD22	1:A:622:PHE:HE2	1.66	0.44
1:A:774:GLY:O	1:A:778:MET:HG3	2.18	0.44
1:A:829:LYS:HA	1:A:829:LYS:HD3	1.77	0.44
1:B:342:HIS:HD2	5:B:976:HOH:O	2.00	0.44
1:A:441:GLU:OE2	1:B:870:LYS:NZ	2.47	0.44
1:B:396:LEU:HD21	1:B:419:HIS:HB2	2.00	0.44
1:A:760:HIS:H	1:A:761:ALA:HA	1.81	0.43
1:B:569:PRO:HG2	1:B:654:PHE:HZ	1.82	0.43
1:A:155:TYR:CD2	1:A:155:TYR:C	2.91	0.43
1:B:378:GLY:HA3	1:B:772:THR:OG1	2.19	0.43
1:B:549:ALA:HB2	1:B:558:THR:HG23	2.00	0.43
1:A:516:GLU:HA	1:A:519:GLU:HB2	2.00	0.43
1:A:760:HIS:N	1:A:761:ALA:HA	2.34	0.43
1:B:565:PRO:HA	1:B:566:ALA:HA	1.75	0.43
1:A:555:ASP:O	1:A:639:LYS:HE2	2.19	0.42
1:B:829:LYS:HD3	1:B:829:LYS:HA	1.70	0.42
1:A:205:ASN:ND2	1:A:266:LYS:HE2	2.31	0.42
1:B:727:ARG:HB3	1:B:743:LEU:HD22	2.00	0.42
1:A:436:MET:HB3	1:A:439:LEU:HD22	2.01	0.42
1:B:322:HIS:HD2	5:B:917:HOH:O	2.02	0.42
1:B:518:TYR:CE1	1:B:527:LEU:HB2	2.54	0.42
1:B:832:LYS:HE3	5:B:1833:HOH:O	2.19	0.42
1:B:326:HIS:HD2	5:B:1090:HOH:O	2.02	0.42
1:B:676:HIS:CE1	1:B:678:HIS:HB2	2.55	0.41
1:A:378:GLY:HA3	1:A:772:THR:OG1	2.20	0.41
1:B:201:LYS:HA	1:B:201:LYS:HD2	1.93	0.41
1:A:118:VAL:O	1:A:120:PRO:HD3	2.21	0.41
1:B:368:ARG:HD3	1:B:368:ARG:HA	1.86	0.41
1:B:427:ASN:HA	1:B:769:PHE:CD2	2.56	0.41
1:A:223:VAL:HG13	1:A:265:LEU:HD13	2.01	0.41
1:A:250:ASP:OD2	1:A:272:ALA:HB3	2.19	0.41
1:B:896:LYS:HB2	1:B:896:LYS:HE2	1.80	0.41
1:A:76:GLU:HG3	1:A:77:THR:HG23	2.03	0.41
1:A:409:HIS:CE1	1:A:485:GLU:OE2	2.66	0.41
1:A:145:TYR:OH	1:A:179:ARG:HD3	2.21	0.40
1:B:326:HIS:CD2	5:B:1090:HOH:O	2.75	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	884/899 (98%)	855 (97%)	24 (3%)	5 (1%)	25	15
1	B	882/899 (98%)	852 (97%)	27 (3%)	3 (0%)	41	31
All	All	1766/1798 (98%)	1707 (97%)	51 (3%)	8 (0%)	29	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ALA
1	A	422	VAL
1	B	422	VAL
1	A	252	GLY
1	A	561	VAL
1	A	251	ASN
1	B	251	ASN
1	B	500	TRP

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	702/711 (99%)	694 (99%)	8 (1%)	73	73
1	B	701/711 (99%)	689 (98%)	12 (2%)	60	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1403/1422 (99%)	1383 (99%)	20 (1%)	67 65

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

Mol	Chain	Res	Type
1	A	61	THR
1	A	250	ASP
1	A	359	ARG
1	A	372	THR
1	A	419	HIS
1	A	526	LEU
1	A	547	HIS
1	A	873	THR
1	B	61	THR
1	B	216	LYS
1	B	236	ASN
1	B	237	ASN
1	B	372	THR
1	B	377	TYR
1	B	419	HIS
1	B	467	THR
1	B	547	HIS
1	B	645	ASP
1	B	743	LEU
1	B	757	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	74	ASN
1	A	93	ASN
1	A	108	ASN
1	A	134	ASN
1	A	137	ASN
1	A	285	GLN
1	A	326	HIS
1	A	397	GLN
1	A	409	HIS
1	A	419	HIS
1	A	483	HIS

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Mol	Chain	Res	Type
1	A	513	ASN
1	A	539	HIS
1	A	543	ASN
1	A	587	ASN
1	A	626	ASN
1	A	671	GLN
1	A	674	ASN
1	A	764	GLN
1	B	74	ASN
1	B	108	ASN
1	B	134	ASN
1	B	148	ASN
1	B	172	HIS
1	B	236	ASN
1	B	237	ASN
1	B	251	ASN
1	B	285	GLN
1	B	322	HIS
1	B	326	HIS
1	B	342	HIS
1	B	397	GLN
1	B	419	HIS
1	B	483	HIS
1	B	513	ASN
1	B	539	HIS
1	B	587	ASN
1	B	676	HIS
1	B	742	GLN
1	B	764	GLN
1	B	841	ASN
1	B	857	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)

3 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	C	1	2	12,12,12	0.54	0	17,17,17	1.00	1 (5%)
2	GAL	C	2	2	11,11,12	1.31	1 (9%)	15,15,17	1.83	3 (20%)
2	FUC	C	3	2	10,10,11	0.69	0	14,14,16	1.32	3 (21%)

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	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GAL	O2-C2	-3.54	1.35	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GAL	C1-O5-C5	4.64	118.48	112.19
2	C	2	GAL	O2-C2-C1	3.96	117.25	109.15
2	C	3	FUC	C1-O5-C5	3.23	120.11	112.78
2	C	2	GAL	O2-C2-C3	2.70	115.54	110.14
2	C	3	FUC	C1-C2-C3	-2.65	106.41	109.67
2	C	1	BGC	O5-C5-C6	2.17	111.83	106.44
2	C	3	FUC	O2-C2-C3	2.02	114.18	110.14

There are no chirality outliers.

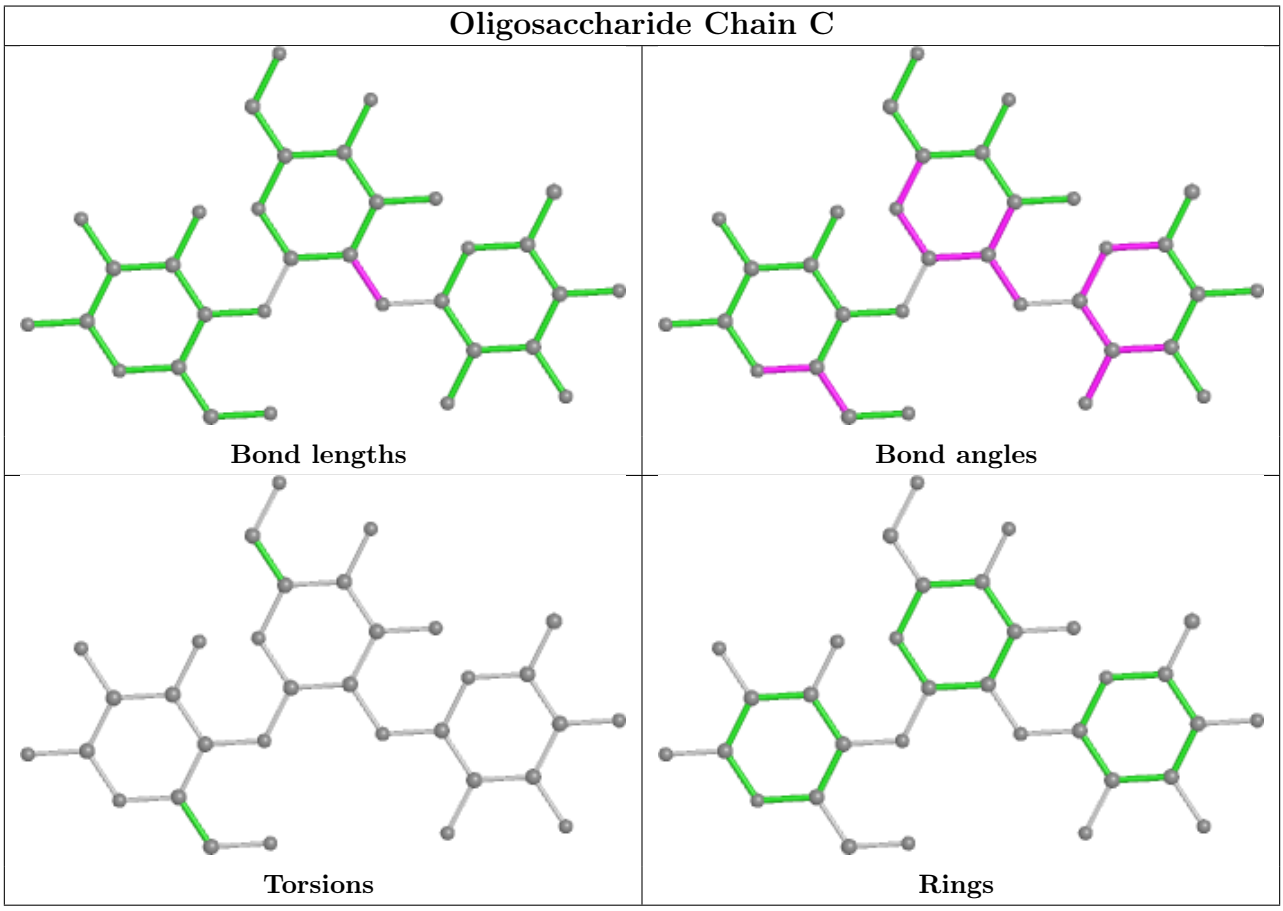
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GAL	1	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 5 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	MES	B	904	-	12,12,12	1.72	1 (8%)	14,16,16	6.99	7 (50%)

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	MES	B	904	-	-	1/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	904	MES	C8-S	-5.31	1.70	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	904	MES	O1S-S-C8	-18.41	84.74	106.92
4	B	904	MES	O3S-S-C8	-12.82	85.03	105.77
4	B	904	MES	O2S-S-C8	-9.73	95.20	106.92
4	B	904	MES	O3S-S-O1S	5.50	124.71	111.27
4	B	904	MES	C5-N4-C3	4.50	118.96	108.83
4	B	904	MES	C7-N4-C5	4.00	121.47	111.23
4	B	904	MES	C7-N4-C3	3.25	119.55	111.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	904	MES	C8-C7-N4-C3

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	886/899 (98%)	-0.39	5 (0%)	89	90	10, 18, 32, 52	0
1	B	884/899 (98%)	-0.52	4 (0%)	91	92	10, 17, 26, 42	0
All	All	1770/1798 (98%)	-0.46	9 (0%)	91	92	10, 17, 29, 52	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	GLY	4.4
1	A	251	ASN	4.3
1	A	250	ASP	3.7
1	B	252	GLY	3.7
1	B	251	ASN	3.3
1	A	262	GLY	3.0
1	B	253	GLU	3.0
1	A	864	ASP	2.8
1	B	618	ASP	2.8

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	C	1	12/12	0.84	0.27	30,40,42,44	0

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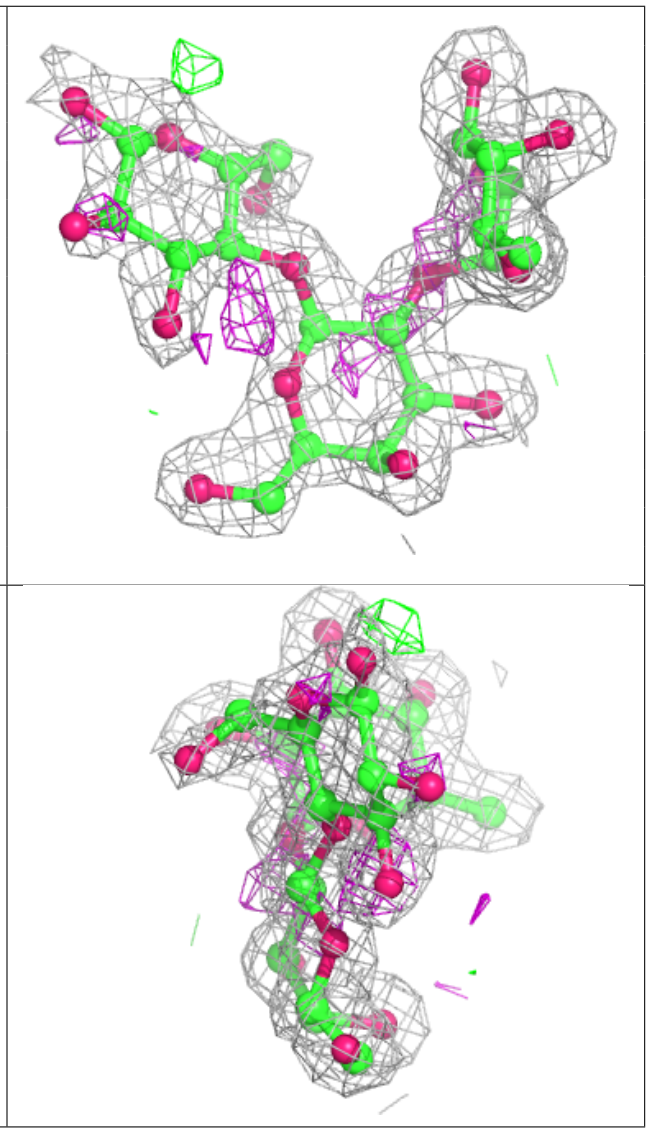
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	C	2	11/12	0.92	0.16	21,23,26,26	0
2	FUC	C	3	10/11	0.94	0.09	16,18,20,20	0

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.

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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
4	MES	B	904	12/12	0.92	0.20	31,41,44,46	0
3	CA	B	903	1/1	0.99	0.04	20,20,20,20	0
3	CA	A	899	1/1	0.99	0.04	24,24,24,24	0
3	CA	A	900	1/1	1.00	0.04	13,13,13,13	0
3	CA	B	902	1/1	1.00	0.05	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.