



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:17 AM BST

PDB ID : 1X38
Title : crystal structure of barley beta-D-glucan glucohydrolase isoenzyme exo1 in complex with gluco-phenylimidazole
Authors : Hrmova, M.; Streltsov, V.A.; Smith, B.J.; Vasella, A.; Varghese, J.N.; Fincher, G.B.
Deposited on : 2005-05-02
Resolution : 1.70 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 ⓘ symbol.

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
buster-report : 1.1.7 (2018)
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

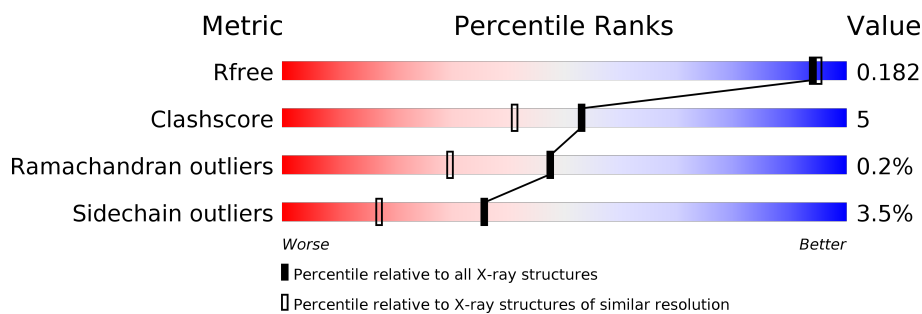
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	602	 91% 8%
2	B	3	 33% 33% 33%
3	C	7	 71% 29%
4	D	5	 60% 40%

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 beta-D-glucan exohydrolase isoenzyme ExoI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4566	2891	787	862	26			

There is a discrepancy between the modelled and reference sequences:

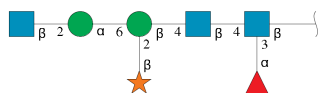
Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	ASN	SEE REMARK 999	GB 4566505

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



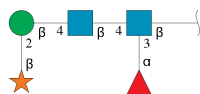
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-xylopyranose-(1-2)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



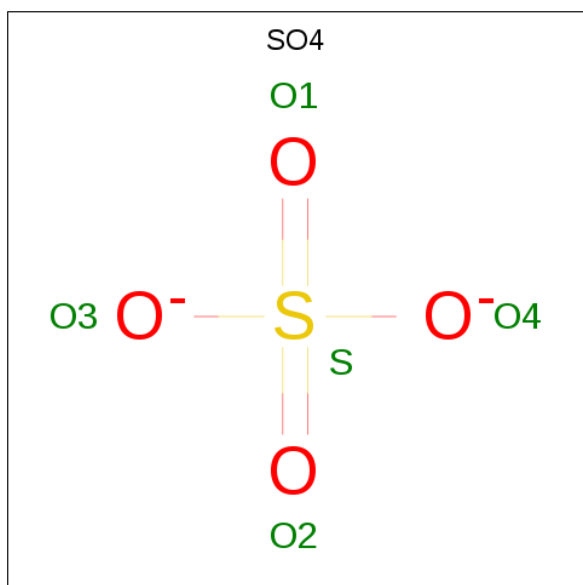
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	0	0	0
			83	47	3	33			

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



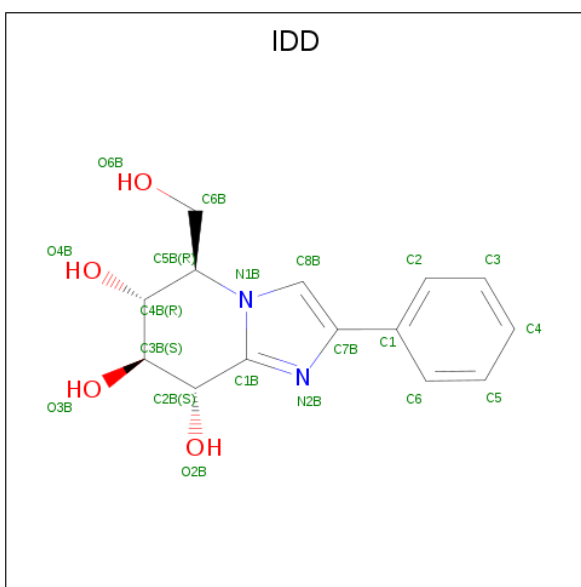
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			58	33	2	23			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (5R,6R,7S,8S)-5-(HYDROXYMETHYL)-2-PHENYL-5,6,7,8-TETRAHYDRO IMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (three-letter code: IDD) (formula: C₁₄H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			7	3	4		
7	A	1	Total	C	O	0	1
			12	6	6		

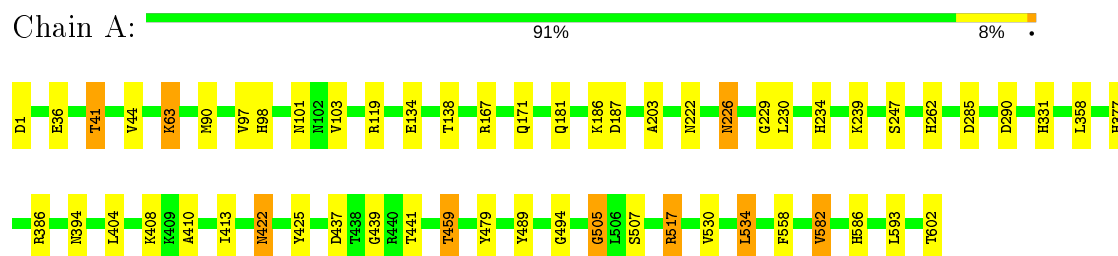
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	931	Total 931	O 931	0	0

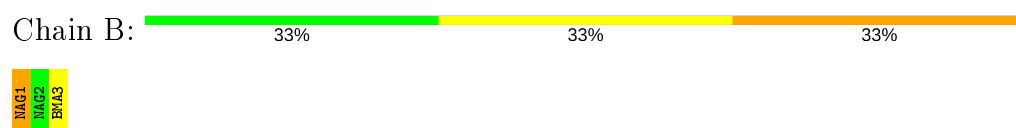
3 Residue-property plots

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. 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. 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.

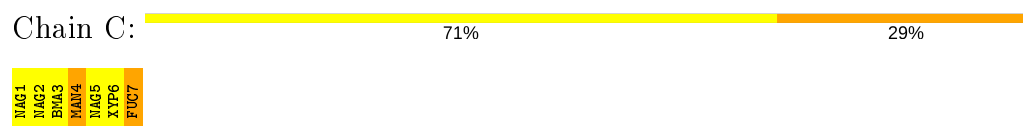
- Molecule 1: beta-D-glucan exohydrolase isoenzyme ExoI



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[beta-D-xylopyranose-(1-2)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.56 Å 100.56 Å 182.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.30 – 1.70 34.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.30-1.70) 99.8 (34.30-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.2.0011	Depositor
R, R_{free}	0.160 , 0.183 0.158 , 0.182	Depositor DCC
R_{free} test set	5168 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5721	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, BMA, NAG, FUC, IDD, MAN, SO4

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	0.54	0/4663	0.61	0/6334

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4566	0	4550	49	1
2	B	39	0	34	1	0
3	C	83	0	63	2	0
4	D	58	0	42	0	0
5	A	5	0	0	0	0
6	A	20	0	16	0	0
7	A	19	0	22	1	0
8	A	931	0	0	11	1
All	All	5721	0	4727	51	1

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 (51) 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:517:ARG:HB2	1:A:517:ARG:NH1	1.41	1.34
1:A:517:ARG:CB	1:A:517:ARG:HH11	1.47	1.27
1:A:41:THR:HG22	1:A:44:VAL:H	1.39	0.86
1:A:394:ASN:HD21	1:A:404:LEU:H	1.18	0.86
1:A:410:ALA:O	1:A:459:THR:HB	1.78	0.83
1:A:41:THR:HG21	8:A:6671:HOH:O	1.84	0.78
1:A:97:VAL:H	1:A:101:ASN:HD21	1.34	0.75
1:A:181:GLN:HE21	1:A:203:ALA:H	1.37	0.72
1:A:422:ASN:HD21	1:A:439:GLY:H	1.37	0.72
1:A:167:ARG:HH11	1:A:171:GLN:HE22	1.39	0.70
1:A:239:LYS:HE2	8:A:6936:HOH:O	1.91	0.70
1:A:505:GLY:N	8:A:6932:HOH:O	2.28	0.65
1:A:422:ASN:ND2	1:A:439:GLY:H	1.95	0.65
1:A:262:HIS:HE1	1:A:285:ASP:H	1.43	0.64
1:A:97:VAL:H	1:A:101:ASN:ND2	1.96	0.63
1:A:119:ARG:HE	7:A:2002[A]:GOL:H2	1.63	0.62
1:A:517:ARG:HB2	1:A:517:ARG:HH11	0.58	0.62
8:A:6766:HOH:O	3:C:7:FUC:H63	2.01	0.60
1:A:479:TYR:HB3	1:A:517:ARG:HH12	1.68	0.59
1:A:234:HIS:HE1	8:A:6196:HOH:O	1.86	0.58
1:A:386:ARG:NH1	8:A:6930:HOH:O	2.33	0.57
1:A:408:LYS:O	1:A:459:THR:HG21	2.04	0.57
1:A:167:ARG:NH1	1:A:171:GLN:HE22	2.02	0.56
1:A:167:ARG:HH11	1:A:171:GLN:NE2	2.01	0.56
1:A:234:HIS:HD2	8:A:6027:HOH:O	1.88	0.56
1:A:262:HIS:CE1	1:A:285:ASP:H	2.23	0.56
1:A:226:ASN:ND2	1:A:229:GLY:H	2.03	0.55
1:A:331:HIS:HD2	8:A:6340:HOH:O	1.90	0.55
1:A:507:SER:OG	8:A:6932:HOH:O	2.18	0.54
1:A:582:VAL:HG11	1:A:593:LEU:HB3	1.89	0.54
1:A:181:GLN:HE22	1:A:247:SER:H	1.57	0.53
1:A:186:LYS:HD3	1:A:186:LYS:H	1.75	0.52
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.94	0.51
1:A:530:VAL:HG13	1:A:534:LEU:HD22	1.92	0.51
1:A:41:THR:CG2	1:A:44:VAL:H	2.19	0.50
1:A:422:ASN:C	1:A:422:ASN:HD22	2.16	0.49
1:A:222:ASN:HB2	2:B:1:NAG:H82	1.96	0.48
1:A:226:ASN:C	1:A:226:ASN:HD22	2.19	0.46
1:A:437:ASP:HB3	1:A:441:THR:HG21	1.98	0.46
1:A:186:LYS:N	1:A:186:LYS:HD3	2.30	0.46
1:A:422:ASN:ND2	1:A:425:TYR:H	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:NAG:H82	3:C:4:MAN:O3	2.18	0.43
1:A:602:THR:HG21	8:A:6307:HOH:O	2.18	0.43
1:A:489:TYR:CD2	1:A:494:GLY:HA3	2.55	0.42
1:A:181:GLN:HE22	1:A:247:SER:N	2.18	0.42
1:A:63:LYS:N	1:A:63:LYS:HE3	2.35	0.42
1:A:558:PHE:HB2	8:A:6652:HOH:O	2.21	0.41
1:A:413:ILE:HG21	1:A:479:TYR:CZ	2.55	0.41
1:A:63:LYS:H	1:A:63:LYS:HE3	1.86	0.41
1:A:103:VAL:HG21	1:A:138:THR:HG21	2.03	0.40
1:A:186:LYS:H	1:A:186:LYS:CD	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LYS:NZ	8:A:6243:HOH:O[3_554]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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	600/602 (100%)	584 (97%)	15 (2%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	GLY

5.3.2 Protein sidechains ⓘ

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	485/485 (100%)	468 (96%)	17 (4%)	36	17

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	36	GLU
1	A	41	THR
1	A	63	LYS
1	A	90	MET
1	A	98	HIS
1	A	187	ASP
1	A	226	ASN
1	A	230	LEU
1	A	290	ASP
1	A	358	LEU
1	A	422	ASN
1	A	459	THR
1	A	517	ARG
1	A	534	LEU
1	A	582	VAL
1	A	586	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	112	ASN
1	A	171	GLN
1	A	181	GLN
1	A	199	ASN
1	A	226	ASN
1	A	234	HIS
1	A	240	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	257	ASN
1	A	262	HIS
1	A	265	GLN
1	A	331	HIS
1	A	333	ASN
1	A	377	HIS
1	A	394	ASN
1	A	422	ASN
1	A	581	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

15 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	NAG	B	1	1,2	14,14,15	0.64	0	17,19,21	1.11	2 (11%)
2	NAG	B	2	2	14,14,15	0.50	0	17,19,21	0.83	0
2	BMA	B	3	2	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
3	NAG	C	2	3	14,14,15	0.57	0	17,19,21	1.04	0
3	BMA	C	3	3	11,11,12	0.57	0	15,15,17	0.76	1 (6%)
3	MAN	C	4	3	11,11,12	0.56	0	15,15,17	0.88	1 (6%)
3	NAG	C	5	3	14,14,15	0.42	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYP	C	6	3	9,9,10	1.21	1 (11%)	10,12,14	0.73	0
3	FUC	C	7	3	10,10,11	0.61	0	14,14,16	0.84	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.57	0	17,19,21	0.83	0
4	NAG	D	2	4	14,14,15	0.49	0	17,19,21	0.60	0
4	BMA	D	3	4	11,11,12	0.55	0	15,15,17	0.79	1 (6%)
4	XYP	D	4	4	9,9,10	1.20	1 (11%)	10,12,14	1.03	1 (10%)
4	FUC	D	5	4	10,10,11	0.58	0	14,14,16	0.72	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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	XYP	C	6	3	-	-	0/1/1/1
3	FUC	C	7	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	XYP	D	4	4	-	-	0/1/1/1
4	FUC	D	5	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4	XYP	O5-C1	-3.23	1.36	1.42
3	C	6	XYP	O5-C1	-3.19	1.36	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4	XYP	C5-O5-C1	2.89	115.96	111.52
2	B	1	NAG	C1-O5-C5	2.76	115.93	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	NAG	C1-O5-C5	2.70	115.85	112.19
2	B	1	NAG	O5-C1-C2	-2.55	107.27	111.29
3	C	7	FUC	O5-C5-C6	2.40	112.49	107.33
2	B	3	BMA	C3-C4-C5	2.20	114.17	110.24
3	C	4	MAN	C1-O5-C5	2.15	115.10	112.19
4	D	3	BMA	O5-C5-C6	2.10	110.49	107.20
3	C	3	BMA	O5-C5-C6	2.05	110.42	107.20
3	C	1	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

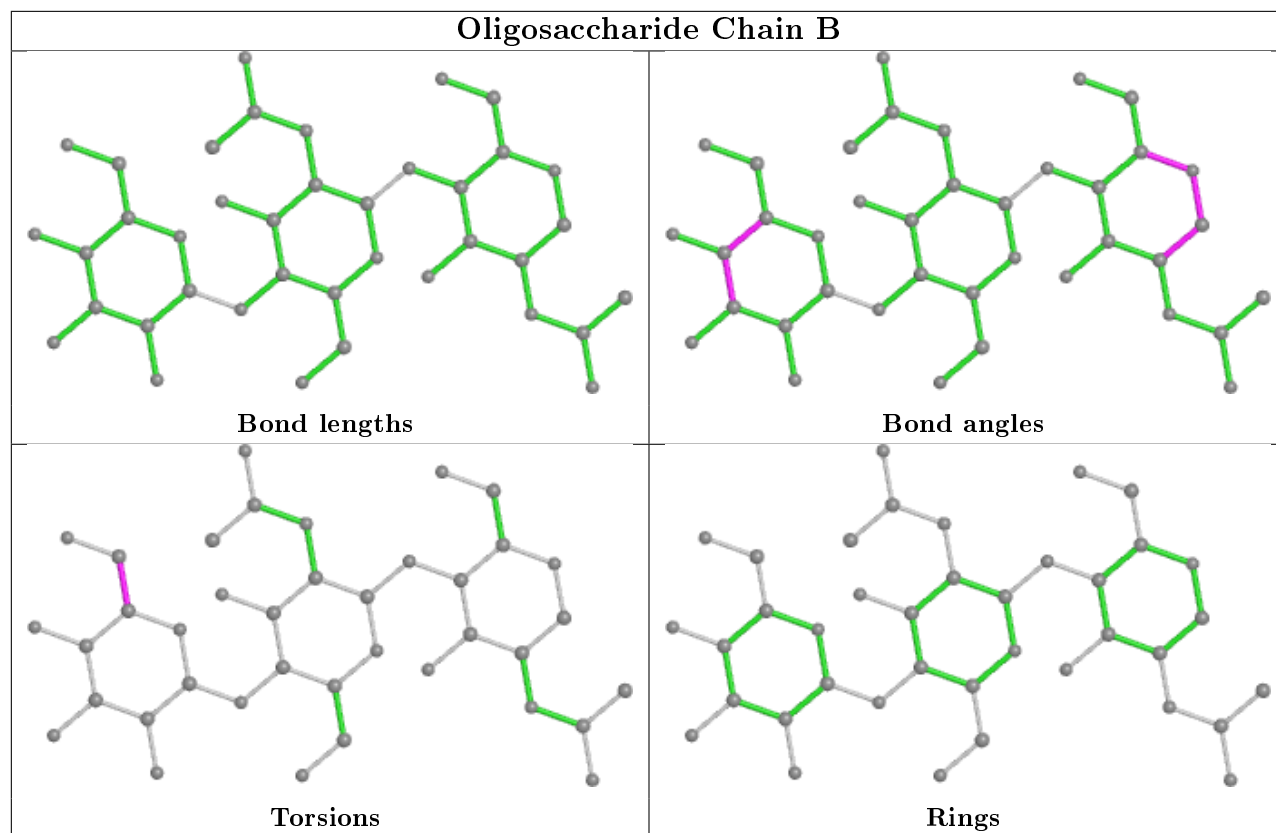
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	B	3	BMA	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

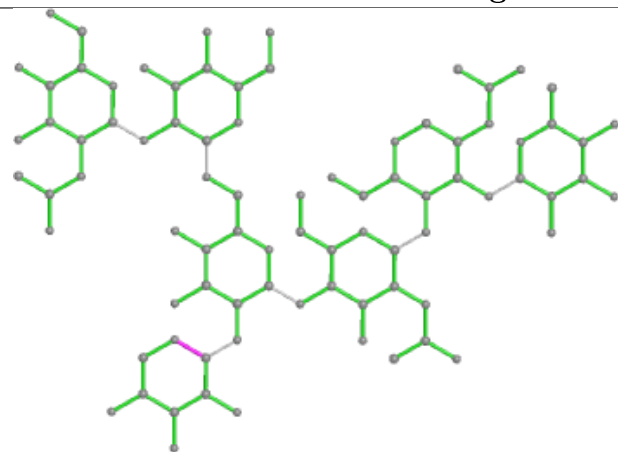
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MAN	1	0
2	B	1	NAG	1	0
3	C	7	FUC	1	0
3	C	2	NAG	1	0

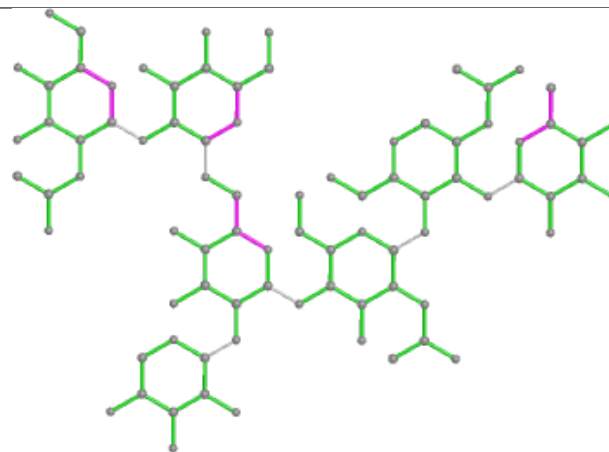
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



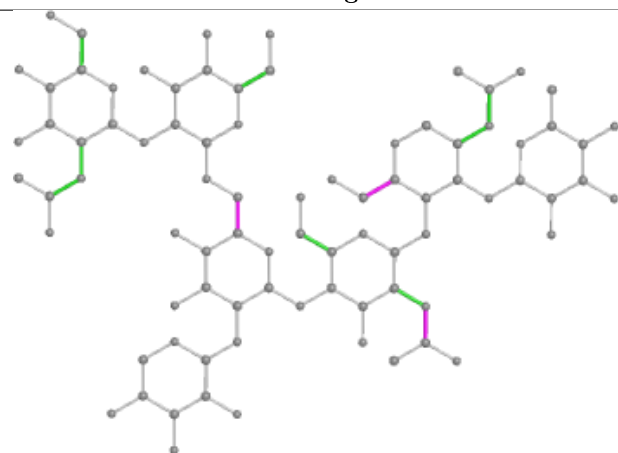
Oligosaccharide Chain C



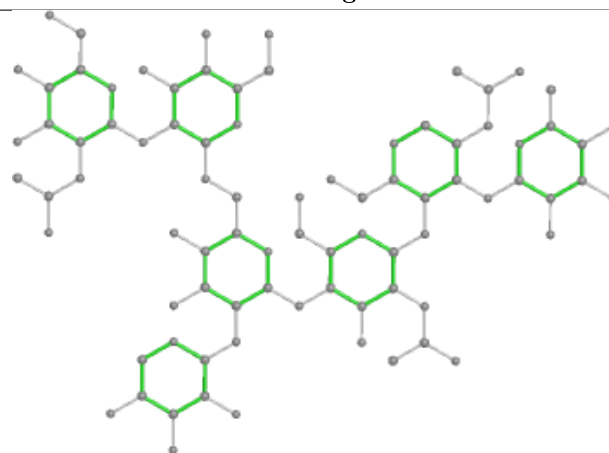
Bond lengths



Bond angles

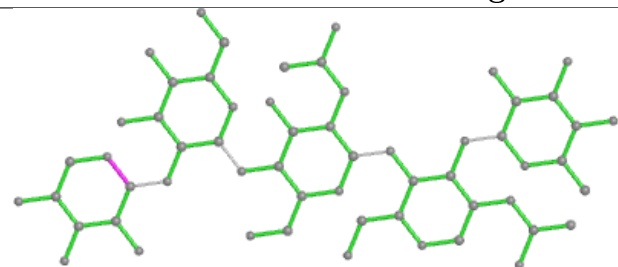


Torsions

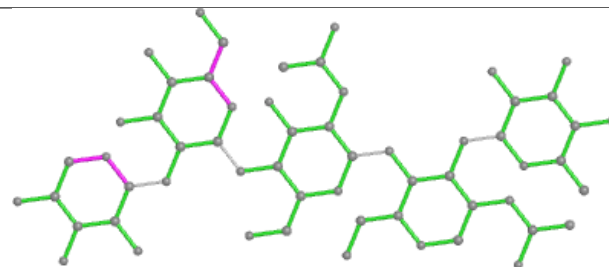


Rings

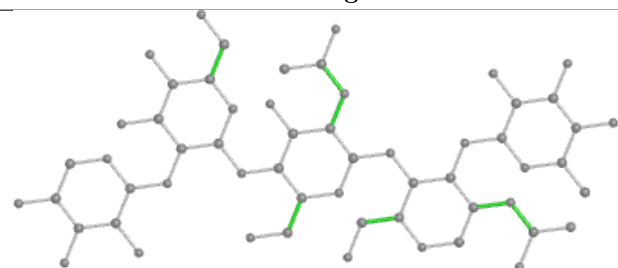
Oligosaccharide Chain D



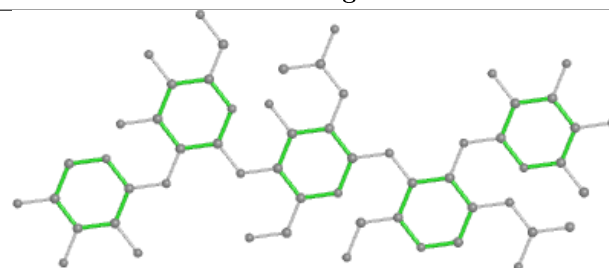
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

6 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
7	GOL	A	2001[B]	-	5,5,5	0.52	0	5,5,5	0.25	0
5	SO4	A	3001	-	4,4,4	0.15	0	6,6,6	0.21	0
7	GOL	A	2001[A]	-	5,5,5	0.51	0	5,5,5	0.34	0
7	GOL	A	2002[A]	-	5,5,5	0.43	0	5,5,5	0.19	0
6	IDD	A	1001	-	19,22,22	1.01	1 (5%)	21,32,32	1.64	5 (23%)
7	GOL	A	2002[B]	-	5,5,5	0.34	0	5,5,5	0.42	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
7	GOL	A	2001[B]	-	-	2/4/4/4	-
7	GOL	A	2001[A]	-	-	0/4/4/4	-
6	IDD	A	1001	-	-	0/6/26/26	0/2/3/3
7	GOL	A	2002[A]	-	-	2/4/4/4	-
7	GOL	A	2002[B]	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	IDD	C1B-C2B	-2.58	1.47	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	IDD	C7B-C8B-N1B	-4.87	102.93	107.96
6	A	1001	IDD	C1-C7B-N2B	2.53	125.03	120.78
6	A	1001	IDD	C2-C1-C7B	-2.47	117.39	121.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	IDD	C8B-C7B-C1	-2.25	124.07	129.15
6	A	1001	IDD	O2B-C2B-C3B	2.05	112.85	108.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

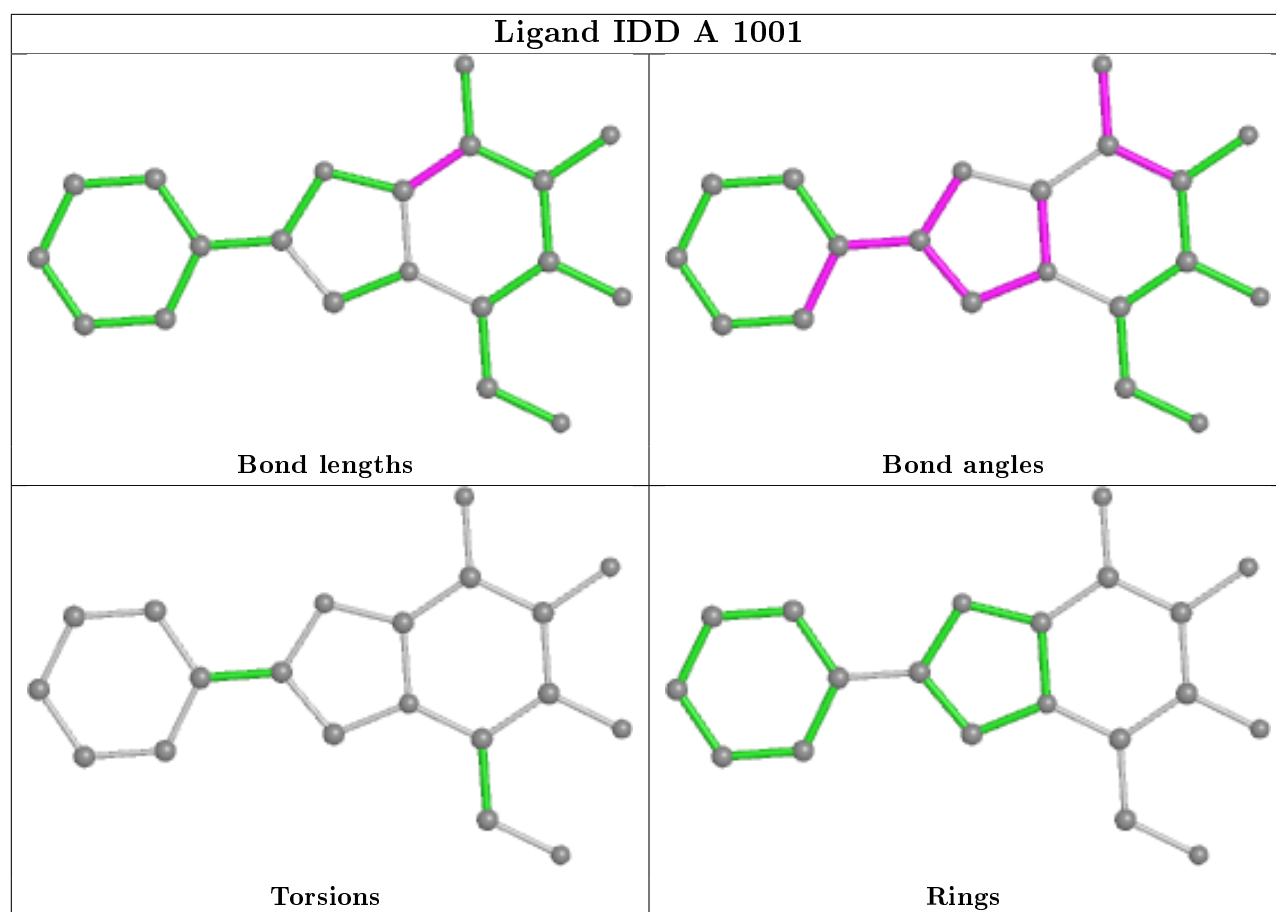
Mol	Chain	Res	Type	Atoms
7	A	2001[B]	GOL	O1-C1-C2-C3
7	A	2002[A]	GOL	O1-C1-C2-O2
7	A	2002[A]	GOL	O1-C1-C2-C3
7	A	2002[B]	GOL	O1-C1-C2-C3
7	A	2002[B]	GOL	O1-C1-C2-O2
7	A	2001[B]	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2002[A]	GOL	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

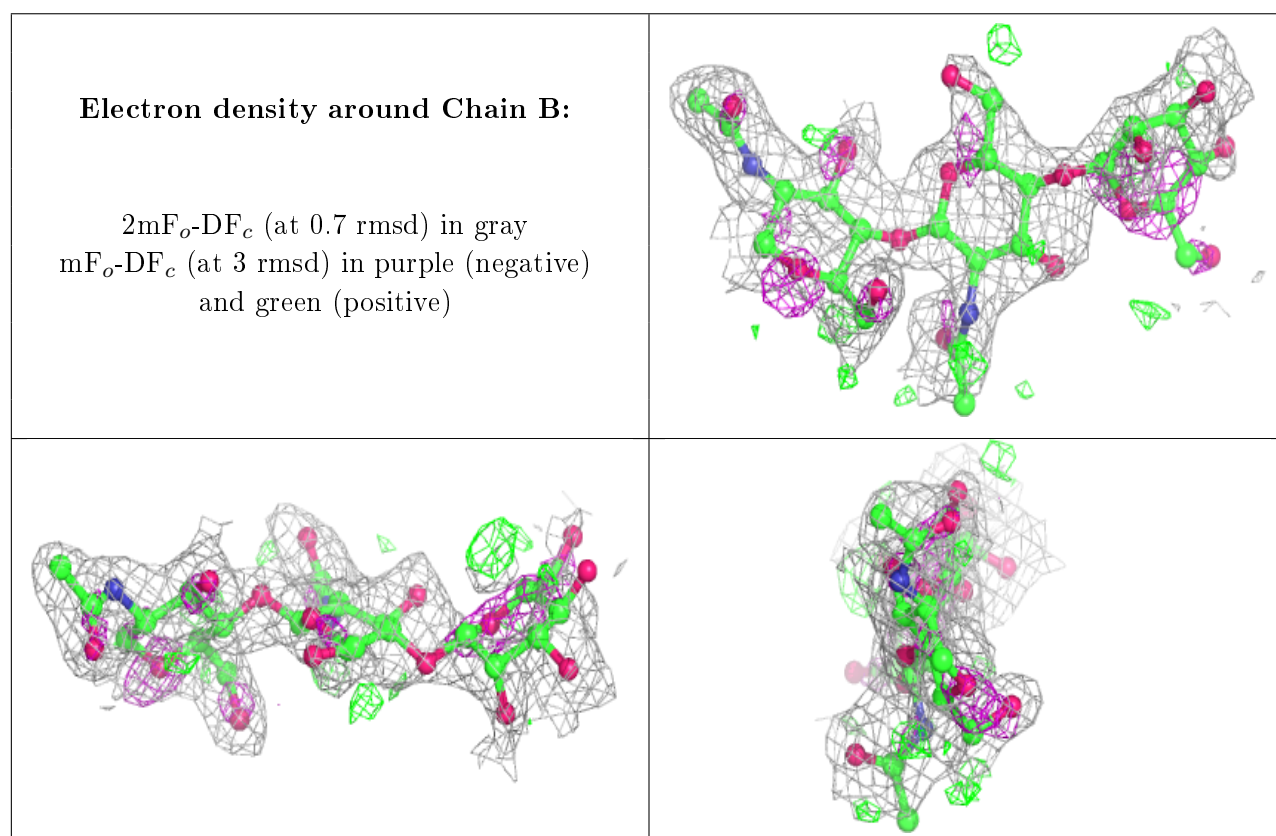
6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

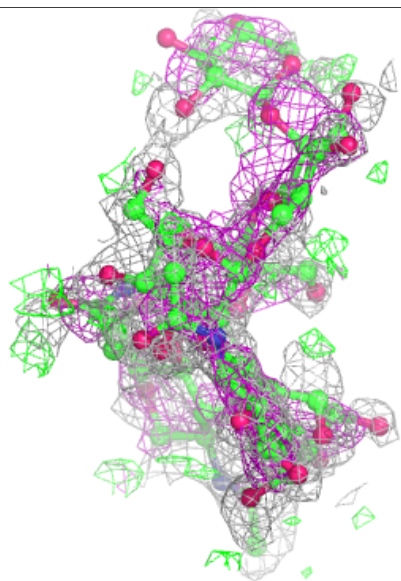
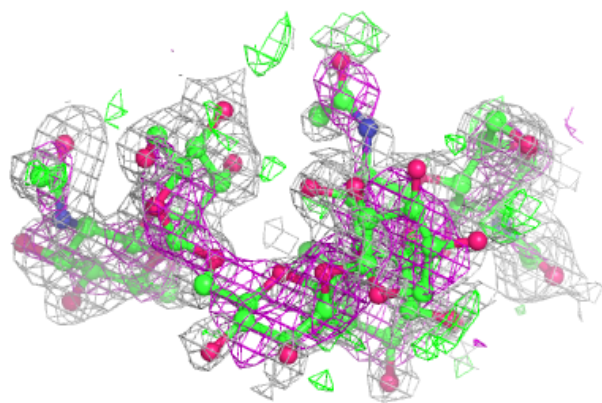
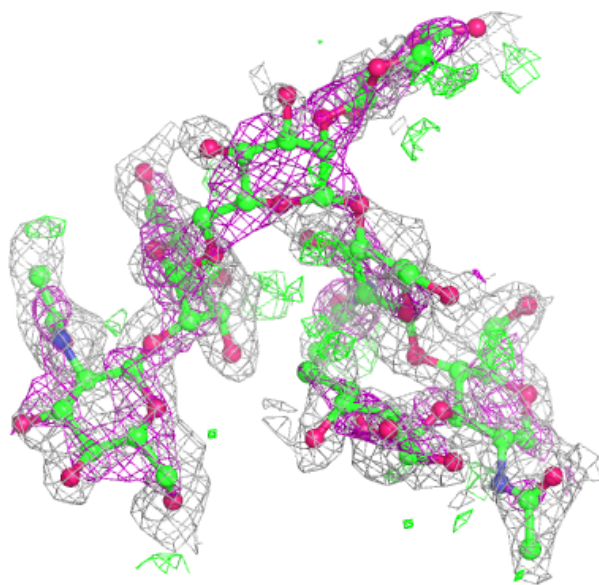
Unable to reproduce the depositors R factor - this section is therefore empty.

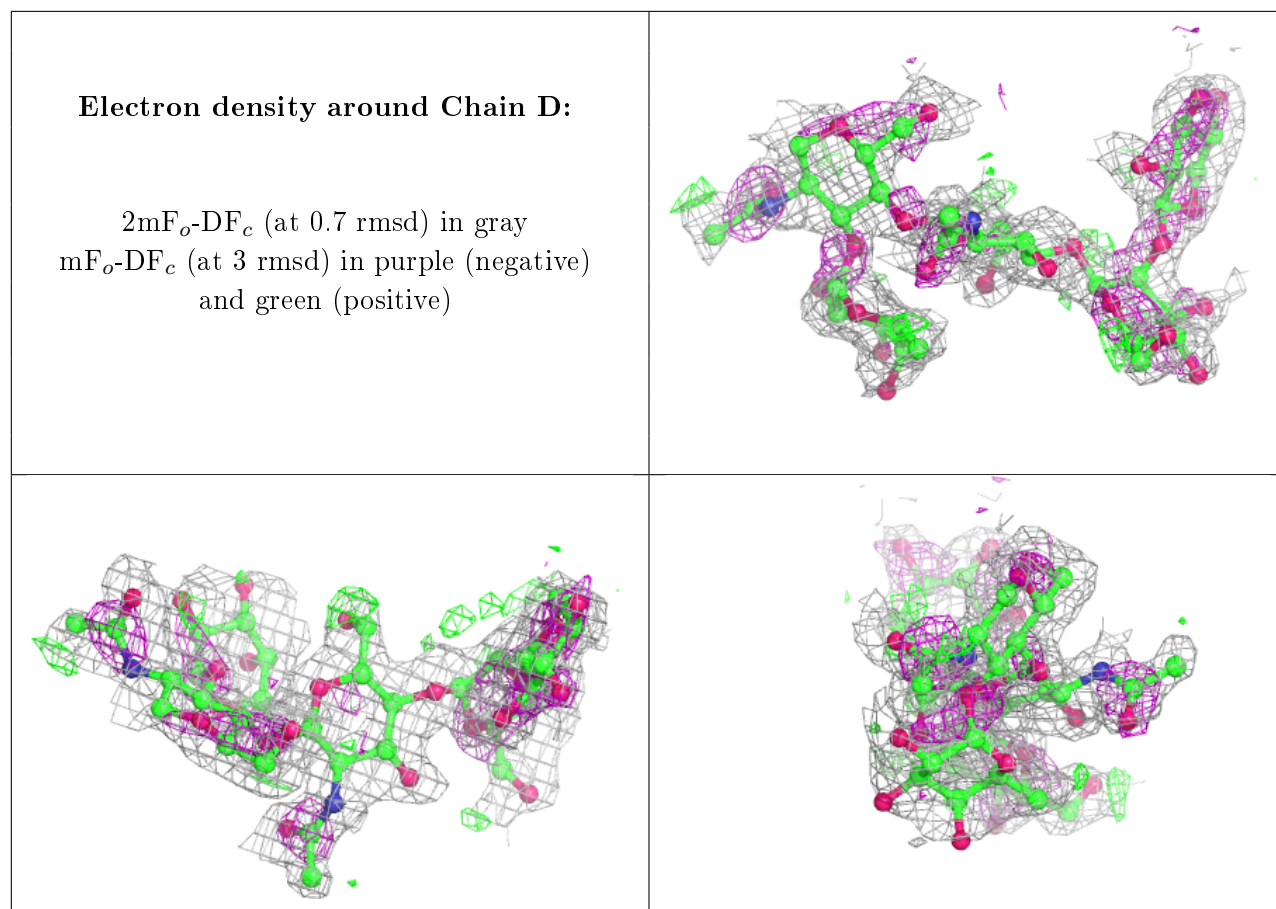
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)

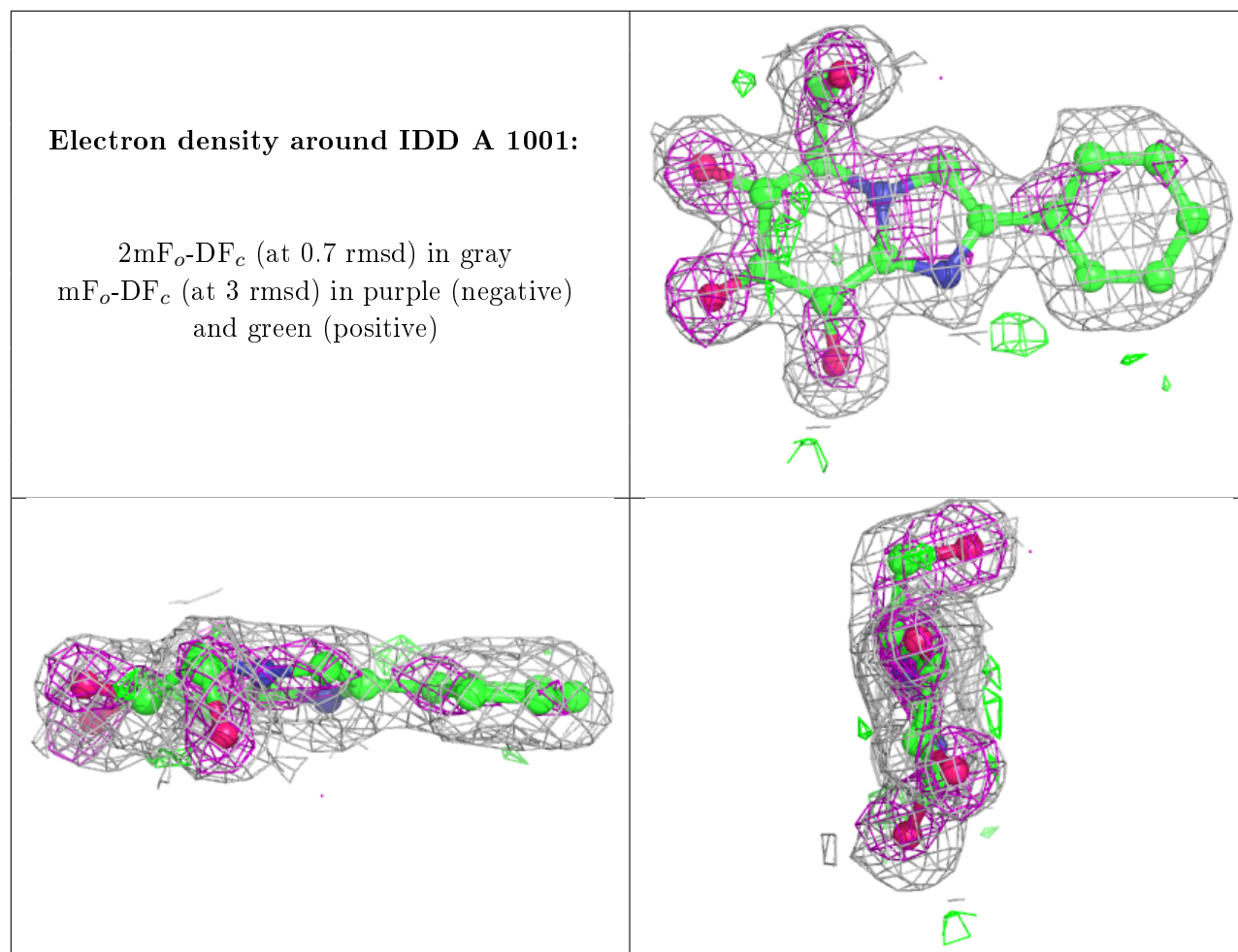




6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.