Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2023 – 02:20 PM EDT

PDB ID	:	2QT6
Title	:	Crystal Structure Determination of a Blue Laccase from Lentinus Tigrinus
Authors	:	Ferraroni, M.; Briganti, F.; Scozzafava, A.
Deposited on	:	2007-08-01
Resolution	:	1.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

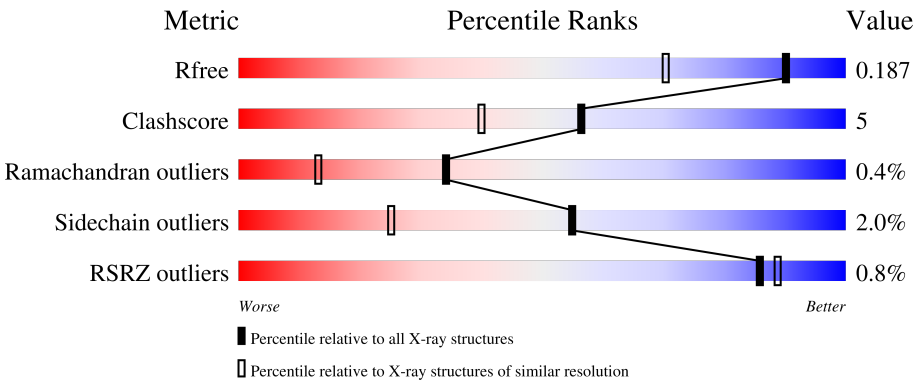
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	498	% 91% 8% •
1	B	498	% 92% 8% •
2	C	6	83% 17%
3	D	6	83% 17%
4	F	2	100%

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Mol	Chain	Length	Quality of chain
4	G	2	100%

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
9	MAN	A	508	X	-	-	-
9	MAN	B	507	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10085 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 Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3836	2430	641	750	15	0	10	0
1	B	498	3828	2427	640	746	15	0	8	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	SER	conflict	UNP Q5EBY5
A	164	LYS	LEU	conflict	UNP Q5EBY5
A	459	ASP	GLU	conflict	UNP Q5EBY5
A	464	VAL	-	expression tag	UNP Q5EBY5
A	465	VAL	-	expression tag	UNP Q5EBY5
A	466	MET	-	expression tag	UNP Q5EBY5
A	467	ALA	-	expression tag	UNP Q5EBY5
A	468	GLU	-	expression tag	UNP Q5EBY5
A	469	ASP	-	expression tag	UNP Q5EBY5
A	470	ILE	-	expression tag	UNP Q5EBY5
A	471	PRO	-	expression tag	UNP Q5EBY5
A	472	ASN	-	expression tag	UNP Q5EBY5
A	473	THR	-	expression tag	UNP Q5EBY5
A	474	VAL	-	expression tag	UNP Q5EBY5
A	475	ASN	-	expression tag	UNP Q5EBY5
A	476	ALA	-	expression tag	UNP Q5EBY5
A	477	ASN	-	expression tag	UNP Q5EBY5
A	478	PRO	-	expression tag	UNP Q5EBY5
A	479	VAL	-	expression tag	UNP Q5EBY5
A	480	PRO	-	expression tag	UNP Q5EBY5
A	481	GLN	-	expression tag	UNP Q5EBY5
A	482	ALA	-	expression tag	UNP Q5EBY5
A	483	TRP	-	expression tag	UNP Q5EBY5
A	484	SER	-	expression tag	UNP Q5EBY5
A	485	ASN	-	expression tag	UNP Q5EBY5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	LEU	-	expression tag	UNP Q5EBY5
A	487	CYS	-	expression tag	UNP Q5EBY5
A	488	PRO	-	expression tag	UNP Q5EBY5
A	489	THR	-	expression tag	UNP Q5EBY5
A	490	TYR	-	expression tag	UNP Q5EBY5
A	491	ASP	-	expression tag	UNP Q5EBY5
A	492	ALA	-	expression tag	UNP Q5EBY5
A	493	LEU	-	expression tag	UNP Q5EBY5
A	494	GLU	-	expression tag	UNP Q5EBY5
A	495	PRO	-	expression tag	UNP Q5EBY5
A	496	SER	-	expression tag	UNP Q5EBY5
A	497	ASN	-	expression tag	UNP Q5EBY5
A	498	GLU	-	expression tag	UNP Q5EBY5
B	16	VAL	SER	conflict	UNP Q5EBY5
B	164	LYS	LEU	conflict	UNP Q5EBY5
B	459	ASP	GLU	conflict	UNP Q5EBY5
B	464	VAL	-	expression tag	UNP Q5EBY5
B	465	VAL	-	expression tag	UNP Q5EBY5
B	466	MET	-	expression tag	UNP Q5EBY5
B	467	ALA	-	expression tag	UNP Q5EBY5
B	468	GLU	-	expression tag	UNP Q5EBY5
B	469	ASP	-	expression tag	UNP Q5EBY5
B	470	ILE	-	expression tag	UNP Q5EBY5
B	471	PRO	-	expression tag	UNP Q5EBY5
B	472	ASN	-	expression tag	UNP Q5EBY5
B	473	THR	-	expression tag	UNP Q5EBY5
B	474	VAL	-	expression tag	UNP Q5EBY5
B	475	ASN	-	expression tag	UNP Q5EBY5
B	476	ALA	-	expression tag	UNP Q5EBY5
B	477	ASN	-	expression tag	UNP Q5EBY5
B	478	PRO	-	expression tag	UNP Q5EBY5
B	479	VAL	-	expression tag	UNP Q5EBY5
B	480	PRO	-	expression tag	UNP Q5EBY5
B	481	GLN	-	expression tag	UNP Q5EBY5
B	482	ALA	-	expression tag	UNP Q5EBY5
B	483	TRP	-	expression tag	UNP Q5EBY5
B	484	SER	-	expression tag	UNP Q5EBY5
B	485	ASN	-	expression tag	UNP Q5EBY5
B	486	LEU	-	expression tag	UNP Q5EBY5
B	487	CYS	-	expression tag	UNP Q5EBY5
B	488	PRO	-	expression tag	UNP Q5EBY5
B	489	THR	-	expression tag	UNP Q5EBY5

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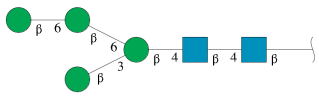
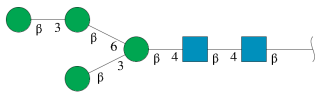
Chain	Residue	Modelled	Actual	Comment	Reference
B	490	TYR	-	expression tag	UNP Q5EBY5
B	491	ASP	-	expression tag	UNP Q5EBY5
B	492	ALA	-	expression tag	UNP Q5EBY5
B	493	LEU	-	expression tag	UNP Q5EBY5
B	494	GLU	-	expression tag	UNP Q5EBY5
B	495	PRO	-	expression tag	UNP Q5EBY5
B	496	SER	-	expression tag	UNP Q5EBY5
B	497	ASN	-	expression tag	UNP Q5EBY5
B	498	GLU	-	expression tag	UNP Q5EBY5

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose -(1-6)-[beta-D-mannopyranose-(1-3)]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
			Total	C	N	O			
2	C	6	72	40	2	30	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-6)-[beta-D-mannopyranose-(1-3)]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
			Total	C	N	O			
3	D	6	72	40	2	30	0	0	0

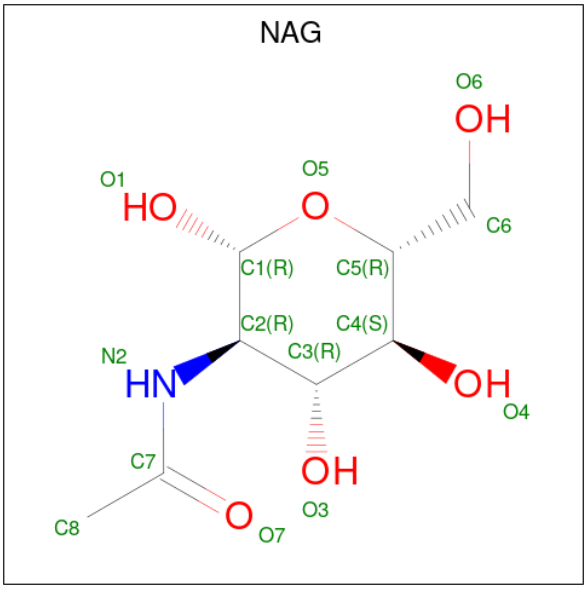
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	G	2	28	16	2	10	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

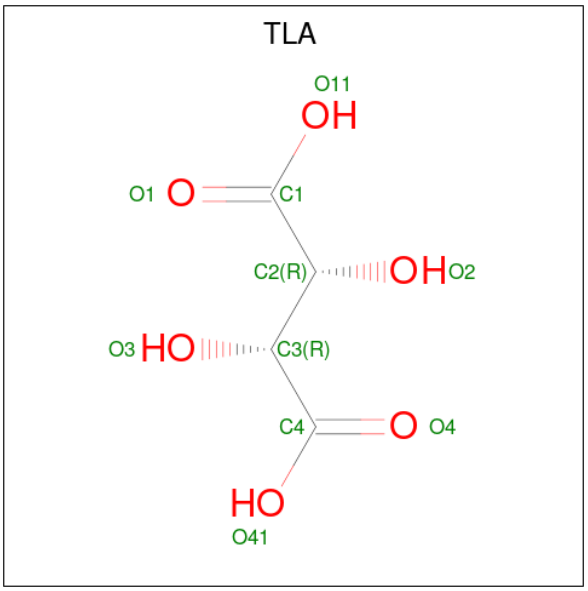
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
5	A	4	4	4	0	0
			Total	Cu		
5	B	4	4	4	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



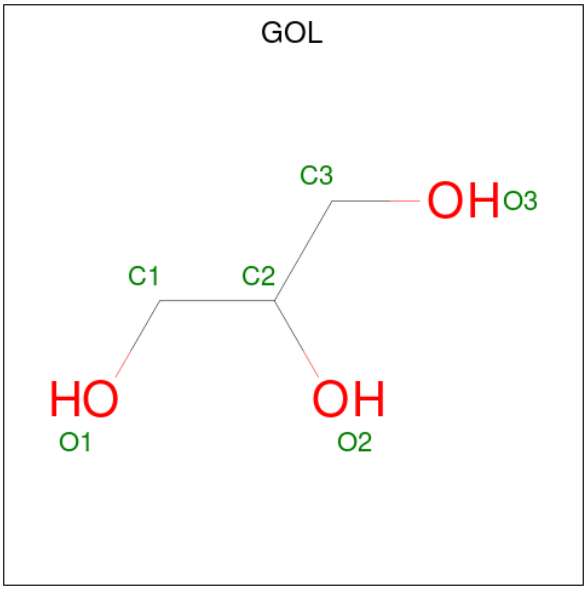
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

- Molecule 7 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



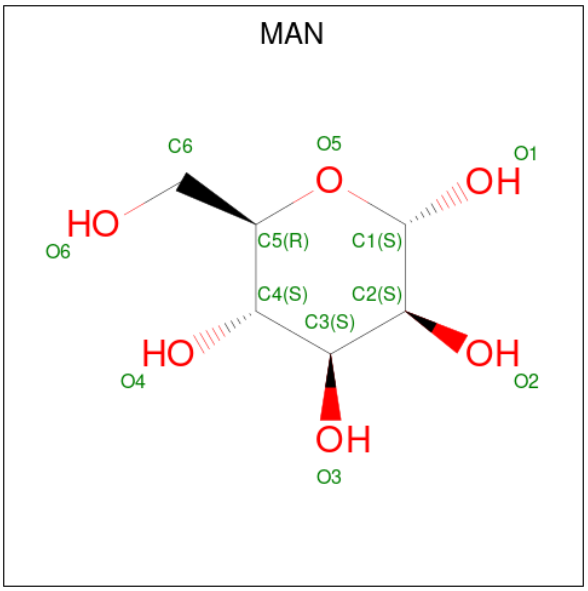
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	4	6	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	6	3	3	0	0
8	B	1	6	3	3	0	0

- Molecule 9 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 11 6 5	0	0
9	B	1	Total C O 11 6 5	0	0

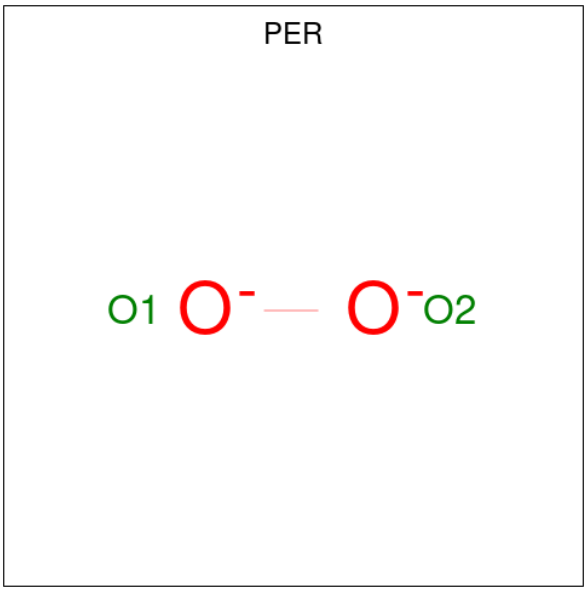
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total Cl 2 2	0	0
11	B	1	Total Cl 1 1	0	0

- Molecule 12 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O 2 2	0	0

- Molecule 13 is water.

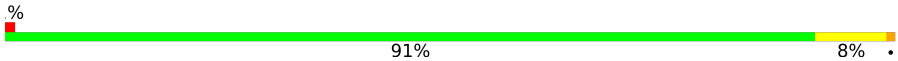
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1139	Total O 1144 1144	0	5
13	B	995	Total O 1000 1000	0	5

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.

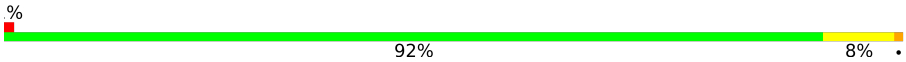
• Molecule 1: Laccase

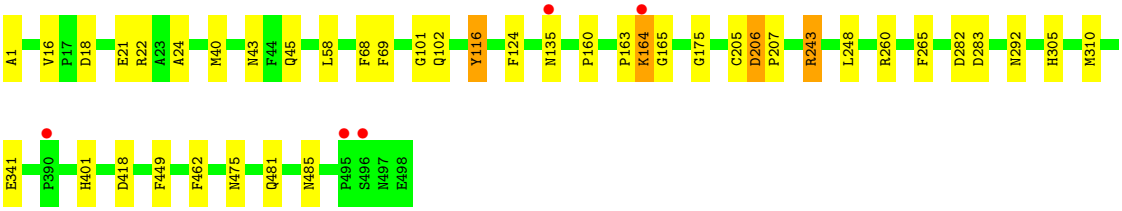
Chain A:



• Molecule 1: Laccase

Chain B:



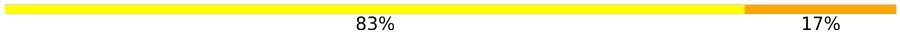


• Molecule 2: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 3: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain F: 100%

NAG1
NAG2

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

Chain G: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.22Å 111.61Å 97.09Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 25.35 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.50) 98.0 (25.35-1.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 1.42Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.182 0.154 , 0.187	Depositor DCC
R_{free} test set	1065 reflections (0.51%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10085	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: BMA, CA, NAG, CU, CL, PER, GOL, MAN, TLA

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	0/4001	0.81	4/5497 (0.1%)
1	B	0.69	0/3983	0.76	2/5476 (0.0%)
All	All	0.70	0/7984	0.79	6/10973 (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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	253	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	A	253	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	205[A]	CYS	CA-CB-SG	-5.17	104.70	114.00
1	A	205[B]	CYS	CA-CB-SG	-5.17	104.70	114.00
1	B	260	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	243	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	HIS	Peptide
1	B	401	HIS	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	3836	0	3609	38	0
1	B	3828	0	3605	34	0
2	C	72	0	61	1	0
3	D	72	0	61	1	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	14	0	13	0	0
7	A	10	0	3	0	0
8	A	6	0	8	3	0
8	B	6	0	8	0	0
9	A	11	0	10	3	0
9	B	11	0	10	0	0
10	A	5	0	0	0	0
10	B	1	0	0	0	0
11	A	2	0	0	1	0
11	B	1	0	0	0	0
12	B	2	0	0	0	0
13	A	1144	0	0	14	0
13	B	1000	0	0	12	1
All	All	10085	0	7438	77	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 (77) 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:164:LYS:H	1:A:164:LYS:HD3	1.18	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:HA	13:A:799:HOH:O	1.58	1.03
1:A:157:LYS:HE2	13:A:622:HOH:O	1.68	0.93
1:A:164:LYS:H	1:A:164:LYS:CD	1.81	0.89
1:B:164:LYS:H	1:B:164:LYS:CD	1.79	0.89
1:B:24:ALA:HA	13:B:602:HOH:O	1.72	0.89
1:A:164:LYS:HD3	1:A:164:LYS:N	1.95	0.81
1:B:16:VAL:HG11	13:B:1353:HOH:O	1.82	0.80
1:B:164:LYS:H	1:B:164:LYS:HD2	1.47	0.80
1:B:22:ARG:NH2	13:B:602:HOH:O	2.18	0.74
1:B:341:GLU:OE1	13:B:601[A]:HOH:O	2.04	0.74
1:B:248:LEU:HG	13:B:741:HOH:O	1.87	0.74
1:B:16:VAL:HG23	13:B:787:HOH:O	1.89	0.73
1:A:16:VAL:HG12	1:A:21:GLU:HA	1.70	0.72
8:A:507:GOL:H31	13:A:1264:HOH:O	1.91	0.71
1:A:260:ARG:NE	1:A:293[A]:GLN:HG2	2.05	0.71
1:B:40[B]:MET:HE2	1:B:101:GLY:HA2	1.73	0.70
1:B:43:ASN:ND2	1:B:45:GLN:HE21	1.90	0.68
1:B:16:VAL:HG12	1:B:21:GLU:HA	1.74	0.68
1:B:164:LYS:HD2	1:B:164:LYS:N	2.04	0.68
9:A:508:MAN:C1	13:A:1216:HOH:O	2.43	0.66
1:A:16:VAL:HG12	1:A:21:GLU:CA	2.25	0.65
1:A:16:VAL:HG23	13:A:637:HOH:O	1.96	0.65
1:A:16:VAL:HG11	13:A:1463:HOH:O	1.97	0.65
1:A:157:LYS:CE	13:A:622:HOH:O	2.36	0.65
1:B:1:ALA:HA	13:B:744:HOH:O	1.98	0.62
1:B:305:HIS:HE1	13:B:873:HOH:O	1.82	0.62
1:A:164:LYS:CD	1:A:164:LYS:N	2.60	0.61
1:B:164:LYS:NZ	13:B:606:HOH:O	2.29	0.60
1:A:305:HIS:HE1	13:A:756:HOH:O	1.84	0.60
1:A:43:ASN:HD21	1:A:45:GLN:HE21	1.48	0.59
1:A:305:HIS:HD2	1:A:418:ASP:O	1.85	0.59
1:B:305:HIS:HD2	1:B:418:ASP:O	1.86	0.59
1:A:40[B]:MET:HE2	1:A:101:GLY:HA2	1.86	0.58
1:B:16:VAL:HG12	1:B:21:GLU:CA	2.32	0.58
1:A:69:PHE:H	1:A:102:GLN:HE22	1.50	0.58
1:A:293[A]:GLN:HG3	13:A:1063:HOH:O	2.03	0.57
1:B:164:LYS:H	1:B:164:LYS:CE	2.17	0.57
1:B:116:TYR:CE1	1:B:205[A]:CYS:SG	2.98	0.57
1:A:113:SER:H	8:A:507:GOL:C3	2.18	0.56
1:B:69:PHE:H	1:B:102:GLN:HE22	1.53	0.56
1:A:443:ASP:HB2	11:A:515:CL:CL	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:H	8:A:507:GOL:H32	1.72	0.55
13:B:1573:HOH:O	3:D:6:BMA:H62	2.07	0.54
1:A:282:ASP:O	1:A:283:ASP:HB2	2.09	0.53
1:A:160:PRO:HG2	1:A:164:LYS:HD2	1.91	0.51
1:B:160:PRO:HG2	1:B:164:LYS:CE	2.40	0.51
1:A:163:PRO:HA	1:A:164:LYS:HD3	1.93	0.51
1:B:163:PRO:HA	1:B:164:LYS:HE3	1.94	0.50
1:A:481:GLN:HE21	1:A:485:ASN:HD21	1.60	0.49
1:B:43:ASN:HD21	1:B:45:GLN:HE21	1.61	0.49
1:B:310[A]:MET:HE2	13:B:1545:HOH:O	2.12	0.49
9:A:508:MAN:O6	13:A:601[A]:HOH:O	2.20	0.48
1:B:16:VAL:HG23	1:B:16:VAL:O	2.14	0.48
1:A:116:TYR:CE1	1:A:205[A]:CYS:SG	3.07	0.47
1:B:160:PRO:HG2	1:B:164:LYS:HE3	1.96	0.47
1:A:481:GLN:HE21	1:A:485:ASN:ND2	2.14	0.46
1:A:360[B]:THR:HG23	1:A:363:ASP:H	1.81	0.45
1:A:135:ASN:ND2	13:A:603:HOH:O	2.31	0.44
1:B:68:PHE:HA	1:B:102:GLN:HE22	1.84	0.43
1:B:165:GLY:HA2	1:B:265:PHE:CE2	2.55	0.42
1:A:295:GLY:HA3	13:A:636:HOH:O	2.18	0.42
1:A:79:PRO:HB2	1:A:82:ILE:HB	2.02	0.42
1:B:475:ASN:ND2	13:B:628:HOH:O	2.52	0.42
9:A:508:MAN:C1	2:C:4:BMA:O3	2.68	0.42
1:A:16:VAL:HG13	13:A:966:HOH:O	2.19	0.42
1:A:43:ASN:ND2	1:A:45:GLN:HE21	2.15	0.42
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.50	0.42
1:B:164:LYS:H	1:B:164:LYS:HE3	1.83	0.41
1:A:40[B]:MET:CE	13:A:1573:HOH:O	2.68	0.41
1:A:260:ARG:CD	1:A:293[A]:GLN:HG2	2.50	0.41
1:B:206:ASP:HB3	1:B:207:PRO:CD	2.50	0.41
1:A:68:PHE:HA	1:A:102:GLN:HE22	1.86	0.41
1:B:18:ASP:HA	1:B:175:GLY:O	2.21	0.40
1:B:282:ASP:O	1:B:283:ASP:HB2	2.22	0.40
1:B:481:GLN:HE21	1:B:485:ASN:HD21	1.69	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)
13:B:895:HOH:O	13:B:908:HOH:O[2_755]	2.03	0.17

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	505/498 (101%)	492 (97%)	11 (2%)	2 (0%)	34	13
1	B	504/498 (101%)	489 (97%)	13 (3%)	2 (0%)	34	13
All	All	1009/996 (101%)	981 (97%)	24 (2%)	4 (0%)	34	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP
1	B	206	ASP
1	B	58	LEU
1	A	58	LEU

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	429/420 (102%)	419 (98%)	10 (2%)	50	20
1	B	427/420 (102%)	419 (98%)	8 (2%)	57	27
All	All	856/840 (102%)	838 (98%)	18 (2%)	55	23

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	TYR
1	A	124	PHE

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Mol	Chain	Res	Type
1	A	164	LYS
1	A	243	ARG
1	A	435	ASN
1	A	449	PHE
1	A	462	PHE
1	A	475	ASN
1	A	494[A]	GLU
1	A	494[B]	GLU
1	B	116	TYR
1	B	124	PHE
1	B	135	ASN
1	B	164	LYS
1	B	243	ARG
1	B	292	ASN
1	B	449	PHE
1	B	462	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	43	ASN
1	A	70	GLN
1	A	91	ASN
1	A	102	GLN
1	A	305	HIS
1	A	315	ASN
1	A	485	ASN
1	B	39	ASN
1	B	43	ASN
1	B	70	GLN
1	B	91	ASN
1	B	102	GLN
1	B	135	ASN
1	B	292	ASN
1	B	305	HIS
1	B	315	ASN
1	B	485	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)

16 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	C	1	2,1	14,14,15	0.87	0	17,19,21	1.98	5 (29%)
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	0.95	1 (5%)
2	BMA	C	3	2	11,11,12	0.41	0	15,15,17	1.54	1 (6%)
2	BMA	C	4	2	11,11,12	0.76	0	15,15,17	4.39	4 (26%)
2	BMA	C	5	2	11,11,12	0.67	0	15,15,17	2.33	4 (26%)
2	BMA	C	6	2	11,11,12	0.78	0	15,15,17	3.63	4 (26%)
3	NAG	D	1	3,1	14,14,15	0.85	0	17,19,21	1.79	5 (29%)
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	1.21	2 (11%)
3	BMA	D	3	3	11,11,12	0.45	0	15,15,17	1.35	2 (13%)
3	BMA	D	4	3	11,11,12	0.62	0	15,15,17	3.71	4 (26%)
3	BMA	D	5	3	11,11,12	0.59	0	15,15,17	2.67	2 (13%)
3	BMA	D	6	3	11,11,12	0.57	0	15,15,17	2.12	4 (26%)
4	NAG	F	1	4,1	14,14,15	0.57	0	17,19,21	1.15	2 (11%)
4	NAG	F	2	4	14,14,15	0.59	0	17,19,21	1.33	3 (17%)
4	NAG	G	1	4,1	14,14,15	0.37	0	17,19,21	1.02	1 (5%)
4	NAG	G	2	4	14,14,15	0.43	0	17,19,21	0.95	1 (5%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	BMA	C	4	2	-	2/2/19/22	0/1/1/1
2	BMA	C	5	2	-	0/2/19/22	0/1/1/1
2	BMA	C	6	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	BMA	D	4	3	-	2/2/19/22	0/1/1/1
3	BMA	D	5	3	-	2/2/19/22	0/1/1/1
3	BMA	D	6	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	BMA	C1-C2-C3	-11.65	95.35	109.67
2	C	4	BMA	C1-O5-C5	-10.78	97.59	112.19
2	C	6	BMA	C1-C2-C3	-10.11	97.24	109.67
3	D	4	BMA	C1-O5-C5	-8.87	100.17	112.19
3	D	4	BMA	C1-C2-C3	-8.81	98.83	109.67
2	C	6	BMA	C1-O5-C5	-8.35	100.88	112.19
3	D	5	BMA	C1-O5-C5	-6.92	102.81	112.19
3	D	5	BMA	C1-C2-C3	-6.80	101.31	109.67
2	C	5	BMA	C1-O5-C5	-6.06	103.97	112.19
3	D	4	BMA	O3-C3-C2	5.26	120.06	109.99
2	C	3	BMA	O3-C3-C4	-4.85	99.14	110.35
2	C	5	BMA	C1-C2-C3	-4.62	103.98	109.67
3	D	6	BMA	C1-C2-C3	-4.45	104.20	109.67
3	D	6	BMA	C1-O5-C5	-4.40	106.23	112.19
2	C	1	NAG	C1-O5-C5	4.33	118.06	112.19
2	C	1	NAG	O5-C1-C2	-4.30	104.50	111.29
2	C	4	BMA	O5-C5-C6	3.56	112.79	107.20
3	D	1	NAG	C1-O5-C5	3.50	116.93	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	BMA	O5-C5-C6	3.45	112.61	107.20
3	D	1	NAG	O7-C7-N2	3.36	128.12	121.95
3	D	6	BMA	C3-C4-C5	3.31	116.15	110.24
3	D	3	BMA	O3-C3-C2	3.23	116.19	109.99
3	D	1	NAG	O5-C1-C2	-3.11	106.38	111.29
4	G	2	NAG	C1-O5-C5	3.09	116.39	112.19
2	C	1	NAG	O5-C5-C6	2.90	111.75	107.20
4	F	2	NAG	C4-C3-C2	2.90	115.26	111.02
2	C	4	BMA	O2-C2-C1	2.79	114.87	109.15
2	C	6	BMA	O5-C5-C6	2.78	111.56	107.20
3	D	1	NAG	O4-C4-C5	-2.75	102.46	109.30
2	C	6	BMA	C3-C4-C5	2.67	115.00	110.24
4	F	1	NAG	O5-C1-C2	-2.65	107.10	111.29
3	D	3	BMA	O3-C3-C4	-2.61	104.31	110.35
3	D	2	NAG	C8-C7-N2	-2.59	111.71	116.10
4	F	2	NAG	C3-C4-C5	2.55	114.79	110.24
4	F	1	NAG	O5-C5-C6	2.44	111.03	107.20
3	D	1	NAG	O7-C7-C8	-2.36	117.68	122.06
2	C	5	BMA	O5-C5-C6	2.28	110.79	107.20
2	C	2	NAG	C1-C2-N2	-2.26	106.62	110.49
3	D	6	BMA	O5-C5-C6	2.23	110.70	107.20
2	C	1	NAG	C3-C4-C5	-2.23	106.26	110.24
2	C	5	BMA	C3-C4-C5	2.13	114.04	110.24
3	D	2	NAG	C1-C2-N2	-2.11	106.89	110.49
4	G	1	NAG	O5-C1-C2	-2.07	108.01	111.29
4	F	2	NAG	O3-C3-C2	-2.06	105.21	109.47
2	C	1	NAG	C4-C3-C2	2.05	114.02	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	6	BMA	C4-C5-C6-O6
3	D	6	BMA	O5-C5-C6-O6
2	C	4	BMA	O5-C5-C6-O6
3	D	5	BMA	C4-C5-C6-O6
2	C	4	BMA	C4-C5-C6-O6
3	D	4	BMA	C4-C5-C6-O6
3	D	5	BMA	O5-C5-C6-O6
3	D	4	BMA	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6

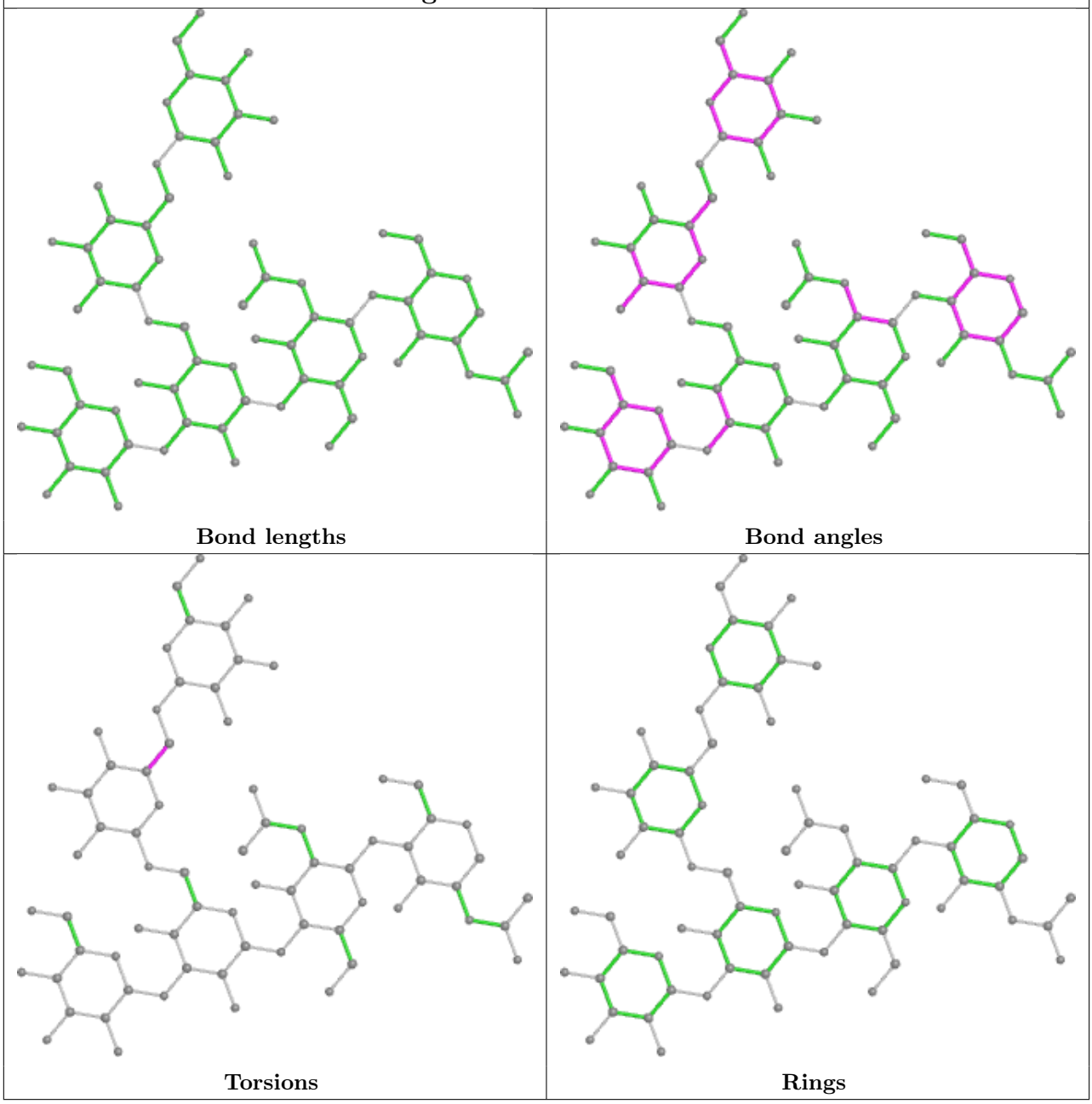
There are no ring outliers.

2 monomers are involved in 2 short contacts:

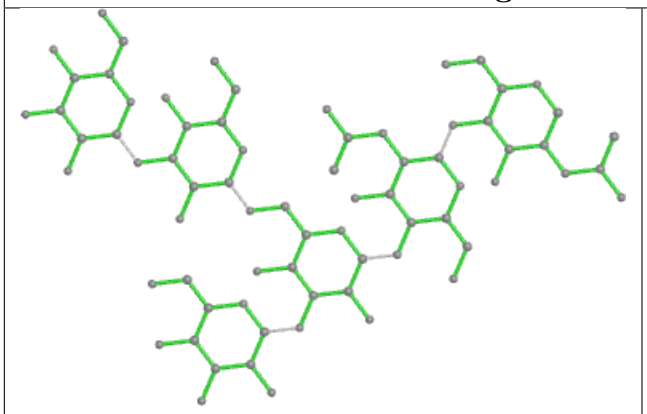
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6	BMA	1	0
2	C	4	BMA	1	0

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

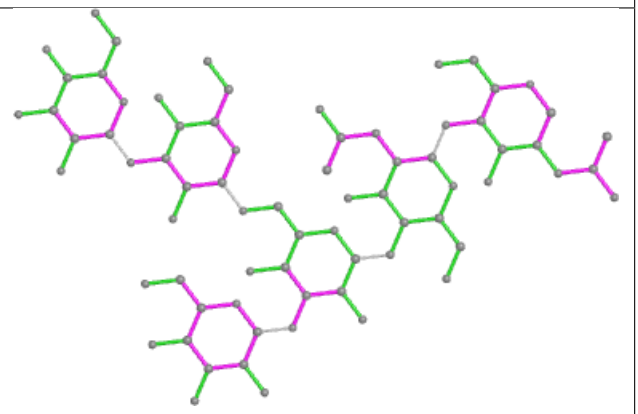
Oligosaccharide Chain C



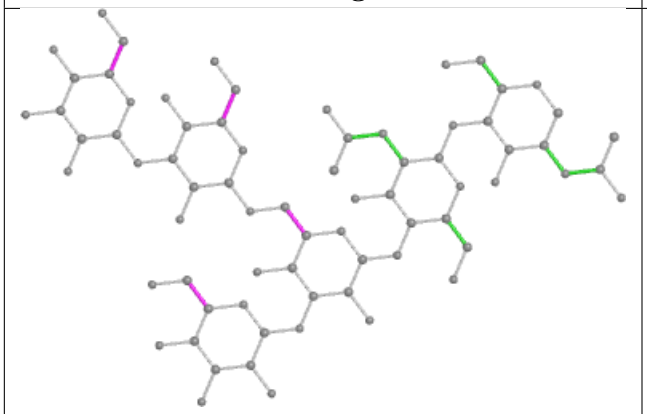
Oligosaccharide Chain D



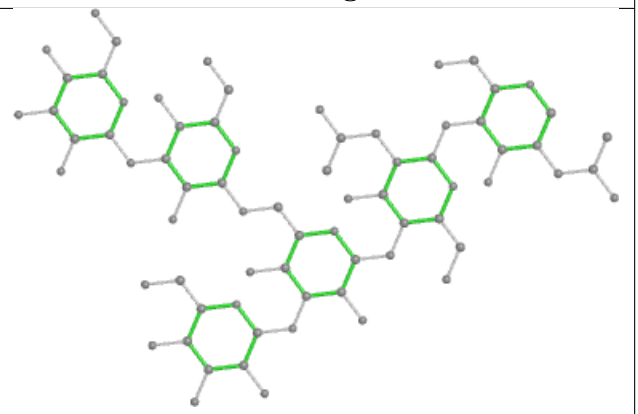
Bond lengths



Bond angles

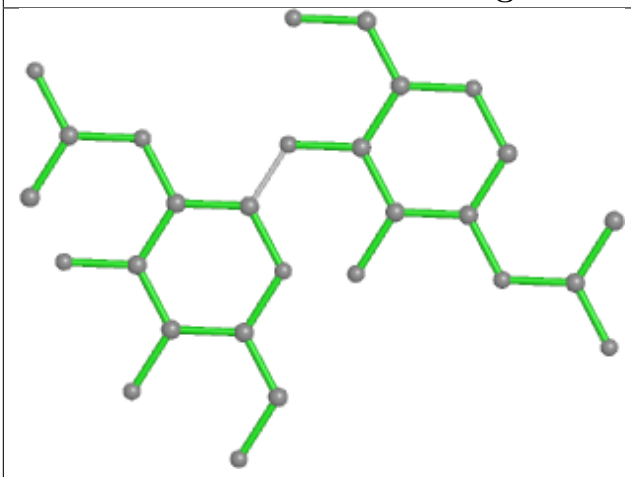


Torsions

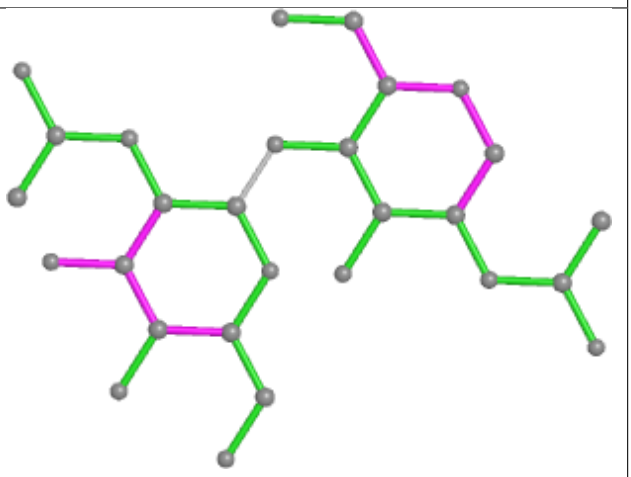


Rings

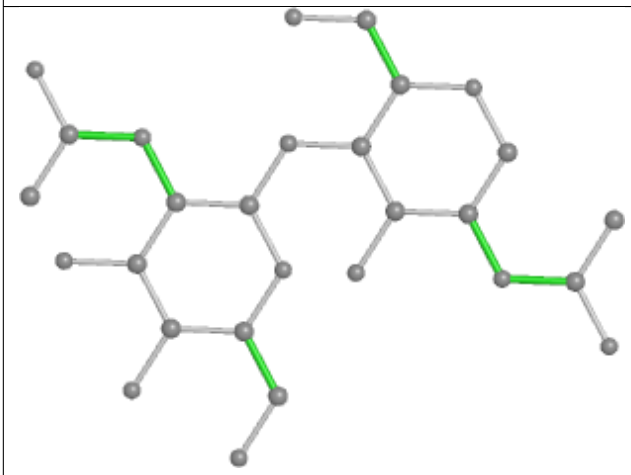
Oligosaccharide Chain F



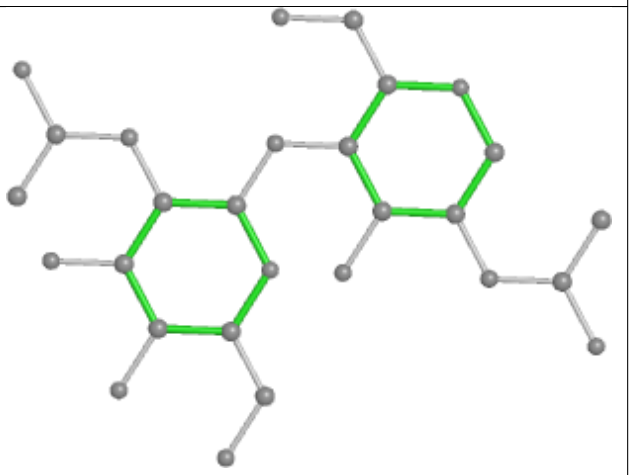
Bond lengths



Bond angles

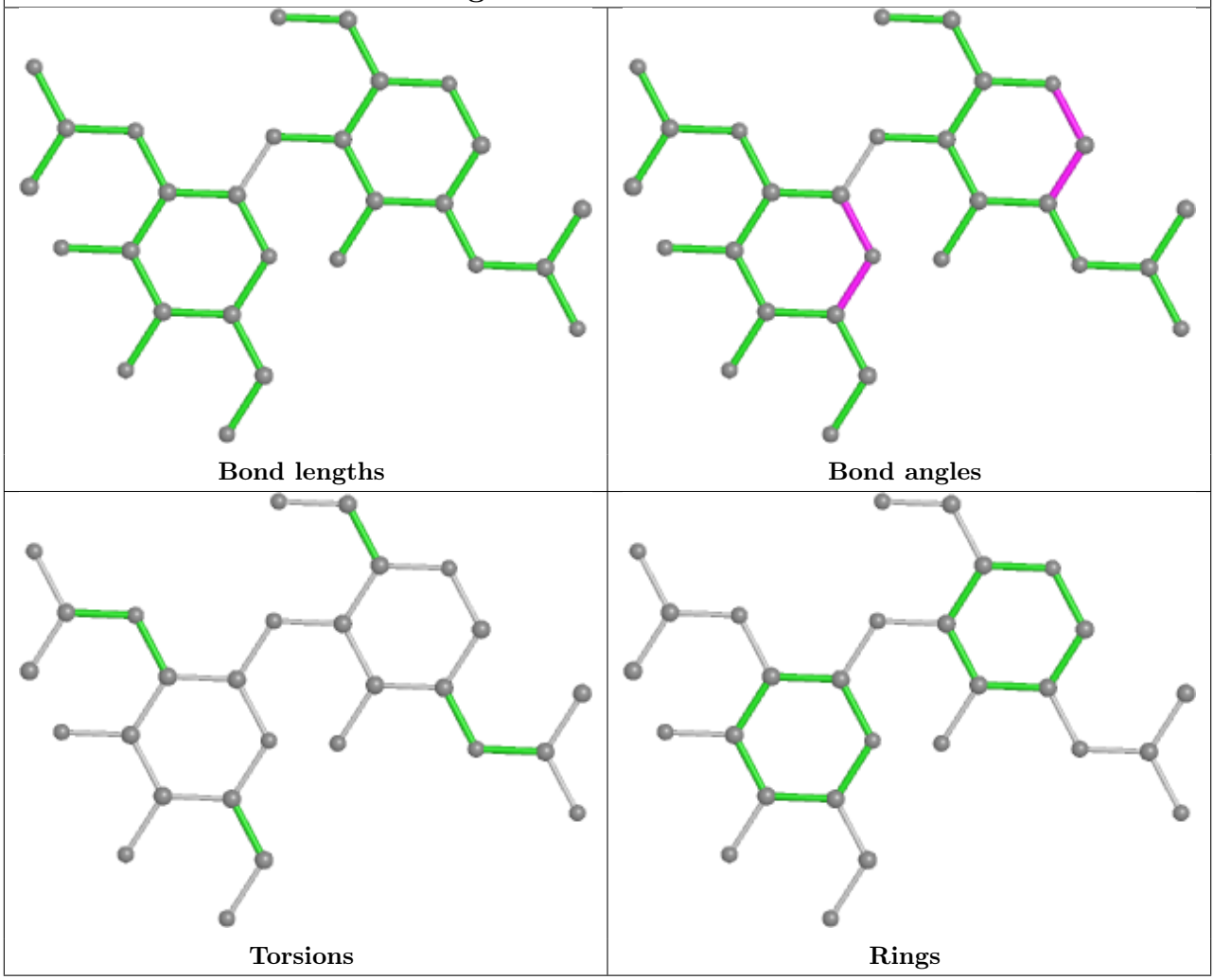


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 17 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
8	GOL	B	506	-	5,5,5	0.45	0	5,5,5	0.67	0
8	GOL	A	507	-	5,5,5	0.51	0	5,5,5	0.69	0
7	TLA	A	506	10	9,9,9	1.07	0	12,12,12	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	505	10,1	14,14,15	0.81	0	17,19,21	1.43	3 (17%)
9	MAN	A	508	-	11,11,12	0.76	0	15,15,17	1.40	2 (13%)
12	PER	B	505	5	0,1,1	-	-	-		
9	MAN	B	507	-	11,11,12	0.62	0	15,15,17	0.80	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
8	GOL	B	506	-	-	0/4/4/4	-
8	GOL	A	507	-	-	2/4/4/4	-
7	TLA	A	506	10	-	0/12/12/12	-
6	NAG	A	505	10,1	-	2/6/23/26	0/1/1/1
9	MAN	A	508	-	1/1/4/5	0/2/19/22	0/1/1/1
9	MAN	B	507	-	1/1/4/5	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	508	MAN	C1-C2-C3	3.21	113.61	109.67
6	A	505	NAG	C8-C7-N2	-2.79	111.38	116.10
6	A	505	NAG	O3-C3-C2	2.67	115.00	109.47
9	A	508	MAN	C3-C4-C5	2.18	114.12	110.24
6	A	505	NAG	O4-C4-C3	-2.14	105.41	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	508	MAN	C5
9	B	507	MAN	C5

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	507	GOL	C1-C2-C3-O3
8	A	507	GOL	O2-C2-C3-O3
9	B	507	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	505	NAG	C4-C5-C6-O6
6	A	505	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	507	GOL	3	0
9	A	508	MAN	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	498/498 (100%)	-0.29	3 (0%)	89	91	15, 19, 27, 35	0
1	B	498/498 (100%)	-0.04	5 (1%)	82	85	16, 23, 33, 40	0
All	All	996/996 (100%)	-0.17	8 (0%)	86	89	15, 20, 30, 40	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	THR	5.1
1	B	495	PRO	3.8
1	B	135	ASN	3.3
1	A	1	ALA	3.0
1	B	496	SER	2.4
1	A	294	THR	2.3
1	B	164	LYS	2.0
1	B	390	PRO	2.0

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
4	NAG	G	2	14/15	0.63	0.27	38,44,48,49	0

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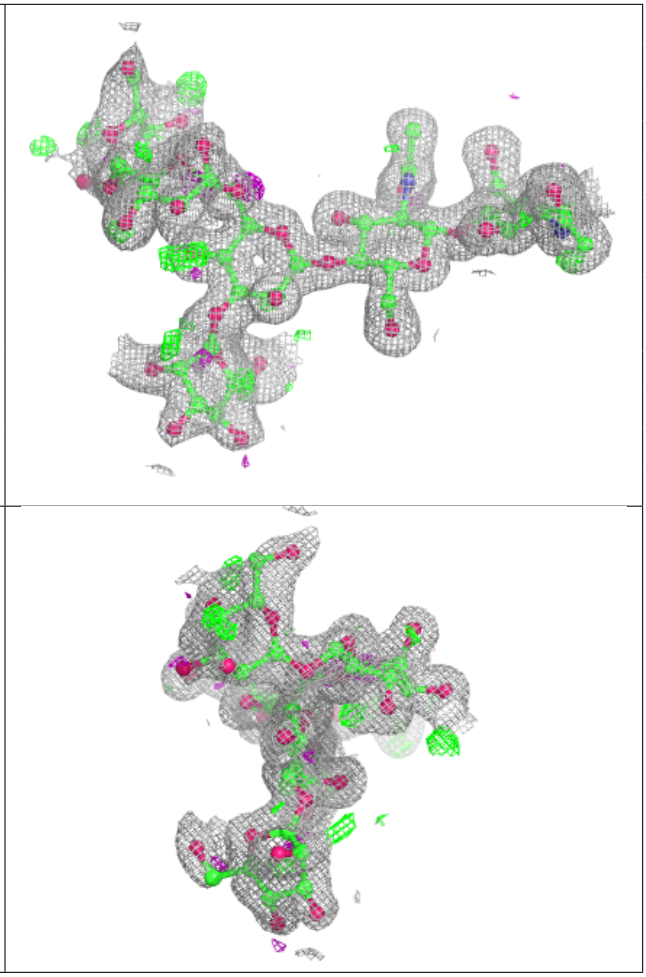
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	C	5	11/12	0.66	0.28	51,53,55,56	0
3	BMA	D	6	11/12	0.67	0.28	48,51,54,57	0
3	BMA	D	4	11/12	0.68	0.25	45,48,49,51	0
3	BMA	D	5	11/12	0.73	0.20	43,46,48,48	0
2	BMA	C	6	11/12	0.76	0.21	40,42,47,49	0
2	BMA	C	4	11/12	0.78	0.22	35,37,43,49	0
4	NAG	F	2	14/15	0.85	0.16	22,28,35,39	0
3	BMA	D	3	11/12	0.88	0.18	31,37,40,46	0
4	NAG	G	1	14/15	0.88	0.09	31,34,37,38	0
2	BMA	C	3	11/12	0.88	0.14	24,28,33,34	0
3	NAG	D	2	14/15	0.89	0.10	19,24,26,28	0
3	NAG	D	1	14/15	0.92	0.09	20,21,23,25	0
2	NAG	C	2	14/15	0.95	0.07	17,19,21,21	0
4	NAG	F	1	14/15	0.96	0.06	18,22,24,25	0
2	NAG	C	1	14/15	0.97	0.07	16,17,20,20	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.

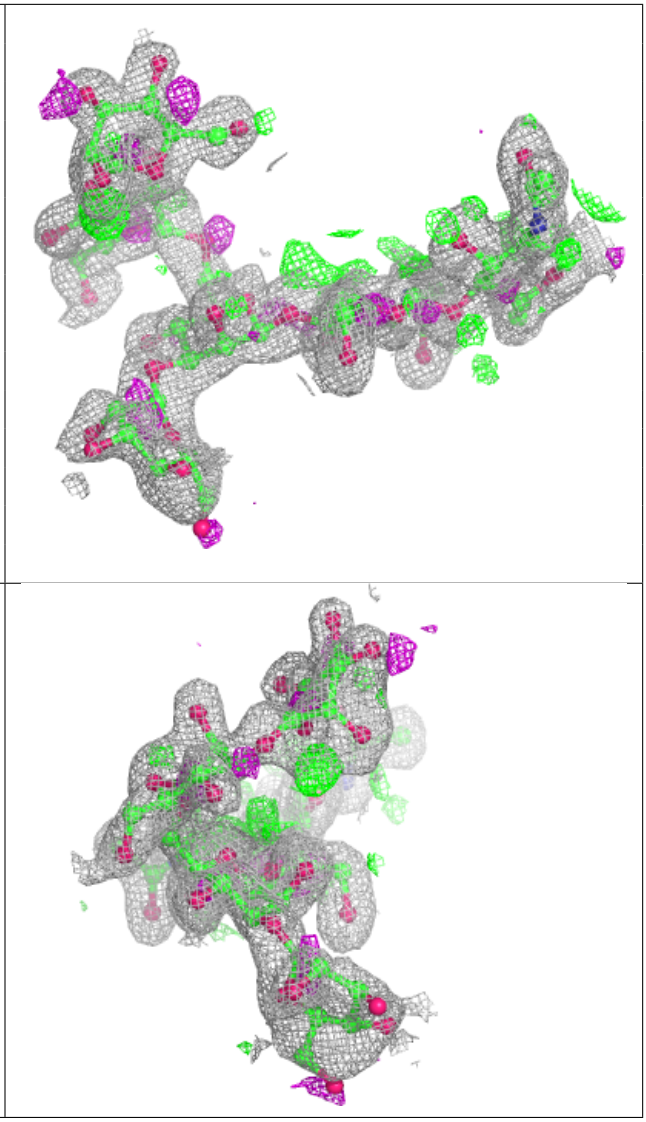
Electron density around Chain C:

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



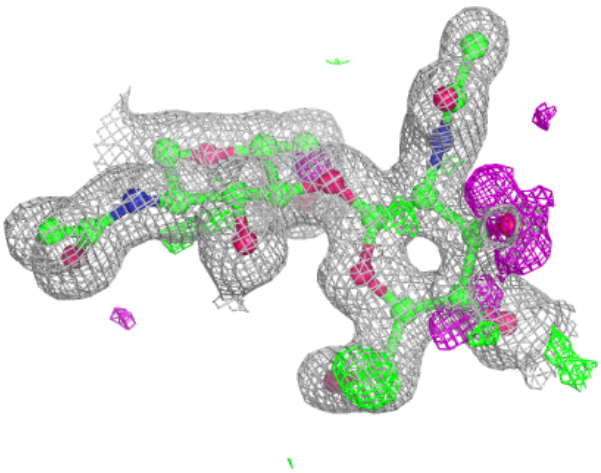
Electron density around Chain D:

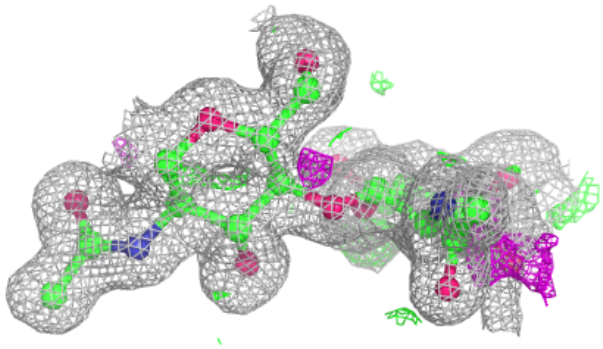
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

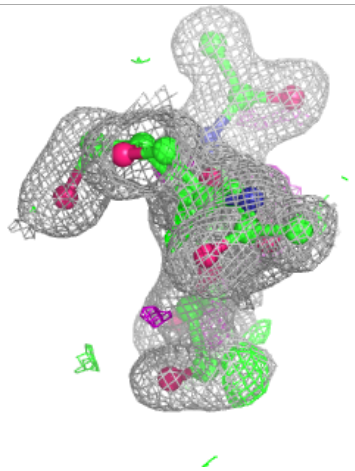


Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

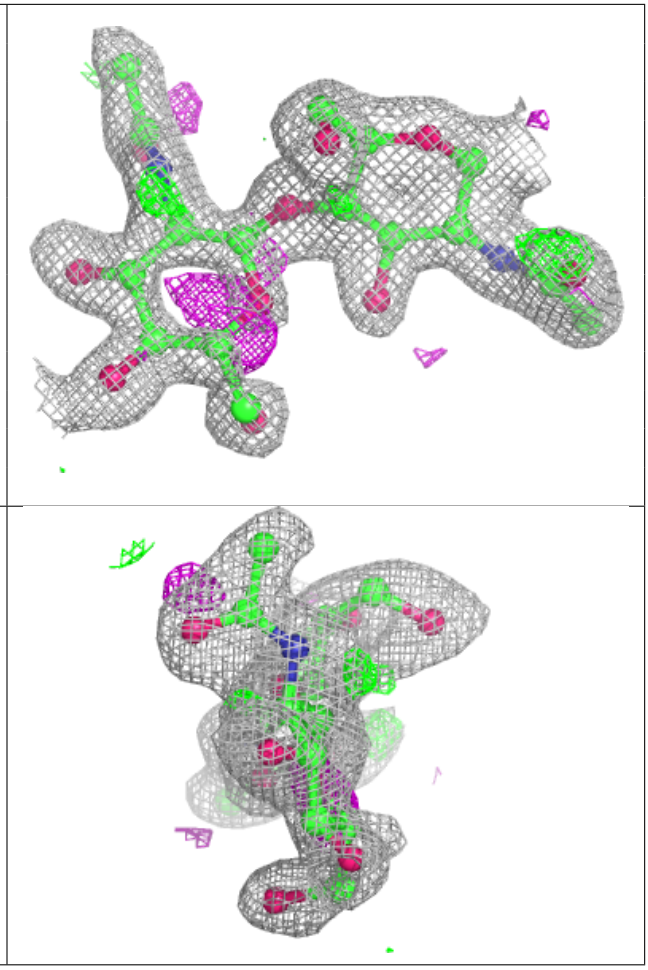






Electron density around Chain G:

$2mF_o$-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
9	MAN	B	507	11/12	0.15	0.35	98,98,99,99	0
9	MAN	A	508	11/12	0.79	0.35	45,51,53,56	0
6	NAG	A	505	14/15	0.82	0.22	21,30,36,41	0
8	GOL	A	507	6/6	0.83	0.14	25,32,34,36	0
12	PER	B	505	2/2	0.92	0.12	23,23,23,33	2
8	GOL	B	506	6/6	0.94	0.08	24,29,30,31	0
7	TLA	A	506	10/10	0.96	0.10	21,23,25,29	0
10	CA	B	508	1/1	0.99	0.11	19,19,19,19	1
5	CU	B	503	1/1	0.99	0.03	26,26,26,26	1
5	CU	A	503	1/1	1.00	0.03	22,22,22,22	1
5	CU	A	504	1/1	1.00	0.03	21,21,21,21	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CU	B	501	1/1	1.00	0.02	24,24,24,24	1
5	CU	B	502	1/1	1.00	0.04	23,23,23,23	1
5	CU	A	501	1/1	1.00	0.03	19,19,19,19	1
10	CA	A	509	1/1	1.00	0.03	20,20,20,20	0
10	CA	A	510	1/1	1.00	0.05	18,18,18,18	0
10	CA	A	511	1/1	1.00	0.03	20,20,20,20	0
10	CA	A	512	1/1	1.00	0.04	18,18,18,18	0
10	CA	A	513	1/1	1.00	0.16	29,29,29,29	0
5	CU	B	504	1/1	1.00	0.03	24,24,24,24	1
11	CL	A	514	1/1	1.00	0.04	29,29,29,29	0
11	CL	A	515	1/1	1.00	0.09	37,37,37,37	0
11	CL	B	509	1/1	1.00	0.05	32,32,32,32	0
5	CU	A	502	1/1	1.00	0.03	19,19,19,19	1

6.5 Other polymers (i)

There are no such residues in this entry.