wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 12:56 AM EDT

PDB ID	:	1ONA
Title	:	CO-CRYSTALS OF CONCANAVALIN A WITH METHYL-3,6-DI-O-(ALPHA-D-MANNOPYRANOSYL)-ALPHA-D-MANNOPYRANOSIDE
Authors	:	Bouckaert, J.; Maes, D.; Poortmans, F.; Wyns, L.; Loris, R.
Deposited on	:	1996-07-07
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

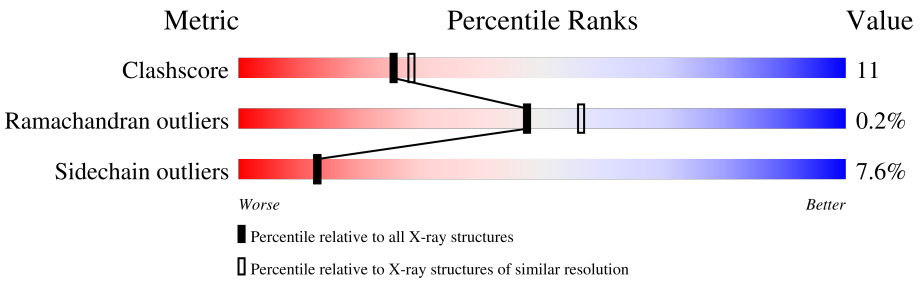
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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%

Mol	Chain	Length	Quality of chain
1	A	237	74% 19% • •
1	B	237	73% 22% • •
1	C	237	75% 19% • •
1	D	237	73% 21% • •
2	E	3	67% 33%
2	F	3	33% 67%
2	G	3	100%
2	H	3	33% 67%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7368 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.

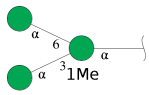
- Molecule 1 is a protein called CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	1755	1111	291	351	2	0	0	0
1	B	231	1755	1111	291	351	2	0	0	0
1	C	231	1755	1111	291	351	2	0	0	0
1	D	231	1755	1111	291	351	2	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866
B	151	ASP	GLU	conflict	UNP P02866
B	155	GLU	ARG	conflict	UNP P02866
C	151	ASP	GLU	conflict	UNP P02866
C	155	GLU	ARG	conflict	UNP P02866
D	151	ASP	GLU	conflict	UNP P02866
D	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	3	35	19	16	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	3	Total C O 35 19 16	0	0	0
2	G	3	Total C O 35 19 16	0	0	0
2	H	3	Total C O 35 19 16	0	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is water.

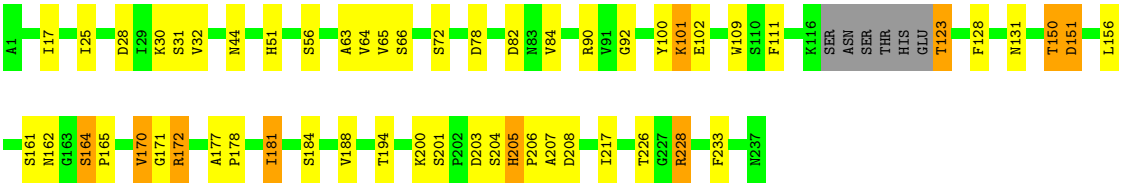
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	47	Total O 47 47	0	0
5	C	50	Total O 50 50	0	0
5	D	53	Total O 53 53	0	0

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. 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.

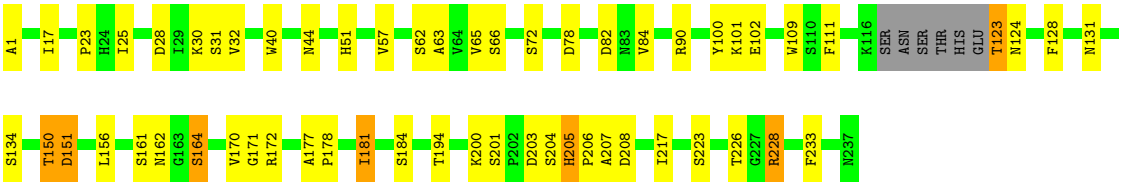
• Molecule 1: CONCANAVALIN A

Chain A:



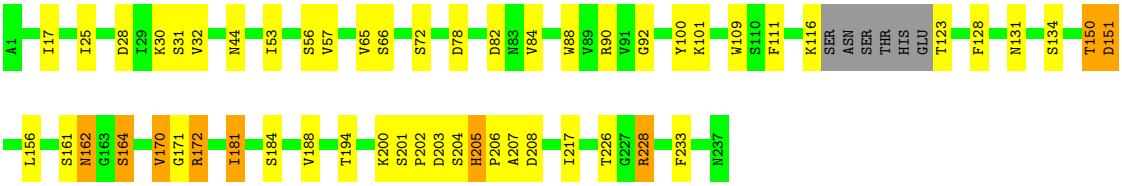
• Molecule 1: CONCANAVALIN A

Chain B:



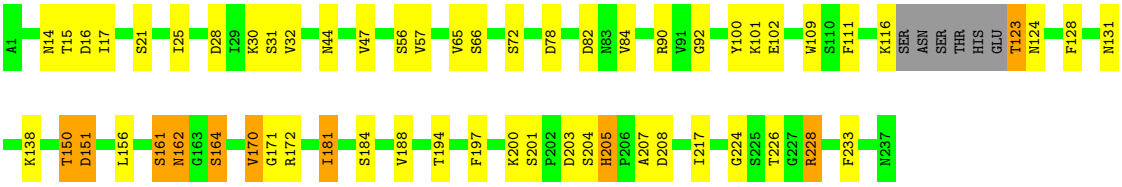
• Molecule 1: CONCANAVALIN A

Chain C:



• Molecule 1: CONCANAVALIN A

Chain D:



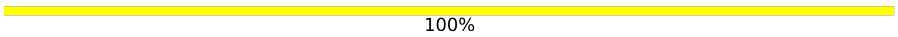
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain E:

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain F:

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain G: 

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]methyl alpha-D-mannopyranoside

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.83Å 64.84Å 125.92Å 90.00° 93.87° 90.00°	Depositor
Resolution (Å)	8.00 – 2.35 15.24 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.35) 69.7 (15.24-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.32Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.282 0.306 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	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	0.84	EDS
Total number of atoms	7368	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 21.40 % 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 7.0631e-03. 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: MN, CA, MMA, MAN

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	0.61	1/1795 (0.1%)	0.82	1/2446 (0.0%)
1	B	0.59	0/1795	0.83	1/2446 (0.0%)
1	C	0.61	1/1795 (0.1%)	0.83	1/2446 (0.0%)
1	D	0.62	1/1795 (0.1%)	0.84	2/2446 (0.1%)
All	All	0.61	3/7180 (0.0%)	0.83	5/9784 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	VAL	CB-CG2	-5.26	1.41	1.52
1	D	170	VAL	CB-CG2	-5.06	1.42	1.52
1	A	170	VAL	CB-CG2	-5.03	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	172	ARG	CB-CG-CD	-5.21	98.05	111.60
1	A	172	ARG	CB-CG-CD	-5.18	98.14	111.60
1	D	161	SER	CB-CA-C	-5.05	100.50	110.10
1	D	172	ARG	CB-CG-CD	-5.04	98.51	111.60
1	B	172	ARG	CB-CG-CD	-5.02	98.56	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1755	0	1701	39	0
1	B	1755	0	1701	41	0
1	C	1755	0	1701	39	0
1	D	1755	0	1701	42	0
2	E	35	0	32	3	0
2	F	35	0	32	2	0
2	G	35	0	32	4	0
2	H	35	0	32	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	50	0	0	1	0
5	B	47	0	0	3	0
5	C	50	0	0	1	0
5	D	53	0	0	2	0
All	All	7368	0	6932	150	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 11.

The worst 5 of 150 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:17:ILE:HD13	1:A:228:ARG:HD3	1.47	0.96
1:C:90:ARG:NH1	1:C:217:ILE:HG22	1.84	0.93
1:B:90:ARG:NH1	1:B:217:ILE:HG22	1.84	0.92
1:C:17:ILE:HD13	1:C:228:ARG:HD3	1.52	0.92
1:B:170:VAL:HG23	1:B:226:THR:HG22	1.52	0.92

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	227/237 (96%)	215 (95%)	12 (5%)	0	100	100
1	B	227/237 (96%)	212 (93%)	15 (7%)	0	100	100
1	C	227/237 (96%)	212 (93%)	14 (6%)	1 (0%)	34	38
1	D	227/237 (96%)	213 (94%)	13 (6%)	1 (0%)	34	38
All	All	908/948 (96%)	852 (94%)	54 (6%)	2 (0%)	47	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	ASN
1	D	162	ASN

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	195/203 (96%)	181 (93%)	14 (7%)	14	14
1	B	195/203 (96%)	179 (92%)	16 (8%)	11	11
1	C	195/203 (96%)	181 (93%)	14 (7%)	14	14
1	D	195/203 (96%)	180 (92%)	15 (8%)	13	12
All	All	780/812 (96%)	721 (92%)	59 (8%)	13	13

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	223	SER
1	D	203	ASP
1	C	151	ASP
1	D	184	SER
1	D	150	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	237	ASN
1	D	41	ASN
1	D	237	ASN
1	B	51	HIS
1	B	131	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)

12 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	MMA	E	1	2	13,13,13	0.38	0	18,18,18	0.83	0
2	MAN	E	2	2	11,11,12	0.61	0	15,15,17	0.94	0
2	MAN	E	3	2	11,11,12	0.61	0	15,15,17	0.80	1 (6%)
2	MMA	F	1	2	13,13,13	0.33	0	18,18,18	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAN	F	2	2	11,11,12	0.43	0	15,15,17	1.29	2 (13%)
2	MAN	F	3	2	11,11,12	0.80	0	15,15,17	0.94	0
2	MMA	G	1	2	13,13,13	0.36	0	18,18,18	0.91	0
2	MAN	G	2	2	11,11,12	0.60	0	15,15,17	1.13	2 (13%)
2	MAN	G	3	2	11,11,12	0.55	0	15,15,17	0.64	0
2	MMA	H	1	2	13,13,13	0.44	0	18,18,18	0.56	0
2	MAN	H	2	2	11,11,12	0.44	0	15,15,17	0.93	1 (6%)
2	MAN	H	3	2	11,11,12	0.46	0	15,15,17	1.04	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MMA	E	1	2	-	2/4/24/24	0/1/1/1
2	MAN	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
2	MMA	F	1	2	-	0/4/24/24	0/1/1/1
2	MAN	F	2	2	-	0/2/19/22	0/1/1/1
2	MAN	F	3	2	-	1/2/19/22	0/1/1/1
2	MMA	G	1	2	-	2/4/24/24	0/1/1/1
2	MAN	G	2	2	-	2/2/19/22	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
2	MMA	H	1	2	-	2/4/24/24	0/1/1/1
2	MAN	H	2	2	-	2/2/19/22	0/1/1/1
2	MAN	H	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	3	MAN	C2-C3-C4	-3.18	105.40	110.89
2	F	2	MAN	C1-C2-C3	2.61	112.87	109.67
2	F	2	MAN	C1-O5-C5	2.45	115.51	112.19
2	G	2	MAN	O5-C5-C6	-2.20	103.75	107.20
2	G	2	MAN	C6-C5-C4	-2.18	107.89	113.00

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	MMA	C2-C1-O1-C7
2	G	1	MMA	O5-C1-O1-C7
2	H	2	MAN	O5-C5-C6-O6
2	G	2	MAN	O5-C5-C6-O6
2	H	2	MAN	C4-C5-C6-O6

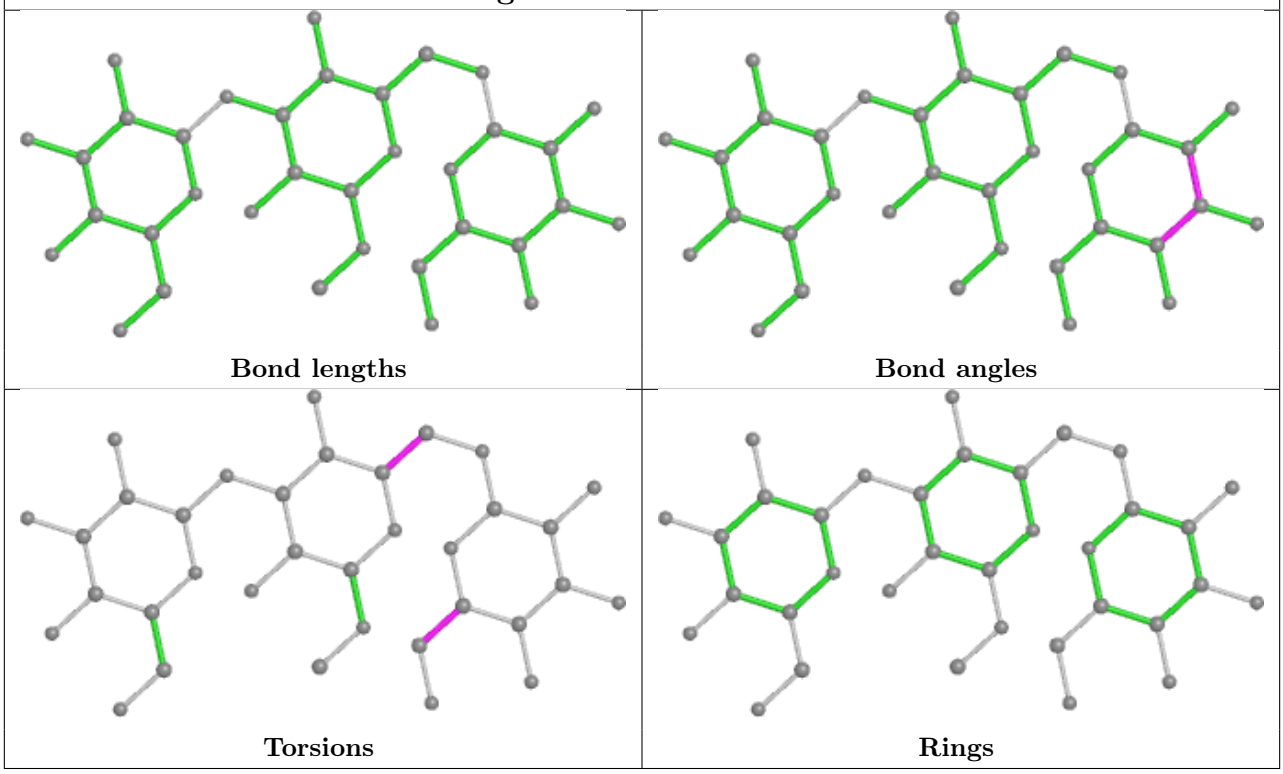
There are no ring outliers.

6 monomers are involved in 13 short contacts:

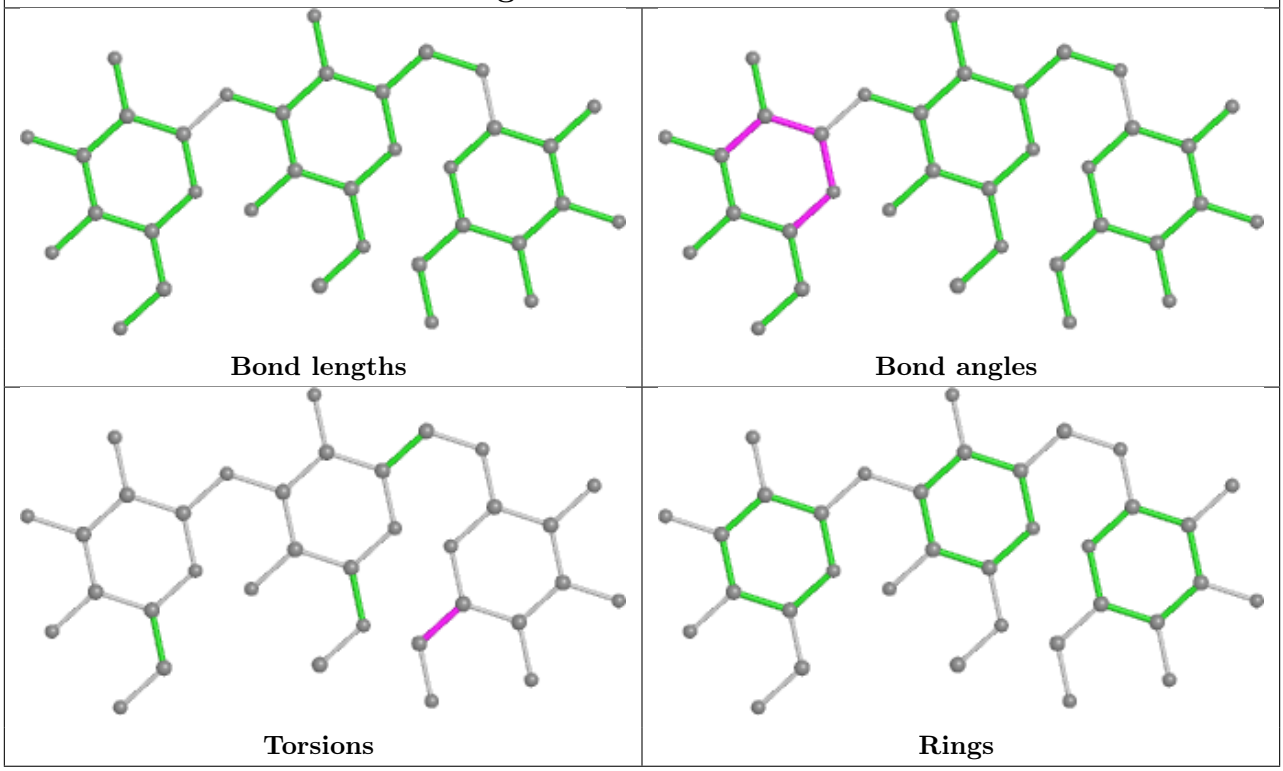
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	MAN	3	0
2	H	3	MAN	1	0
2	F	3	MAN	2	0
2	G	3	MAN	3	0
2	G	1	MMA	1	0
2	H	2	MAN	3	0

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

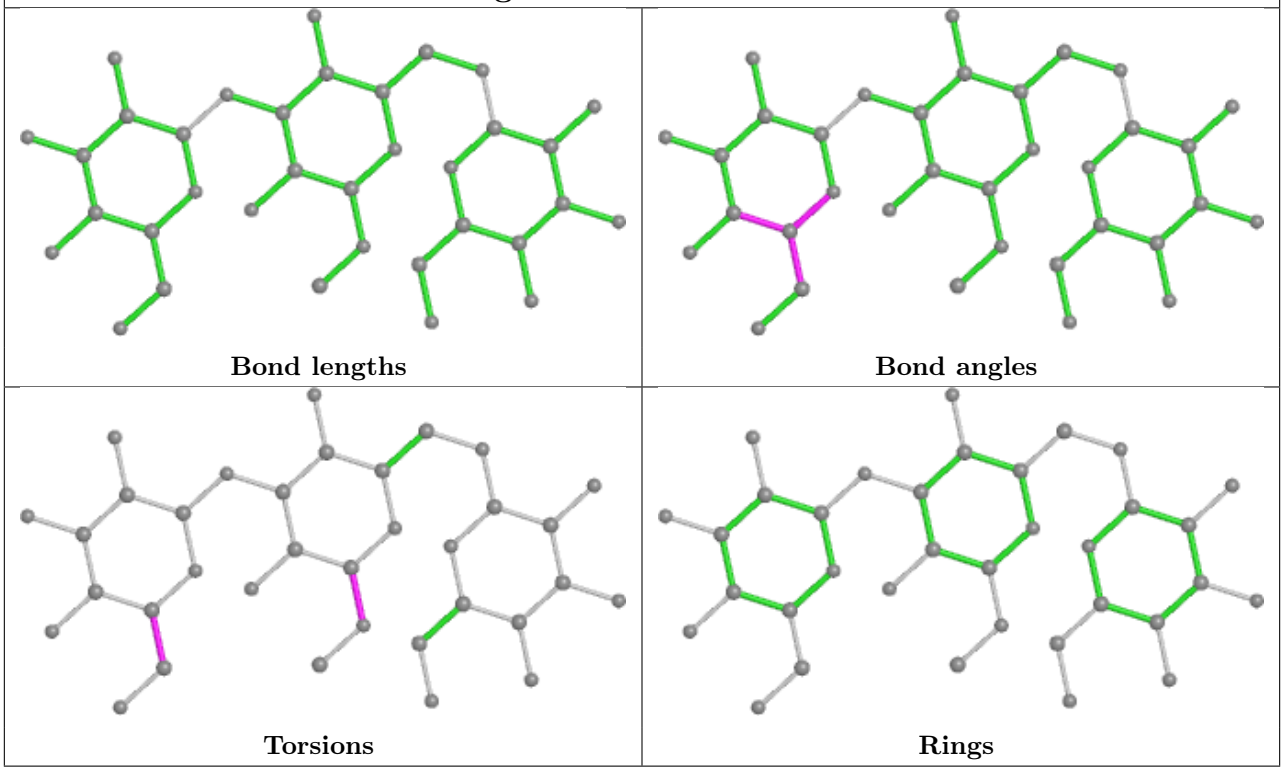
Oligosaccharide Chain E

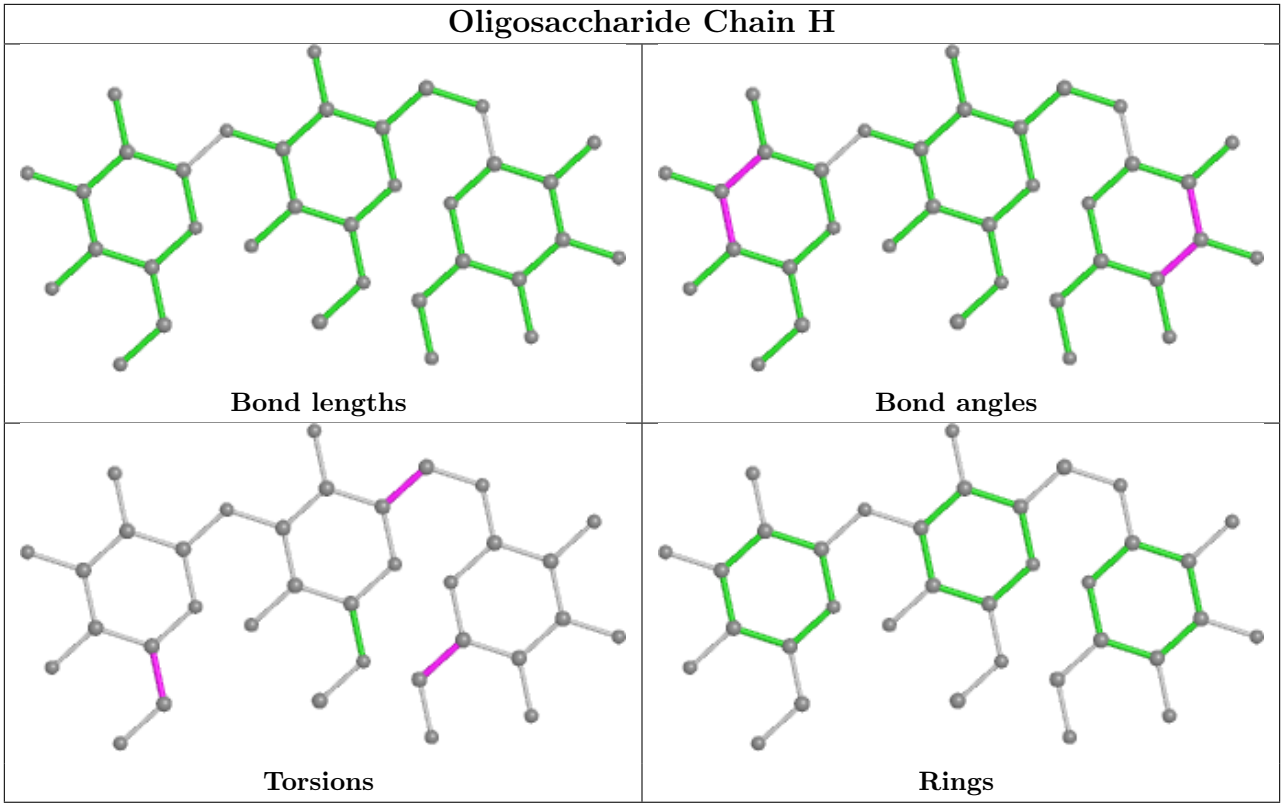


Oligosaccharide Chain F



Oligosaccharide Chain G





5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

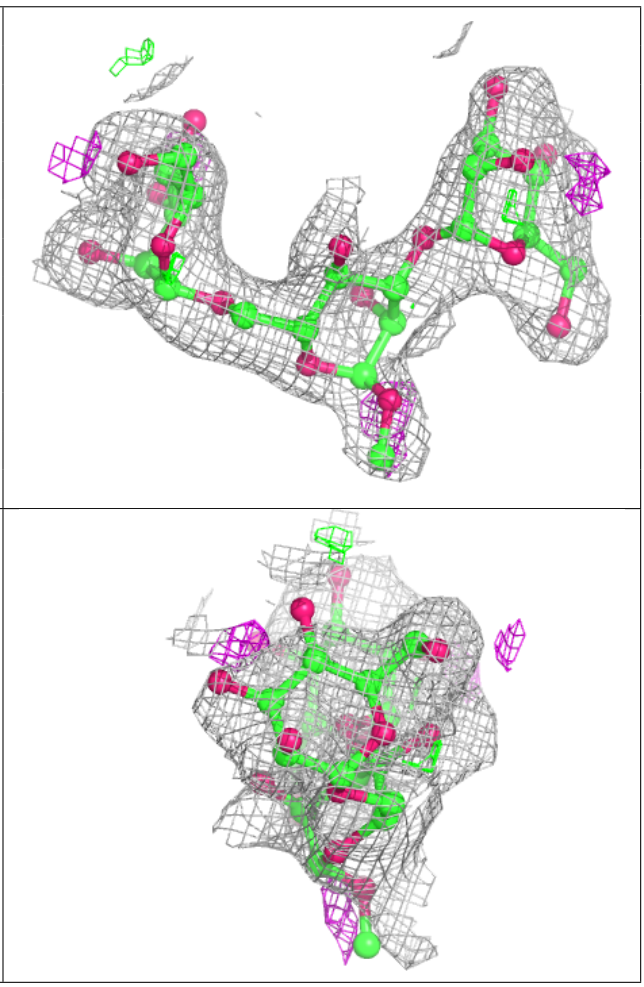
6.3 Carbohydrates (i)

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.

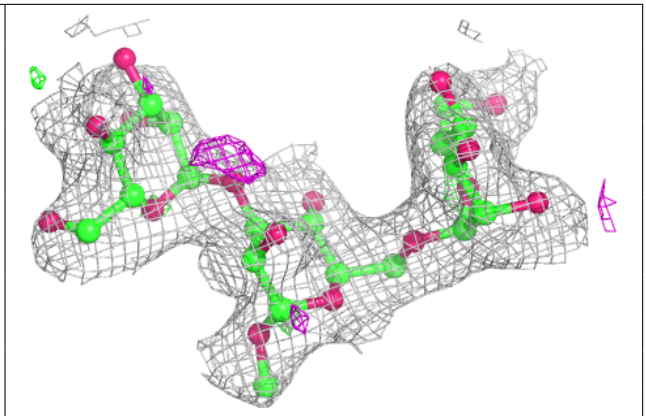
Electron density around Chain E:

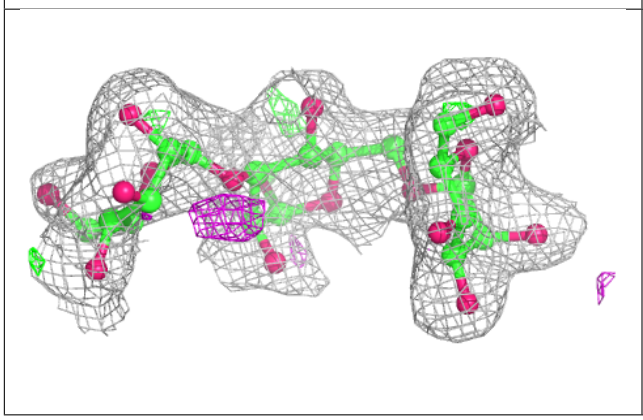
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

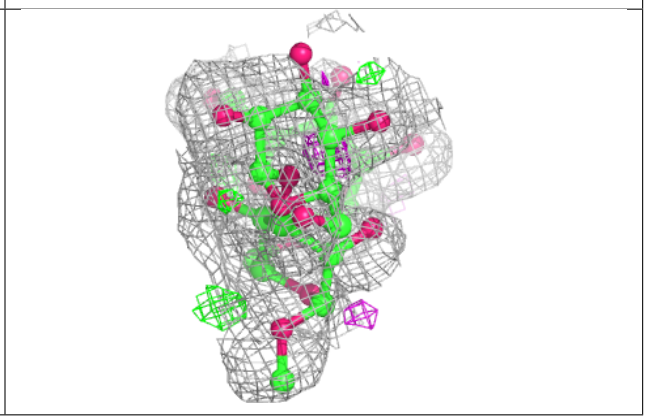


Electron density around Chain F:

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

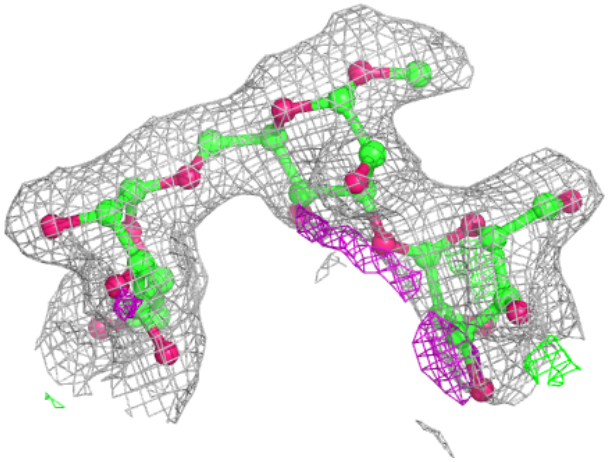


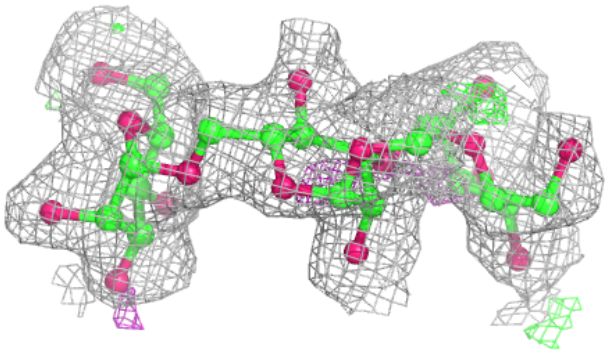




Electron density around Chain G:

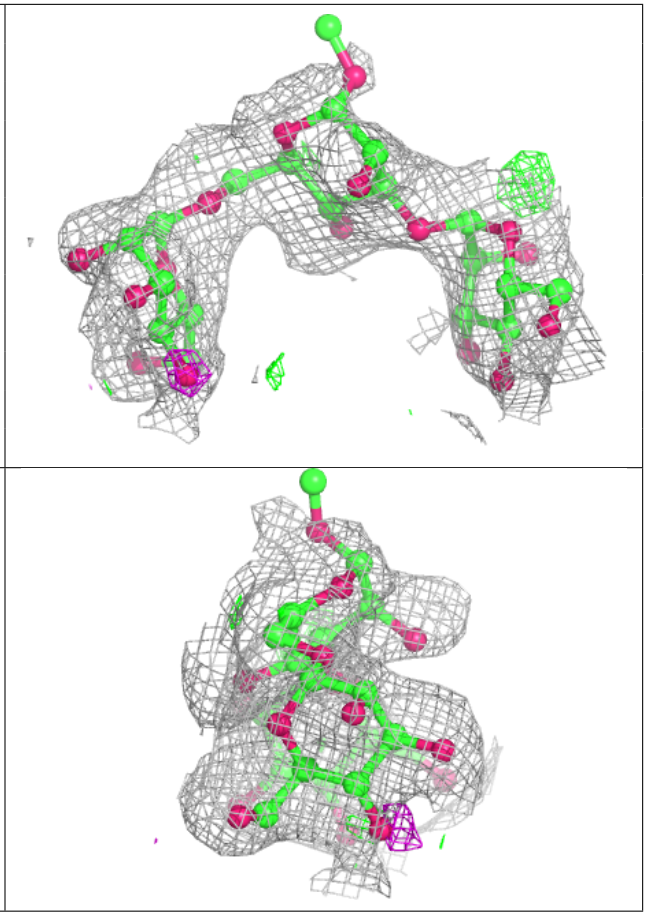
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around Chain H:

$2mF_o$-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)

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

6.5 Other polymers (i)

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