

wwPDB X-ray Structure Validation Summary Report (i)

Apr 13, 2022 – 12:09 pm BST

PDB ID : 7Q1Y

Title : X-ray structure of human A2ML1

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2021-10-22 Deposited on

4.40 Å(reported) Resolution

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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.4, CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.27

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0267

CCP4 7.1.010 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

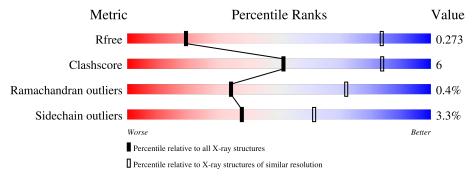
Validation Pipeline (wwPDB-VP)

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 4.40 Å.

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



Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)

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	1436	78%	16%			
1	В	1436	80%	14%			
2	С	3	100%				
2	D	3	67%	33%			
2	Е	3	33% 33%	33%			
2	F	3	67%	33%			
2	I	3		67%			

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Mol	Chain	Length	Quality of chain				
3	G	2	100%				
3	Н	2	50%	50%			



2 Entry composition (i)

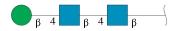
There are 4 unique types of molecules in this entry. The entry contains 21765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-2-macroglobulin-like protein 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	1374	Total 10729	C 6858	N 1761	O 2058	S 52	0	0	0
1	В	1374	Total 10729	C 6858	N 1761	O 2058	S 52	0	0	0

• 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	С	3	Total C N O 39 22 2 15	0	0	0
2	D	3	Total C N O 39 22 2 15	0	0	0
2	Е	3	Total C N O 39 22 2 15	0	0	0
2	F	3	Total C N O 39 22 2 15	0	0	0
2	I	3	Total C N O 39 22 2 15	0	0	0

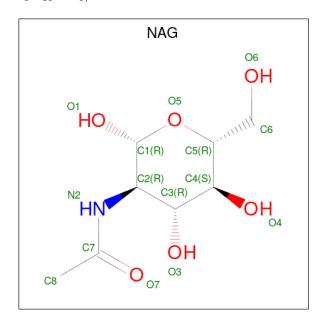
• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





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

 \bullet Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



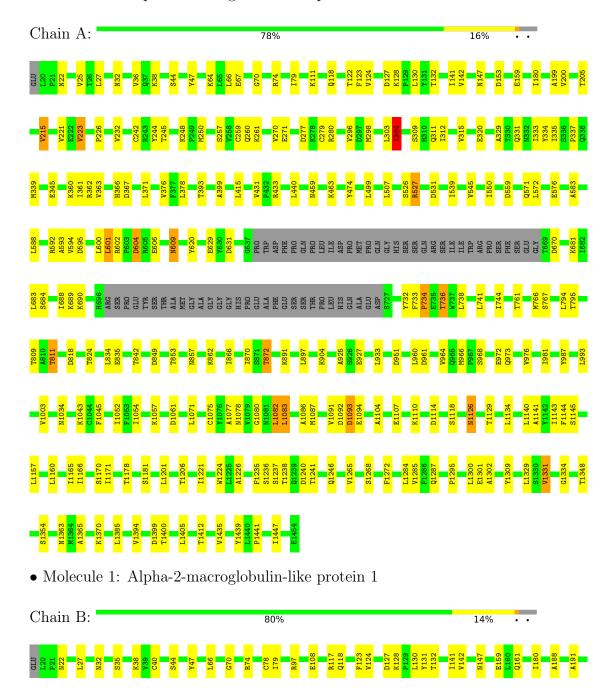
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O	0	0
			14 8 1 5		
4	Α	1	Total C N O	0	0
	71	1	14 8 1 5		O D
4	В	1	Total C N O	0	0
4	Б	1	14 8 1 5	U	U
4	В	1	Total C N O	0	0
4	D	1	14 8 1 5	U	U



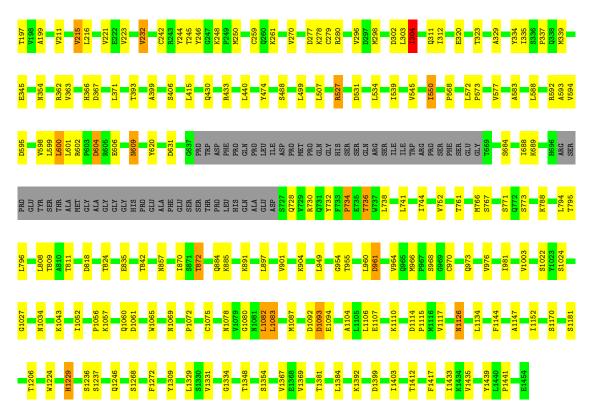
3 Residue-property plots (i)

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: Alpha-2-macroglobulin-like protein 1







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

Chain C: 100%

NAG1 NAG2 BMA3

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

Chain D: 67% 33%

NAG1 NAG2 BMA3

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

Chain E: 33% 33% 33%

NAG1 NAG2 BMA3

 $\bullet \ \, \text{Molecule 2: beta-D-mannopyranose-} (1\text{-}4)\text{-}2\text{-}acetamido-2\text{-}deoxy-beta-D-glucopyranose-} (1\text{-}4)\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}$

Chain F: 67% 33%





 $\bullet \ \, \text{Molecule 2: beta-D-mannopyranose-} (1\text{-}4)\text{-}2\text{-}acetamido-2\text{-}deoxy-beta-D-glucopyranose-} (1\text{-}4)\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}2\text{-}acetamido-2\text{-}$

Chain I: 33% 67%



 $\bullet \ \, \text{Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$

Chain G: 100%

NAG1 NAG2

 \bullet Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50% 50%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	320.15Å 320.15Å 321.94Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 - 4.40	Depositor
Resolution (A)	49.90 - 4.28	EDS
% Data completeness	99.8 (49.37-4.40)	Depositor
(in resolution range)	99.5 (49.90-4.28)	EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.97 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P. P.	0.238 , 0.276	Depositor
R, R_{free}	0.237 , 0.273	DCC
R_{free} test set	2000 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	294.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21765	wwPDB-VP
Average B, all atoms (Å ²)	342.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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, NAG

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.37	0/10975	0.58	0/14922	
1	В	0.36	0/10975	0.58	$1/14922 \ (0.0\%)$	
All	All	0.37	0/21950	0.58	1/29844~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	970	CYS	CA-CB-SG	-6.62	102.09	114.00

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	10729	0	10606	130	0
1	В	10729	0	10607	113	0
2	С	39	0	34	1	0
2	D	39	0	34	0	0
2	Е	39	0	34	2	0
2	F	39	0	34	0	0
2	I	39	0	34	0	0
3	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Н	28	0	25	0	0
4	A	28	0	26	0	0
4	В	28	0	26	0	0
All	All	21765	0	21485	241	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 6.

The worst 5 of 241 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:128:LYS:NZ	1:B:734:PRO:O	2.01	0.93
1:A:128:LYS:NZ	1:A:734:PRO:O	2.02	0.92
1:A:147:ASN:O	1:A:527:ARG:NH1	2.10	0.85
1:B:904:LYS:NZ	1:B:1399:ASP:OD2	2.12	0.83
1:A:360:LYS:NZ	1:A:459:ASN:OD1	2.11	0.83

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	Perce	ntiles
1	A	1368/1436 (95%)	1304 (95%)	58 (4%)	6 (0%)	34	72
1	В	$1368/1436 \ (95\%)$	1304 (95%)	58 (4%)	6 (0%)	34	72
All	All	2736/2872 (95%)	2608 (95%)	116 (4%)	12 (0%)	34	72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	VAL

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Mol	Chain	Res	Type
1	A	1181	SER
1	В	215	VAL
1	В	1092	ASP
1	В	1181	SER

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	Percentile	\mathbf{s}
1	A	$1201/1253\ (96\%)$	1164 (97%)	37 (3%)	40 63	
1	В	1201/1253~(96%)	1158 (96%)	43 (4%)	35 60	
All	All	2402/2506~(96%)	2322 (97%)	80 (3%)	38 61	

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	736	THR
1	В	1082	LEU
1	В	766	MET
1	В	955	THR
1	В	1134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	22	ASN
1	В	152	ASN
1	В	772	GLN

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)

19 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	Во	ond leng	ths	В	ond ang	les
IVIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	С	1	1,2	14,14,15	0.52	0	17,19,21	0.49	0
2	NAG	С	2	2	14,14,15	0.80	1 (7%)	17,19,21	0.67	0
2	BMA	С	3	2	11,11,12	1.75	4 (36%)	15,15,17	0.99	0
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	0.62	0
2	NAG	D	2	2	14,14,15	0.69	0	17,19,21	0.51	0
2	BMA	D	3	2	11,11,12	1.59	4 (36%)	15,15,17	1.04	0
2	NAG	Е	1	1,2	14,14,15	0.52	0	17,19,21	0.75	0
2	NAG	Е	2	2	14,14,15	0.46	0	17,19,21	1.31	2 (11%)
2	BMA	Е	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.12	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.42	0	17,19,21	0.69	0
2	NAG	F	2	2	14,14,15	0.58	0	17,19,21	0.55	0
2	BMA	F	3	2	11,11,12	1.82	4 (36%)	15,15,17	1.11	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.30	0	17,19,21	0.44	0
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	0.65	1 (5%)
3	NAG	Н	1	1,3	14,14,15	0.36	0	17,19,21	0.70	0
3	NAG	Н	2	3	14,14,15	0.88	1 (7%)	17,19,21	0.56	0
2	NAG	I	1	1,2	14,14,15	0.30	0	17,19,21	0.52	0
2	NAG	I	2	2	14,14,15	0.80	1 (7%)	17,19,21	0.63	0
2	BMA	I	3	2	11,11,12	1.27	2 (18%)	15,15,17	0.90	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	С	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	0/6/23/26	0/1/1/1
2	BMA	С	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	NAG	Ε	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Ε	2	2	-	1/6/23/26	0/1/1/1
2	BMA	Ε	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Н	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Н	2	3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
2	D	3	BMA	C1-C2	3.28	1.59	1.52
2	С	3	BMA	C1-C2	3.15	1.59	1.52
2	F	3	BMA	C1-C2	3.06	1.59	1.52
2	F	3	BMA	C4-C3	2.94	1.59	1.52
3	Н	2	NAG	O5-C1	2.60	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	E	3	BMA	C1-O5-C5	3.17	116.48	112.19
2	Е	2	NAG	C3-C4-C5	2.88	115.37	110.24
2	Е	2	NAG	C2-N2-C7	2.71	126.76	122.90
2	F	3	BMA	O5-C5-C6	2.14	110.55	107.20
3	G	2	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:



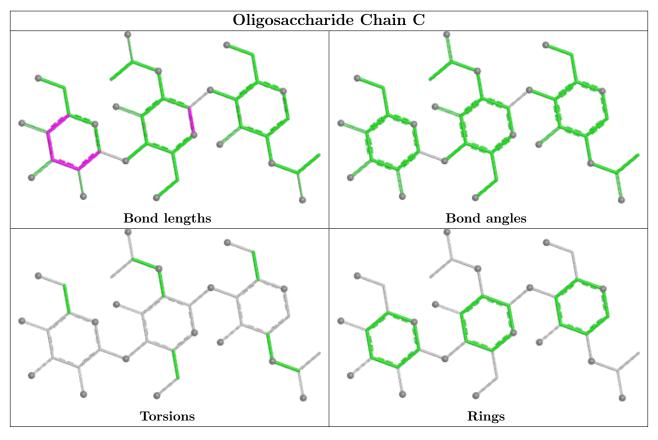
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
3	Н	2	NAG	O5-C5-C6-O6
3	Н	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6

There are no ring outliers.

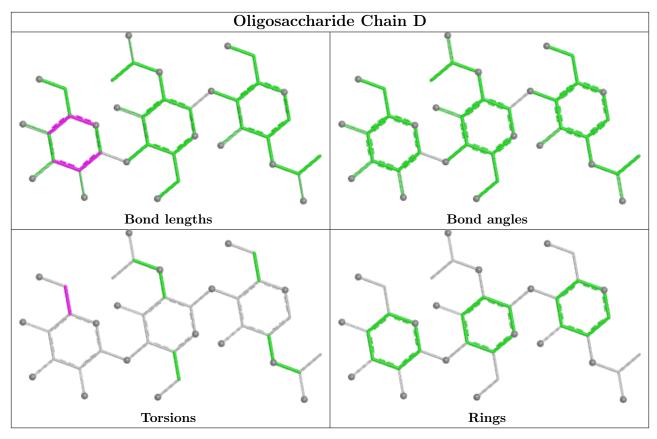
3 monomers are involved in 4 short contacts:

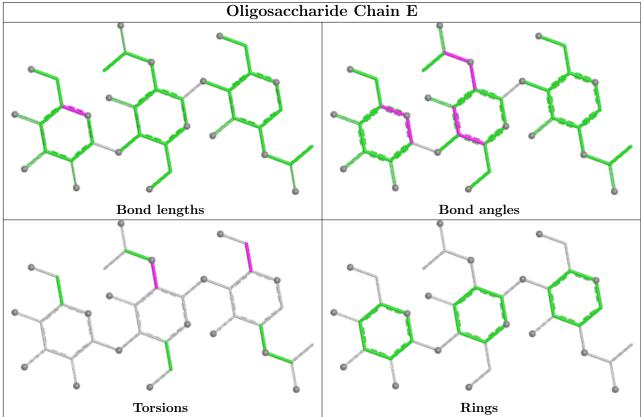
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1	NAG	1	0
2	Е	3	BMA	2	0
3	G	1	NAG	1	0

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

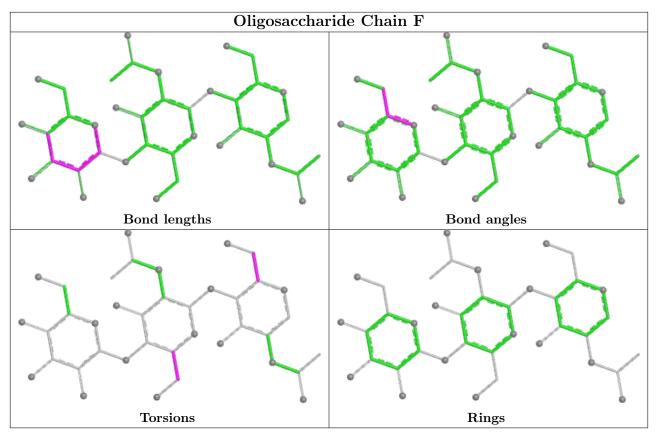


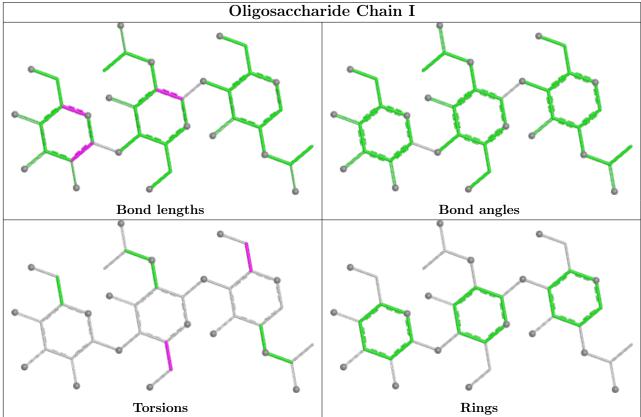




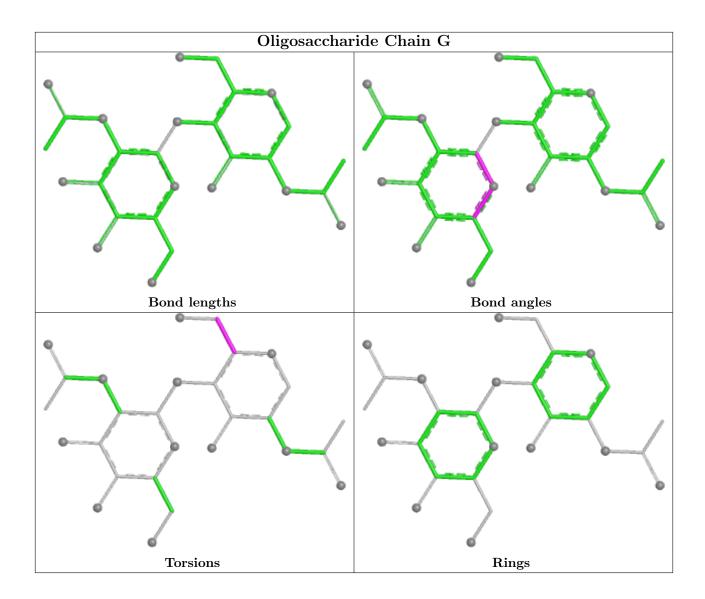




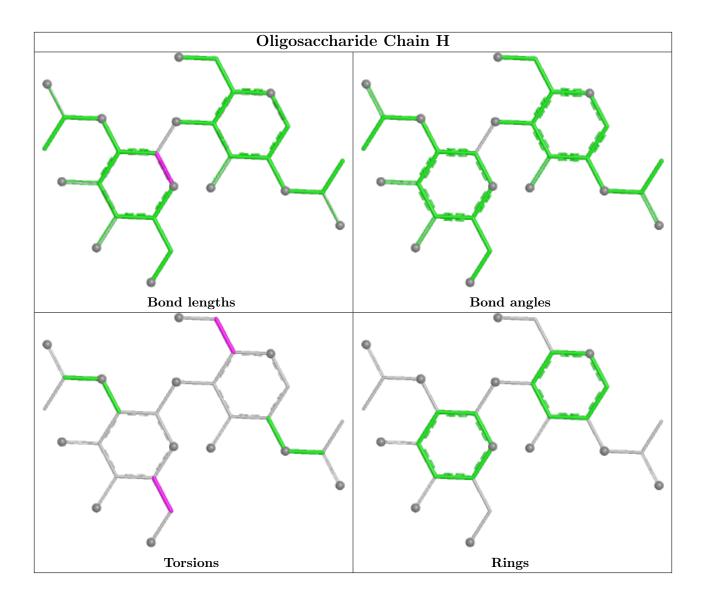












5.6 Ligand geometry (i)

4 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).

1/4	ol	Type	Chain	Res	Link	Bo	ond leng	В	ond ang	les	
101	.01	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	1	NAG	В	1502	1	14,14,15	0.85	1 (7%)	17,19,21	2.00	3 (17%)
4	1	NAG	A	1501	1	14,14,15	0.48	0	17,19,21	0.43	0
4	1	NAG	A	1502	1	14,14,15	0.27	0	17,19,21	0.42	0



Mol	Type	Chain	Pos	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
WIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	В	1501	1	14,14,15	0.43	0	17,19,21	0.54	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
4	NAG	В	1502	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	В	1501	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
4	В	1502	NAG	C1-C2	2.51	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
4	В	1502	NAG	C2-N2-C7	7.15	133.08	122.90
4	В	1502	NAG	C1-C2-N2	2.70	115.10	110.49
4	В	1502	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	1502	NAG	C4-C5-C6-O6
4	В	1502	NAG	O5-C5-C6-O6
4	В	1502	NAG	C8-C7-N2-C2
4	В	1502	NAG	O7-C7-N2-C2
4	A	1501	NAG	O5-C5-C6-O6

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.

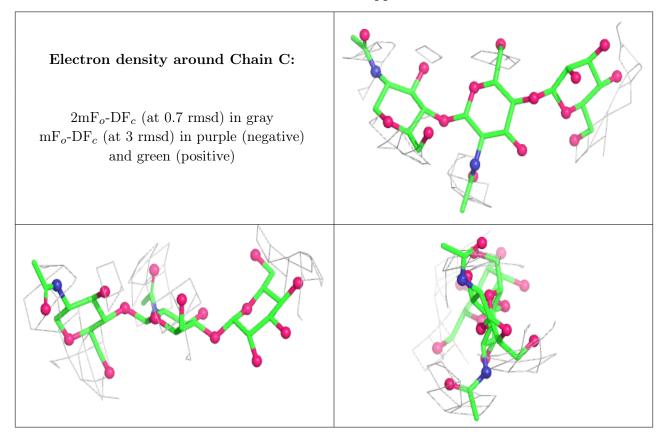
6.2 Non-standard residues in protein, DNA, RNA chains (i)

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.

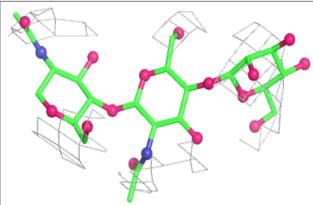
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

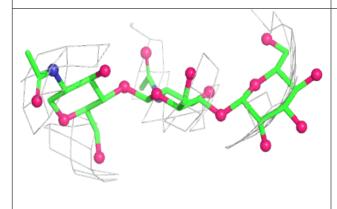


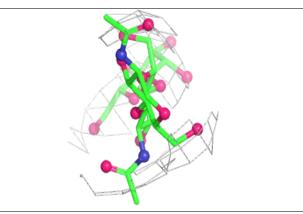


Electron density around Chain D:

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

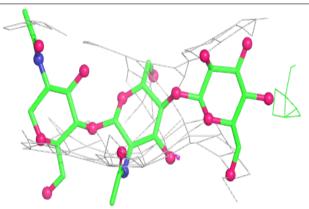


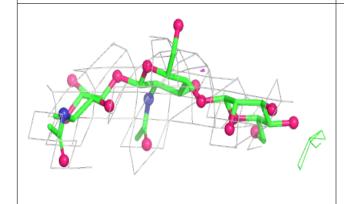


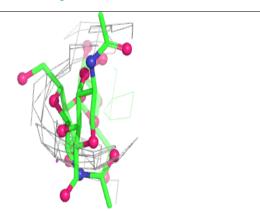


Electron density around Chain E:

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



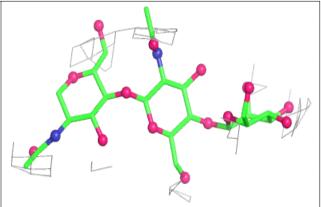


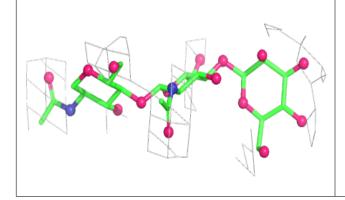


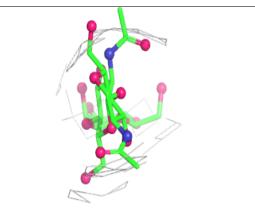


Electron density around Chain F:

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

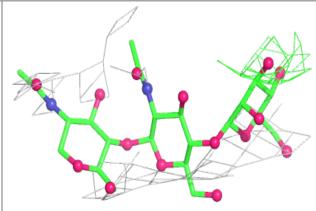


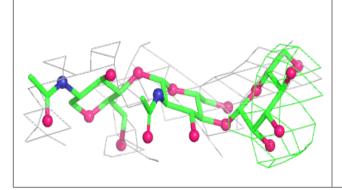


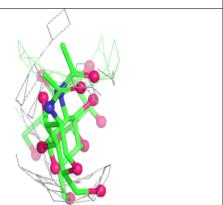


Electron density around Chain I:

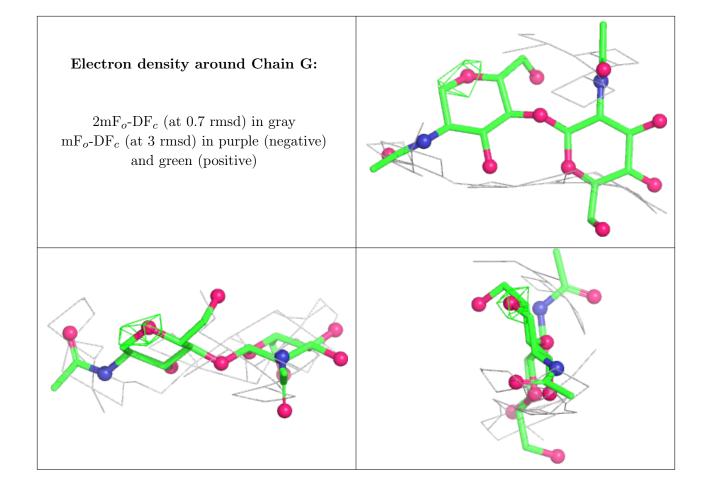
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



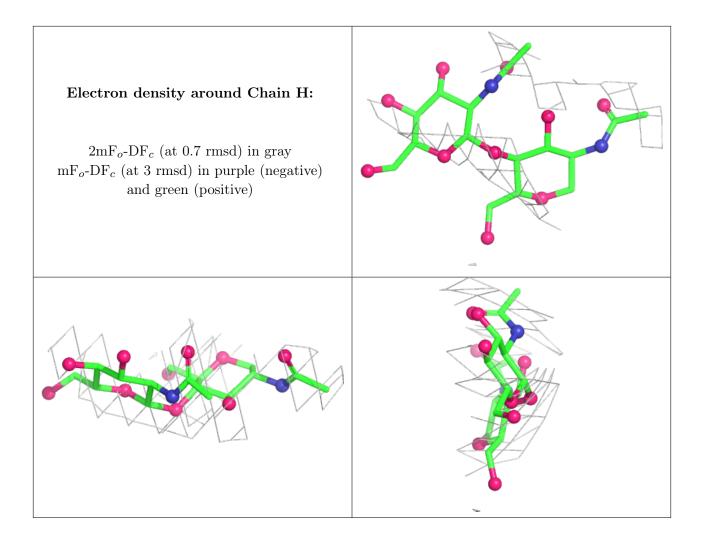












6.4 Ligands (i)

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.

