



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 07:12 AM BST

PDB ID : 1TYE
Title : Structural basis for allostery in integrins and binding of ligand-mimetic therapeutics to the platelet receptor for fibrinogen
Authors : Xiao, T.; Takagi, J.; Collier, B.S.; Wang, J.-H.; Springer, T.A.
Deposited on : 2004-07-07
Resolution : 2.90 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 ⓘ 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
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

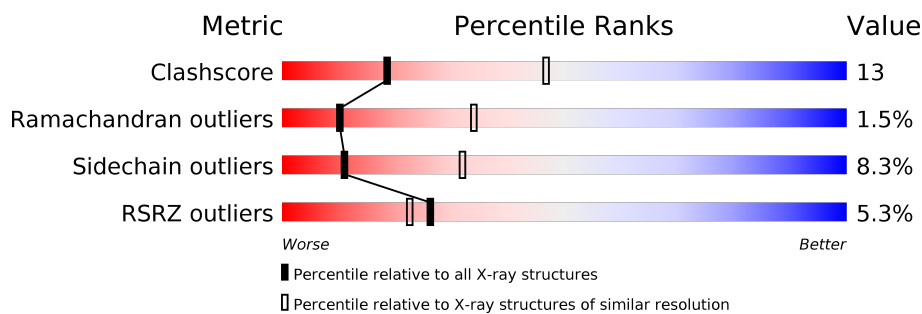
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	452	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	C	452	<div> <div>%</div> <div>74%</div> <div>20%</div> <div>5%</div> <div>•</div> </div>
1	E	452	<div> <div>%</div> <div>74%</div> <div>21%</div> <div>5%</div> <div>•</div> </div>
2	B	440	<div> <div>9%</div> <div>64%</div> <div>33%</div> <div>•</div> </div>
2	D	440	<div> <div>5%</div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
2	F	440	<div> <div>13%</div> <div>72%</div> <div>24%</div> <div>•</div> </div>
3	G	4	<div> <div>25%</div> <div>75%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	4	
4	H	5	

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
3	NAG	I	2	-	-	X	-
4	BMA	H	4	-	-	-	X
6	NAG	F	1015	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21019 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			
1	C	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			
1	E	452	Total	C	N	O	S	0	0	0
			3468	2203	597	660	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			
2	D	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			
2	F	440	Total	C	N	O	S	0	0	0
			3400	2125	574	672	29			

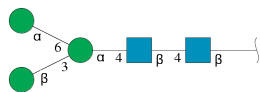
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyrano

se-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

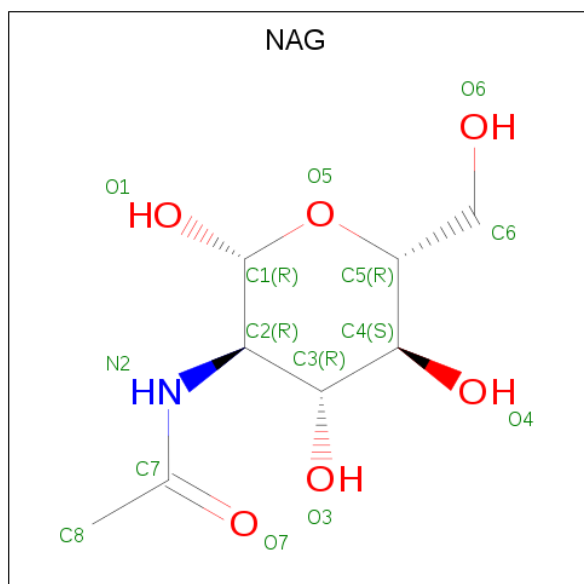


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

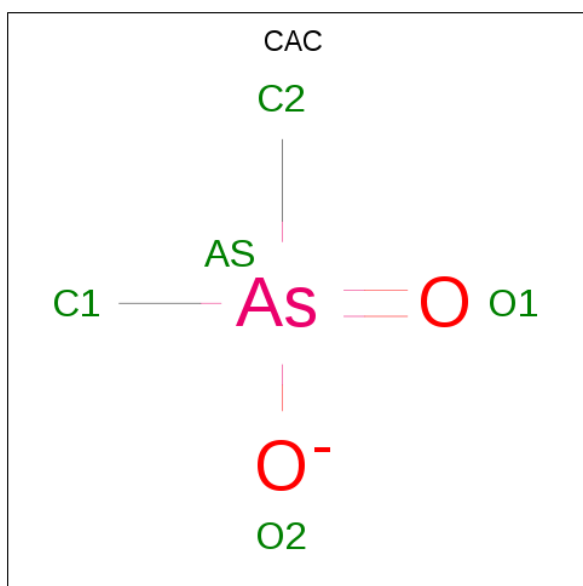
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Ca	0	0
			2	2		
5	E	4	Total	Ca	0	0
			4	4		
5	B	2	Total	Ca	0	0
			2	2		
5	C	4	Total	Ca	0	0
			4	4		
5	A	4	Total	Ca	0	0
			4	4		
5	F	2	Total	Ca	0	0
			2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	As	C	O	0	0
			5	1	2	2		
7	D	1	Total	As	C	O	0	0
			5	1	2	2		
7	F	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0
8	F	1	Total Mg 1 1	0	0

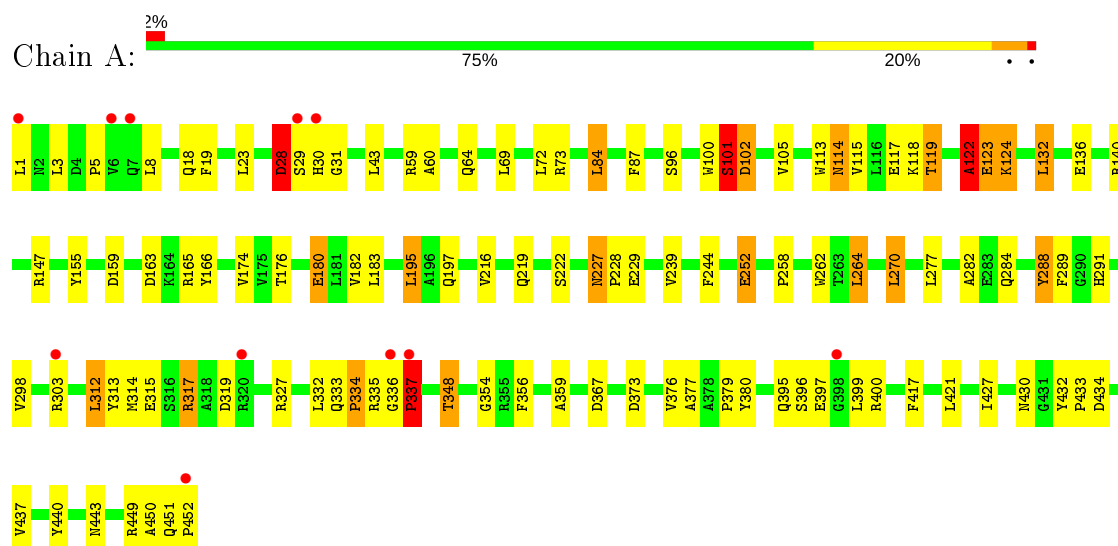
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	22	Total O 22 22	0	0
9	B	16	Total O 16 16	0	0
9	C	20	Total O 20 20	0	0
9	D	19	Total O 19 19	0	0
9	E	28	Total O 28 28	0	0
9	F	15	Total O 15 15	0	0

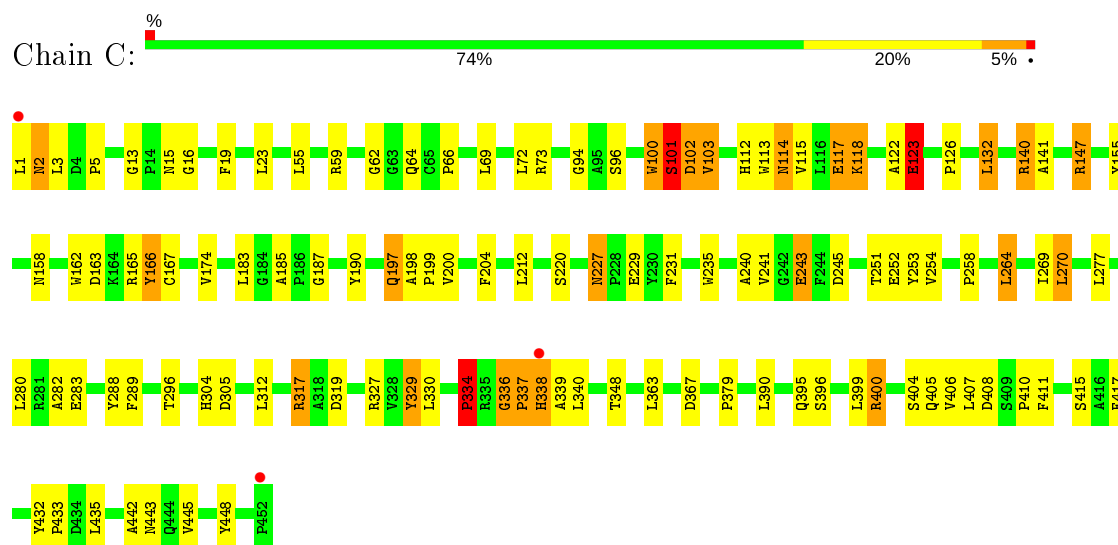
3 Residue-property plots

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 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.

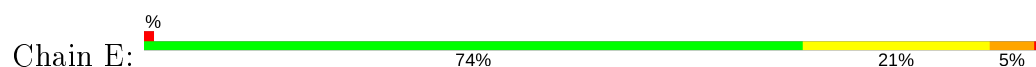
• Molecule 1: Integrin alpha-IIb

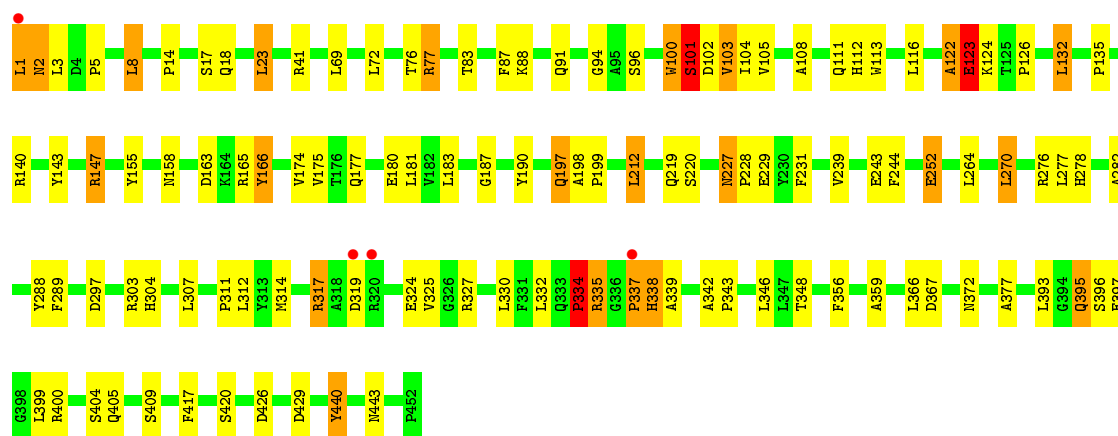


• Molecule 1: Integrin alpha-IIb

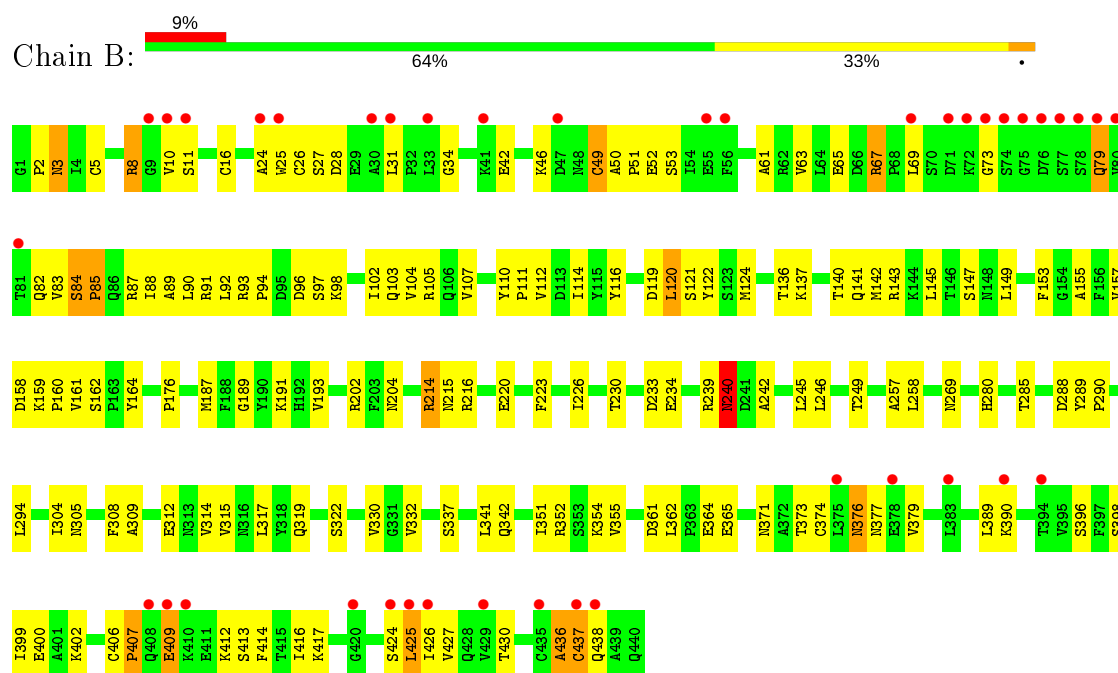


• Molecule 1: Integrin alpha-IIb

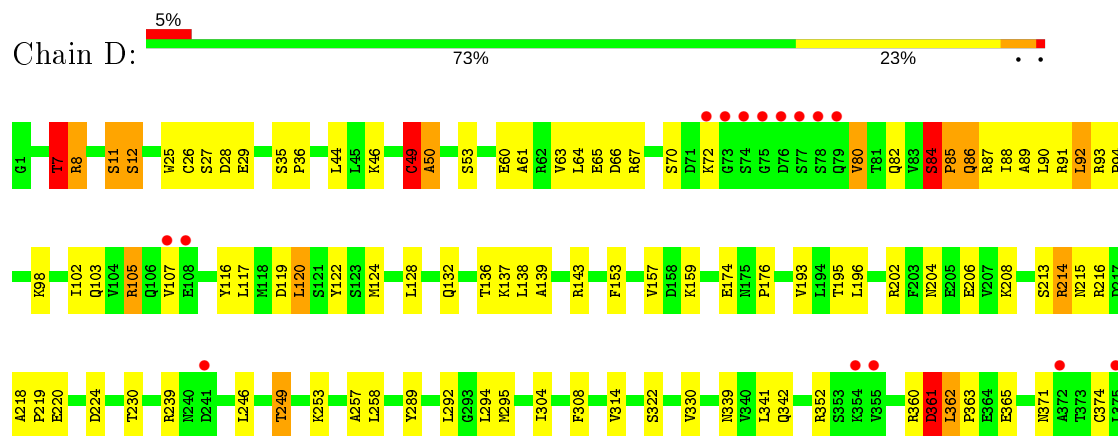


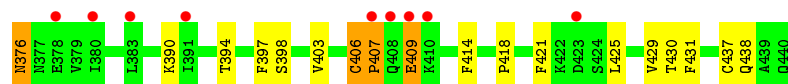


• Molecule 2: Integrin beta-3

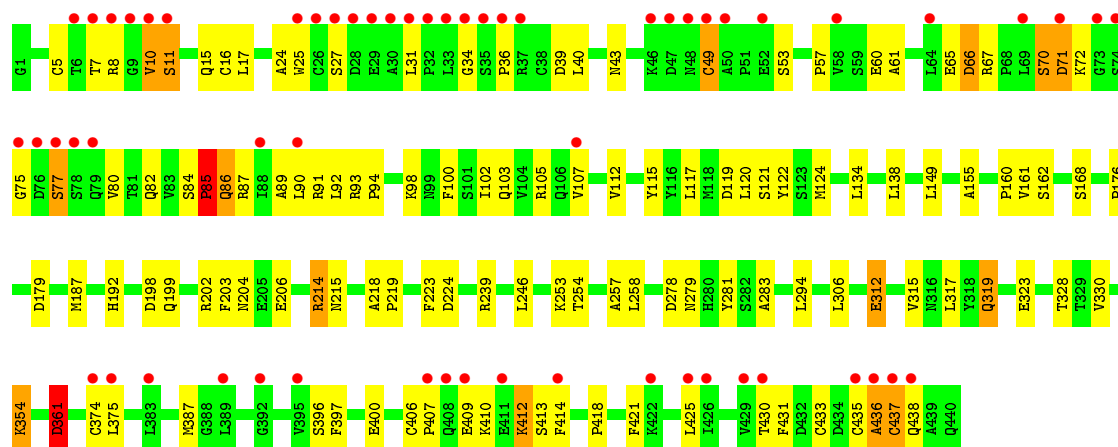
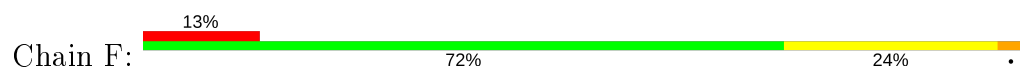


• Molecule 2: Integrin beta-3





• Molecule 2: Integrin beta-3



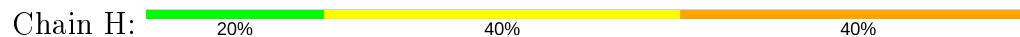
• Molecule 3: beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	332.09 Å 332.09 Å 88.29 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 47.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.90) 98.3 (47.28-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.91 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.254 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21019	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, CA, CAC, 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	0.75	9/3564 (0.3%)	0.86	11/4857 (0.2%)
1	C	0.60	7/3564 (0.2%)	0.95	17/4857 (0.4%)
1	E	0.61	4/3564 (0.1%)	0.88	12/4857 (0.2%)
2	B	0.40	0/3461	0.80	6/4693 (0.1%)
2	D	0.68	5/3461 (0.1%)	0.78	9/4693 (0.2%)
2	F	0.39	0/3461	0.73	9/4693 (0.2%)
All	All	0.59	25/21075 (0.1%)	0.84	64/28650 (0.2%)

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	4
1	C	0	5
1	E	0	3
2	D	0	3
2	F	0	1
All	All	0	16

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	85	PRO	N-CD	28.23	1.87	1.47
1	A	101	SER	CB-OG	22.05	1.71	1.42
1	A	123	GLU	CB-CG	17.06	1.84	1.52
1	E	123	GLU	C-N	-16.41	0.96	1.34
1	E	122	ALA	C-N	13.02	1.64	1.34

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	SER	C-N-CD	-26.08	63.23	120.60
1	C	101	SER	O-C-N	-24.91	82.84	122.70
1	E	123	GLU	O-C-N	-18.48	93.12	122.70
1	C	334	PRO	CA-N-CD	-16.12	88.93	111.50
1	A	122	ALA	O-C-N	-15.63	97.70	122.70

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TRP	Mainchain
1	A	122	ALA	Mainchain,Peptide
1	A	28	ASP	Mainchain
1	C	100	TRP	Mainchain,Peptide
1	C	101	SER	Mainchain

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	3468	0	3300	85	0
1	C	3468	0	3299	75	0
1	E	3468	0	3297	84	0
2	B	3400	0	3350	110	0
2	D	3400	0	3349	91	0
2	F	3400	0	3350	85	0
3	G	50	0	43	6	0
3	I	50	0	43	9	0
4	H	61	0	52	5	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
6	B	28	0	26	2	0
6	D	28	0	26	0	0
6	E	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	28	0	26	3	0
7	B	5	0	0	1	0
7	D	5	0	0	1	0
7	F	5	0	0	1	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	A	22	0	0	1	0
9	B	16	0	0	0	0
9	C	20	0	0	1	0
9	D	19	0	0	0	0
9	E	28	0	0	1	0
9	F	15	0	0	0	0
All	All	21019	0	20174	541	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 13.

The worst 5 of 541 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)
2:D:85:PRO:CB	2:D:85:PRO:CG	1.76	1.59
1:A:123:GLU:CG	1:A:123:GLU:CB	1.84	1.52
1:C:117:GLU:C	1:C:117:GLU:CA	1.84	1.45
1:A:101:SER:CB	1:A:101:SER:OG	1.70	1.38
2:D:85:PRO:CD	2:D:85:PRO:N	1.87	1.37

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	450/452 (100%)	404 (90%)	40 (9%)	6 (1%)	12	37
1	C	450/452 (100%)	409 (91%)	34 (8%)	7 (2%)	9	32
1	E	450/452 (100%)	414 (92%)	33 (7%)	3 (1%)	22	54
2	B	438/440 (100%)	390 (89%)	39 (9%)	9 (2%)	7	26
2	D	438/440 (100%)	387 (88%)	43 (10%)	8 (2%)	8	29
2	F	438/440 (100%)	386 (88%)	45 (10%)	7 (2%)	9	32
All	All	2664/2676 (100%)	2390 (90%)	234 (9%)	40 (2%)	10	34

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
2	B	85	PRO
1	C	101	SER
1	C	102	ASP
1	C	123	GLU

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	360/360 (100%)	329 (91%)	31 (9%)	10	30
1	C	360/360 (100%)	327 (91%)	33 (9%)	9	27
1	E	360/360 (100%)	328 (91%)	32 (9%)	9	29
2	B	392/392 (100%)	361 (92%)	31 (8%)	12	34
2	D	392/392 (100%)	358 (91%)	34 (9%)	10	30
2	F	392/392 (100%)	365 (93%)	27 (7%)	15	41
All	All	2256/2256 (100%)	2068 (92%)	188 (8%)	11	32

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	288	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	174	GLU
2	F	206	GLU
1	C	317	ARG
2	D	46	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	304	HIS
2	D	15	GLN
2	F	82	GLN
1	C	338	HIS
1	C	395	GLN

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 ⓘ

13 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	$\# Z > 2$
3	NAG	G	1	3,2	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
3	MAN	G	3	3	11,11,12	0.70	0	15,15,17	1.36	2 (13%)
3	BMA	G	4	3	11,11,12	0.47	0	15,15,17	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	H	1	2,4	14,14,15	0.43	0	17,19,21	0.76	1 (5%)
4	NAG	H	2	4	14,14,15	0.62	0	17,19,21	0.85	0
4	MAN	H	3	4	11,11,12	0.74	0	15,15,17	1.14	2 (13%)
4	BMA	H	4	4	11,11,12	0.49	0	15,15,17	0.58	0
4	MAN	H	5	4	11,11,12	0.56	0	15,15,17	0.57	0
3	NAG	I	1	3,2	14,14,15	0.43	0	17,19,21	0.72	0
3	NAG	I	2	3	14,14,15	0.69	0	17,19,21	0.84	1 (5%)
3	MAN	I	3	3	11,11,12	0.64	0	15,15,17	0.97	1 (6%)
3	BMA	I	4	3	11,11,12	0.51	0	15,15,17	0.64	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
3	NAG	G	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	MAN	G	3	3	-	1/2/19/22	0/1/1/1
3	BMA	G	4	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	MAN	H	3	4	-	2/2/19/22	0/1/1/1
4	BMA	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	MAN	I	3	3	-	1/2/19/22	0/1/1/1
3	BMA	I	4	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	C3-C4-C5	3.57	116.61	110.24
4	H	3	MAN	C1-C2-C3	2.97	113.32	109.67
3	I	3	MAN	C1-C2-C3	2.88	113.20	109.67
3	I	2	NAG	C4-C3-C2	2.47	114.64	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	C1-C2-C3	2.29	112.48	109.67

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2

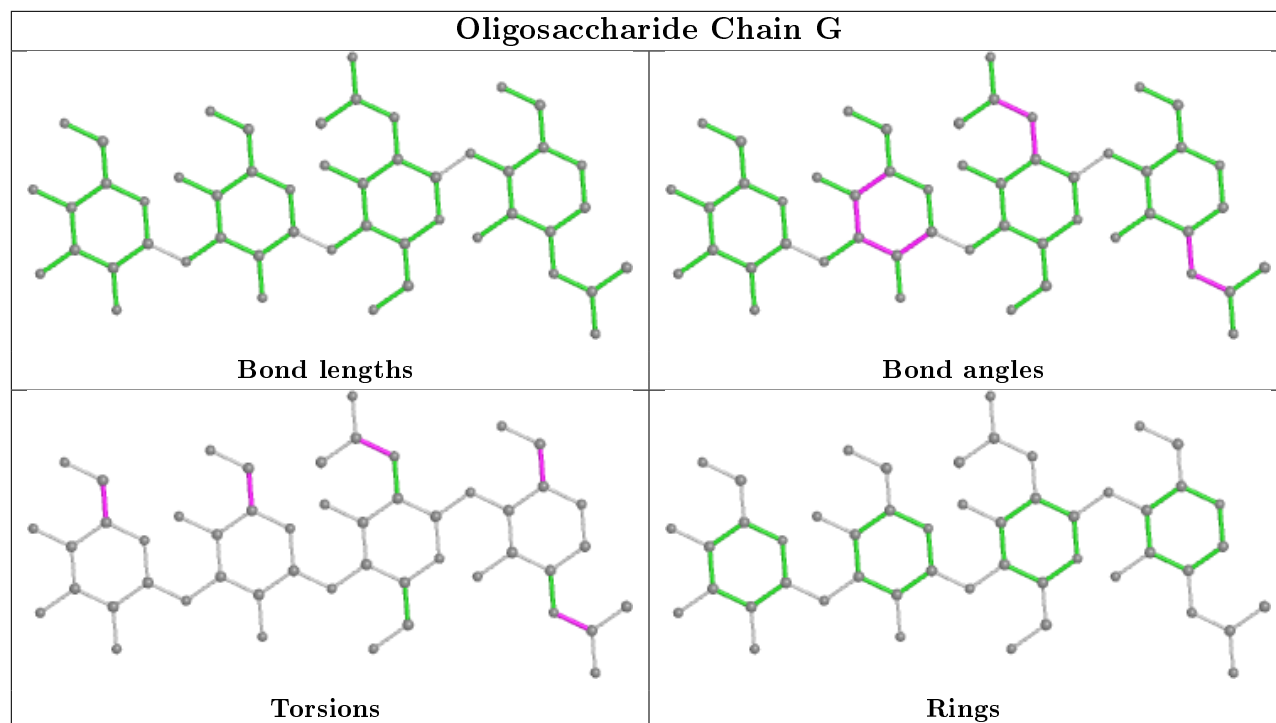
There are no ring outliers.

12 monomers are involved in 20 short contacts:

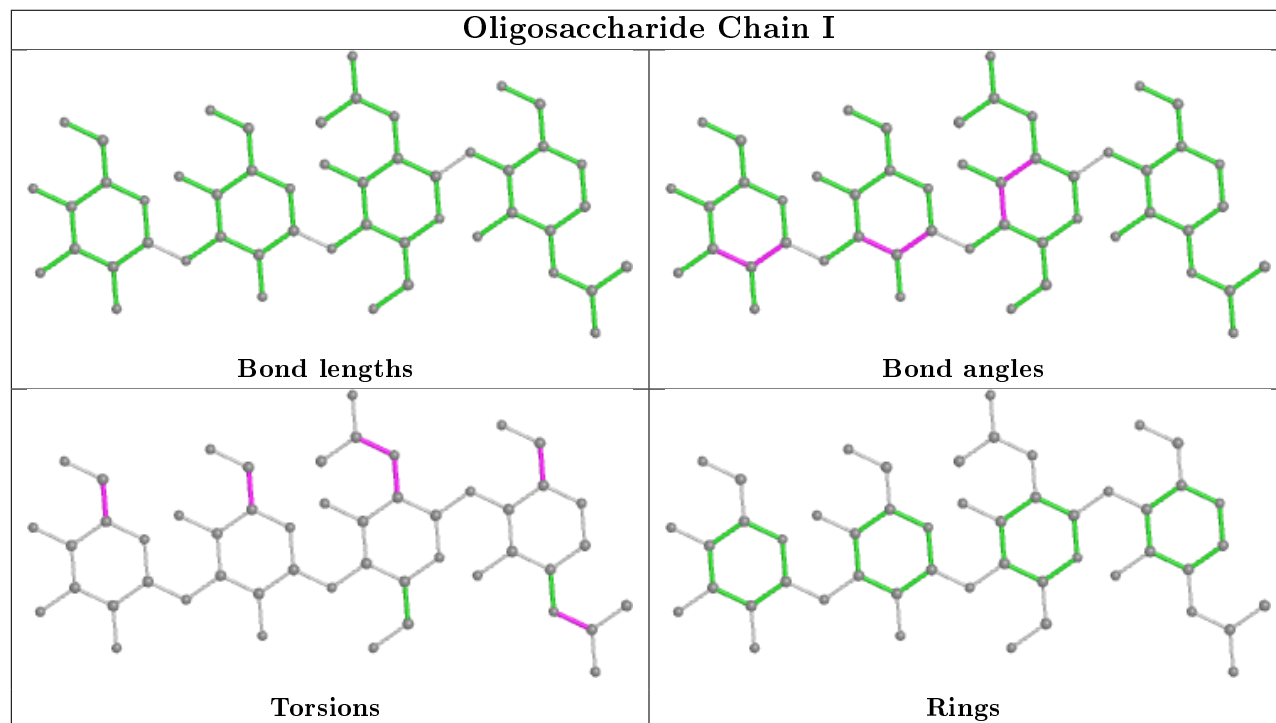
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	MAN	5	0
4	H	4	BMA	1	0
3	I	1	NAG	6	0
4	H	1	NAG	2	0
4	H	3	MAN	3	0
4	H	2	NAG	4	0
3	G	2	NAG	5	0
3	G	4	BMA	1	0
3	I	2	NAG	7	0
3	G	1	NAG	1	0
3	I	3	MAN	3	0
3	I	4	BMA	1	0

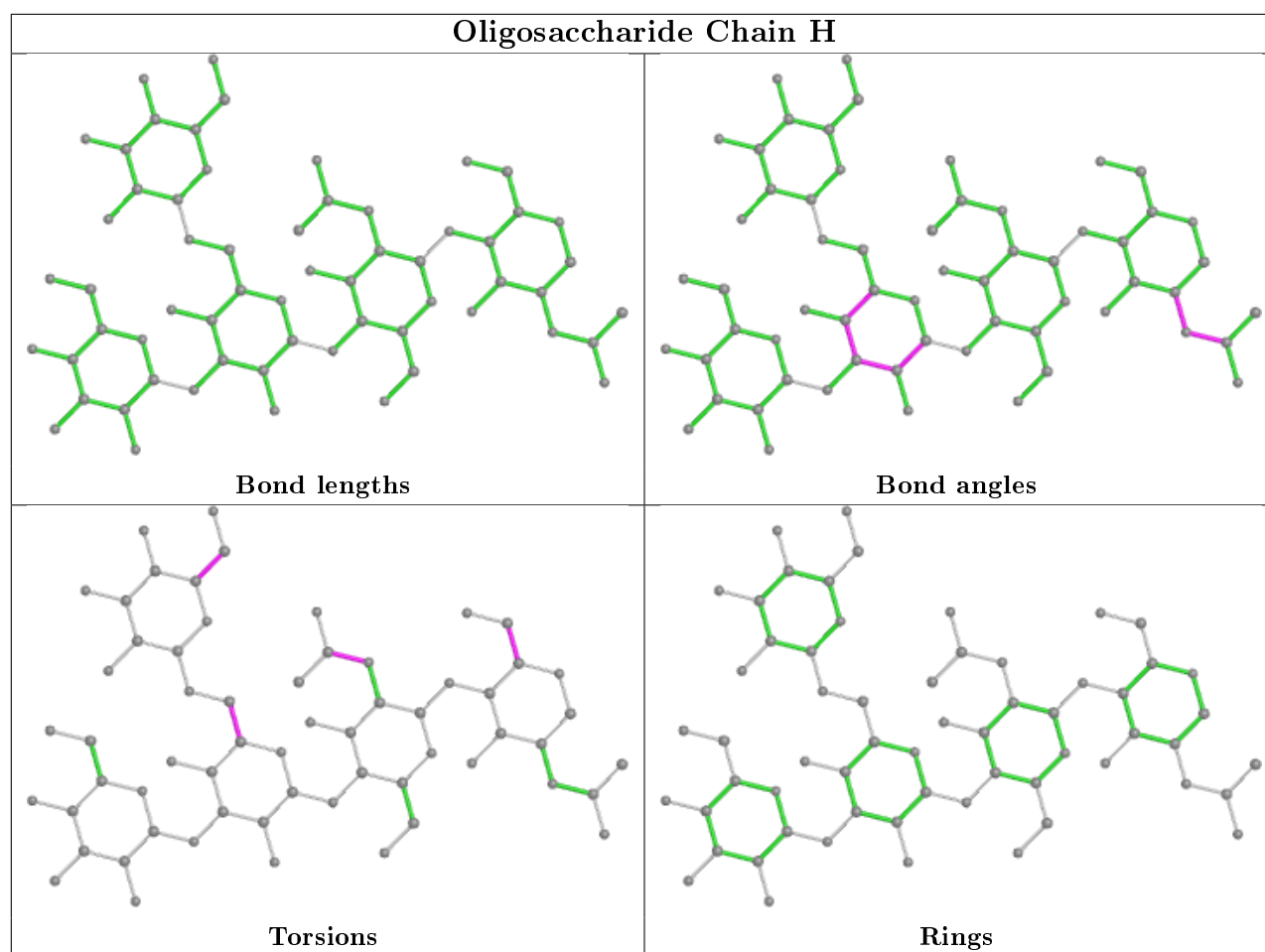
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G



Oligosaccharide Chain I





5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 21 are monoatomic - leaving 10 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	$\# Z > 2$
6	NAG	D	1007	2	14,14,15	0.55	0	17,19,21	0.57	0
6	NAG	F	1020	2	14,14,15	0.44	0	17,19,21	0.77	1 (5%)
7	CAC	B	1301	8	0,4,4	0.00	-	0,6,6	0.00	-
7	CAC	D	1302	8	0,4,4	0.00	-	0,6,6	0.00	-
6	NAG	D	1013	2	14,14,15	0.50	0	17,19,21	0.86	1 (5%)
6	NAG	E	1014	1	14,14,15	0.69	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CAC	F	1303	8	0,4,4	0.00	-	0,6,6	0.00	-
6	NAG	B	1001	2	14,14,15	0.50	0	17,19,21	0.74	0
6	NAG	F	1015	2	14,14,15	0.59	0	17,19,21	0.61	0
6	NAG	B	1006	2	14,14,15	0.51	0	17,19,21	0.66	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
6	NAG	D	1007	2	-	2/6/23/26	0/1/1/1
6	NAG	F	1020	2	-	2/6/23/26	0/1/1/1
6	NAG	D	1013	2	-	4/6/23/26	0/1/1/1
6	NAG	E	1014	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1001	2	-	4/6/23/26	0/1/1/1
6	NAG	F	1015	2	-	4/6/23/26	0/1/1/1
6	NAG	B	1006	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1013	NAG	C2-N2-C7	-2.60	119.20	122.90
6	F	1020	NAG	C2-N2-C7	-2.12	119.89	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1014	NAG	C8-C7-N2-C2
6	E	1014	NAG	O7-C7-N2-C2
6	F	1015	NAG	C8-C7-N2-C2
6	F	1015	NAG	O7-C7-N2-C2
6	B	1001	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1020	NAG	2	0
7	B	1301	CAC	1	0
7	D	1302	CAC	1	0
7	F	1303	CAC	1	0
6	F	1015	NAG	1	0
6	B	1006	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	3
2	D	2
1	C	2
1	A	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	122:ALA	C	123:GLU	N	1.64
1	D	7:THR	C	8:ARG	N	1.19
1	D	84:SER	C	85:PRO	N	1.17
1	C	100:TRP	C	101:SER	N	1.09
1	C	101:SER	C	102:ASP	N	1.07

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	452/452 (100%)	0.11	11 (2%) 59 56	19, 52, 91, 113	2 (0%)
1	C	452/452 (100%)	-0.07	3 (0%) 87 87	24, 47, 87, 108	2 (0%)
1	E	452/452 (100%)	-0.05	4 (0%) 84 84	26, 45, 79, 107	2 (0%)
2	B	440/440 (100%)	0.47	40 (9%) 9 6	31, 75, 118, 120	8 (1%)
2	D	440/440 (100%)	0.32	24 (5%) 25 21	27, 67, 108, 120	8 (1%)
2	F	440/440 (100%)	0.62	59 (13%) 3 2	36, 97, 120, 120	8 (1%)
All	All	2676/2676 (100%)	0.23	141 (5%) 26 22	19, 58, 117, 120	30 (1%)

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	73	GLY	13.8
2	B	76	ASP	13.5
2	D	76	ASP	10.0
2	B	75	GLY	9.9
2	D	75	GLY	9.2

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

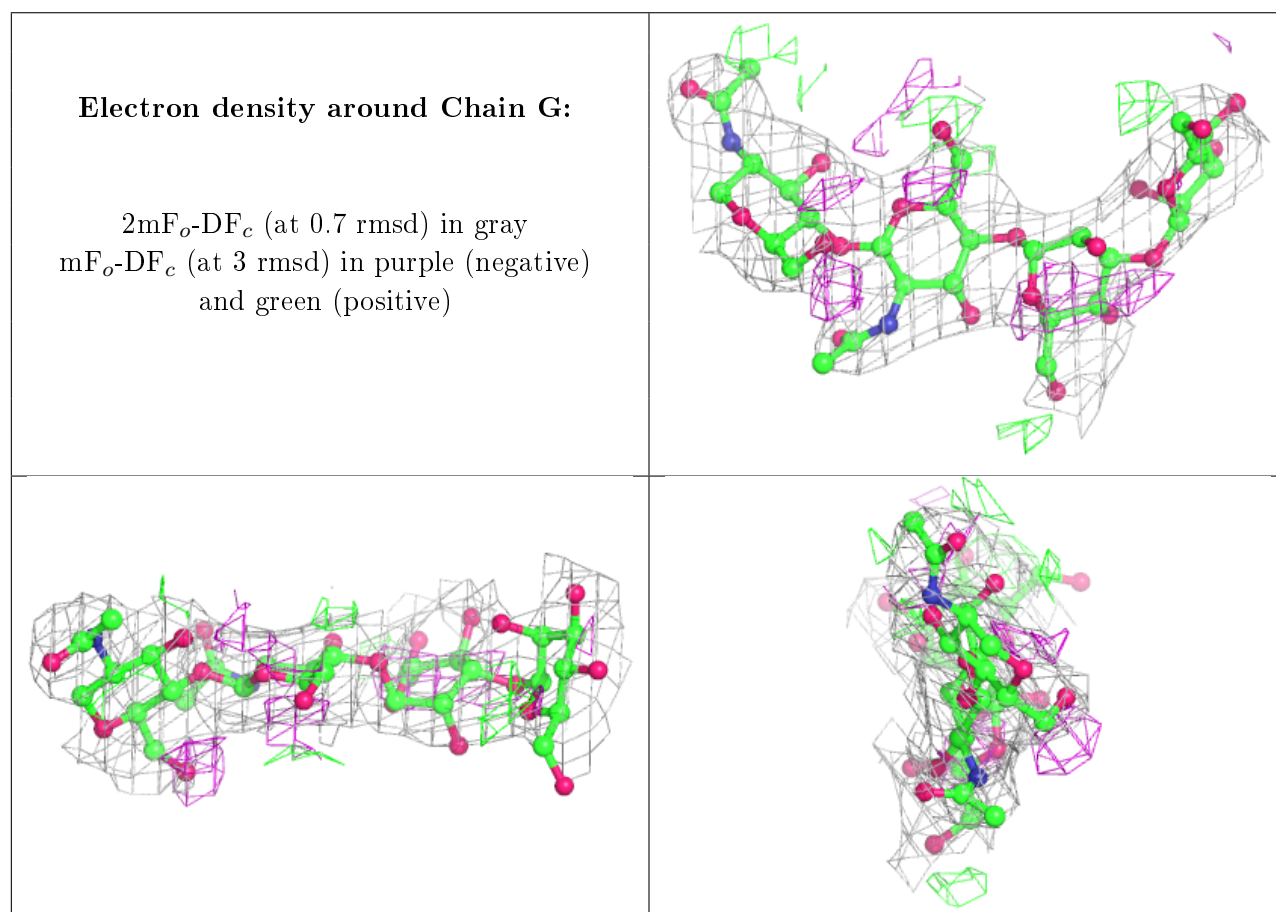
There are no non-standard protein/DNA/RNA residues in this entry.

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.

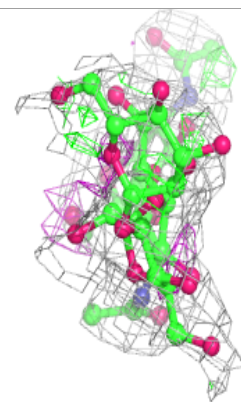
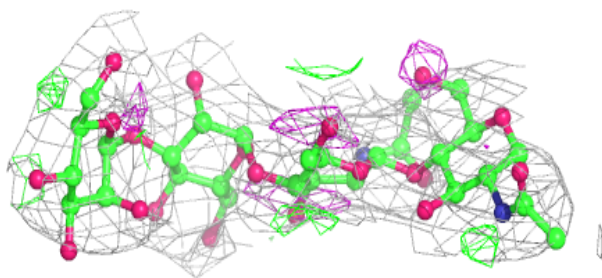
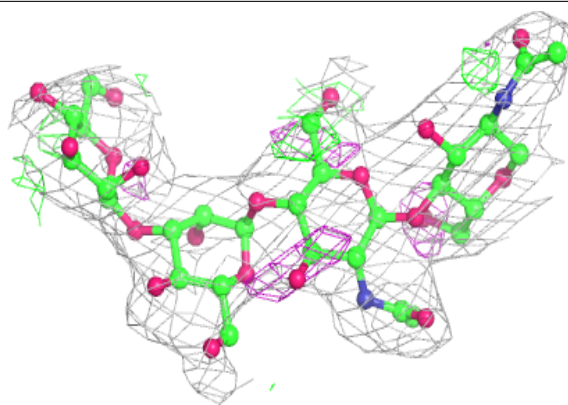
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	H	3	11/12	0.65	0.33	103,110,113,116	0
4	MAN	H	5	11/12	0.72	0.39	117,118,119,119	0
3	MAN	G	3	11/12	0.73	0.37	103,107,108,111	0
4	BMA	H	4	11/12	0.77	0.47	115,116,117,117	0
4	NAG	H	2	14/15	0.78	0.21	77,81,87,95	0
3	MAN	I	3	11/12	0.80	0.28	97,101,102,103	0
3	NAG	I	2	14/15	0.84	0.28	77,81,86,91	0
3	BMA	G	4	11/12	0.84	0.27	112,113,114,115	0
3	BMA	I	4	11/12	0.84	0.21	102,103,104,104	0
3	NAG	G	2	14/15	0.85	0.28	77,82,88,96	0
3	NAG	I	1	14/15	0.93	0.21	53,59,66,69	0
3	NAG	G	1	14/15	0.94	0.17	53,59,61,69	0
4	NAG	H	1	14/15	0.95	0.12	48,52,58,68	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.

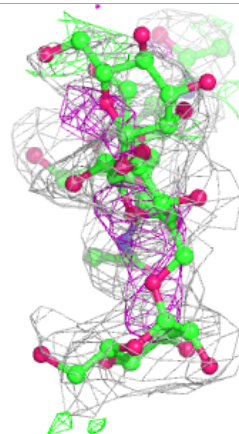
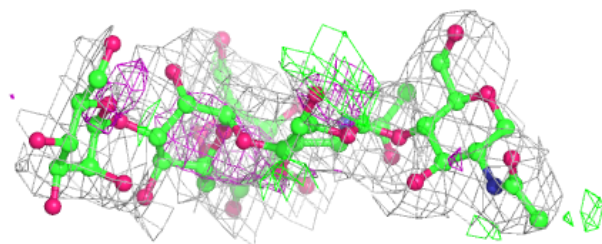
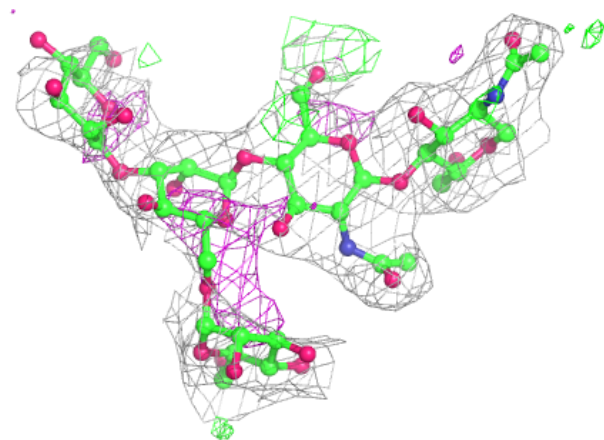


Electron density around Chain I:

$2mF_o-DF_c$ (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 ⓘ

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
6	NAG	F	1015	14/15	0.64	0.42	118,119,120,120	0
5	CA	A	1407	1/1	0.73	0.07	68,68,68,68	0
5	CA	F	1416	1/1	0.77	0.06	63,63,63,63	0
6	NAG	E	1014	14/15	0.77	0.30	87,92,95,95	0
6	NAG	D	1007	14/15	0.78	0.29	101,104,105,105	0
6	NAG	F	1020	14/15	0.78	0.26	109,112,113,114	0
5	CA	A	1406	1/1	0.79	0.07	73,73,73,73	0
6	NAG	D	1013	14/15	0.81	0.17	92,94,96,96	0
5	CA	E	1421	1/1	0.83	0.08	65,65,65,65	0
5	CA	F	1417	1/1	0.84	0.18	42,42,42,42	0
5	CA	C	1411	1/1	0.85	0.09	58,58,58,58	0
6	NAG	B	1001	14/15	0.85	0.28	109,111,113,114	0
5	CA	E	1420	1/1	0.85	0.08	51,51,51,51	0
6	NAG	B	1006	14/15	0.85	0.30	102,103,103,103	0
5	CA	C	1414	1/1	0.86	0.07	68,68,68,68	0
5	CA	C	1413	1/1	0.87	0.07	70,70,70,70	0
5	CA	A	1404	1/1	0.89	0.06	61,61,61,61	0
8	MG	D	1408	1/1	0.91	0.13	18,18,18,18	0
5	CA	D	1409	1/1	0.92	0.14	54,54,54,54	0
7	CAC	F	1303	5/5	0.93	0.19	114,114,115,115	0
5	CA	E	1419	1/1	0.94	0.12	35,35,35,35	0
5	CA	C	1412	1/1	0.95	0.12	46,46,46,46	0
8	MG	F	1415	1/1	0.95	0.13	32,32,32,32	0
5	CA	B	1402	1/1	0.95	0.15	48,48,48,48	0
5	CA	A	1405	1/1	0.96	0.07	75,75,75,75	0
7	CAC	B	1301	5/5	0.97	0.21	100,101,102,102	0
7	CAC	D	1302	5/5	0.97	0.17	96,96,98,98	0
5	CA	B	1403	1/1	0.97	0.20	28,28,28,28	0
5	CA	D	1410	1/1	0.97	0.21	24,24,24,24	0
5	CA	E	1418	1/1	0.98	0.09	48,48,48,48	0
8	MG	B	1401	1/1	0.99	0.12	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.