



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:48 AM UTC

PDB ID : 5AMC / pdb_00005amc
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta fluorogenic fragment 4-10
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2015-03-10
Resolution : 1.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

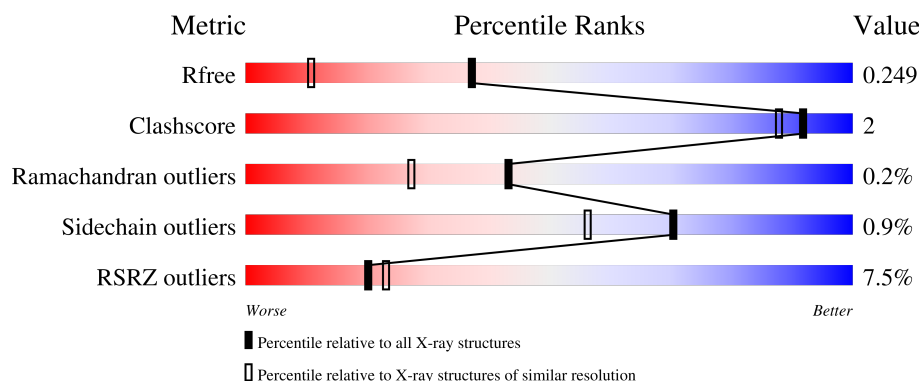
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 $\leq 5\%$. 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	629	8% 92% . .
2	B	629	7% 92% . .
3	C	2	100%
3	F	2	100%
4	D	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	2	 100%
5	E	4	 100%
6	H	3	 33%  67%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 11113 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 ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	3	0
			4969	3190	852	908	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	13	GLU	ASP	conflict	UNP P12821
A	14	ASP	GLU	conflict	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	ARG	engineered mutation	UNP P12821

- Molecule 2 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	607	Total	C	N	O	S	0	1	0
			4951	3181	849	902	19			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821

Continued on next page...

Continued from previous page...

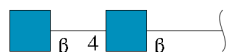
Chain	Residue	Modelled	Actual	Comment	Reference
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	ARG	engineered mutation	UNP P12821

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



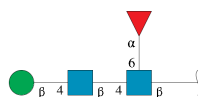
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



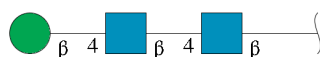
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



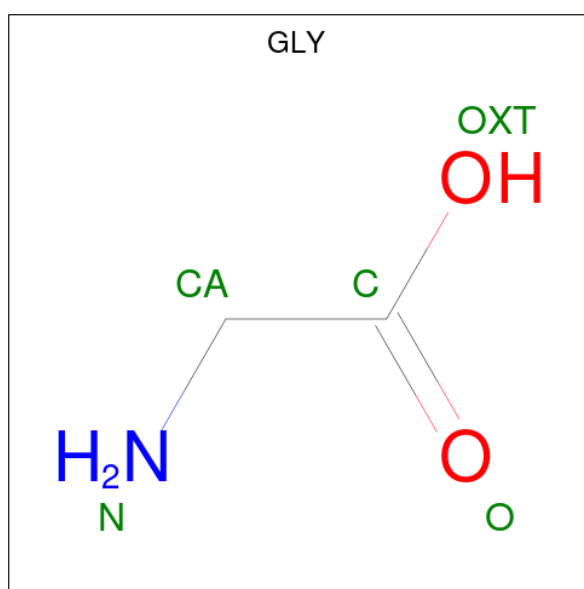
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 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.



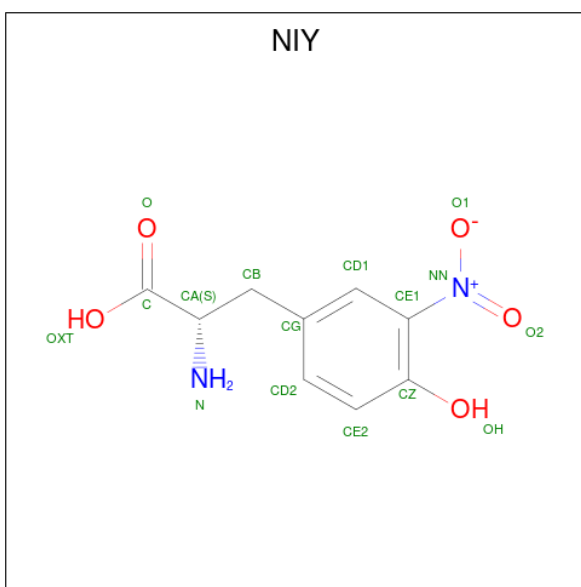
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			4	2	1	1		
7	B	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 8 is META-NITRO-TYROSINE (CCD ID: NIY) (formula: C₉H₁₀N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 16	C 9	N 2	O 5	0	0
8	B	1	Total 16	C 9	N 2	O 5	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Zn 1 1	0	0
9	B	1	Total Zn 1 1	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

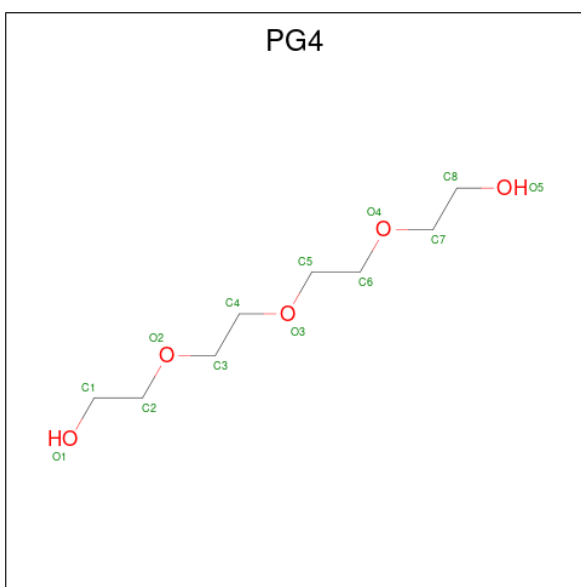
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0
10	B	1	Total Cl 1 1	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



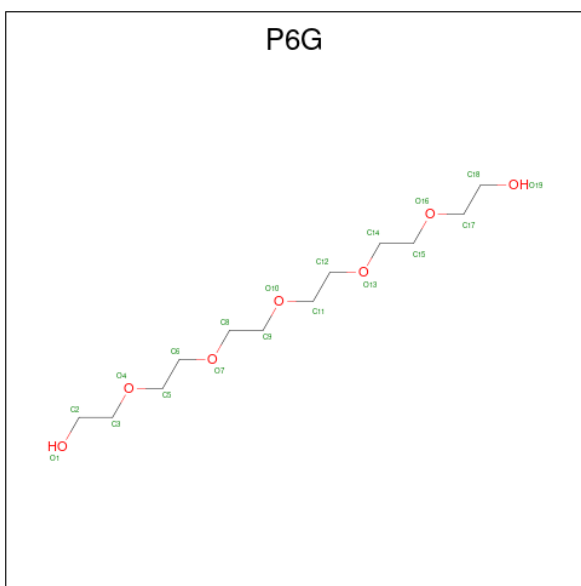
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		
11	A	1	Total	C	O	0	0
			7	4	3		
11	A	1	Total	C	O	0	0
			7	4	3		
11	B	1	Total	C	O	0	0
			7	4	3		
11	B	1	Total	C	O	0	0
			7	4	3		
11	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			19	12	7		

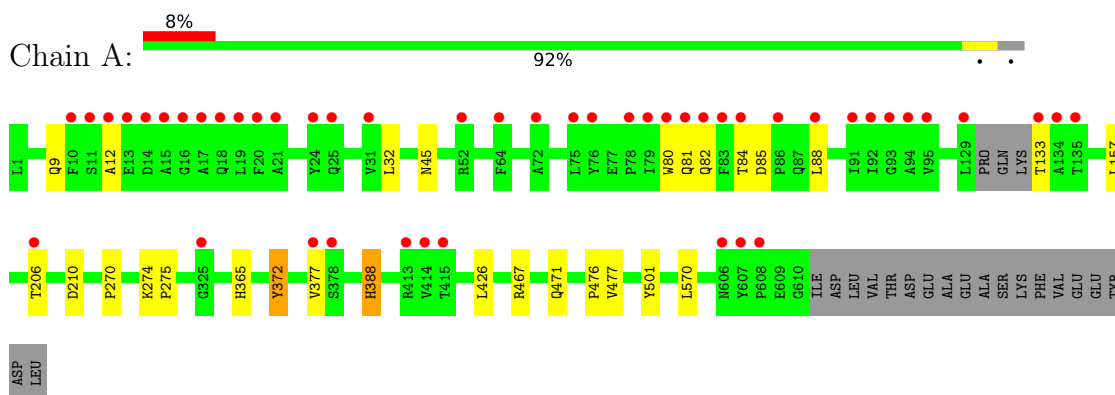
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	510	Total 510	O 510	0	0
14	B	376	Total 376	O 376	0	0

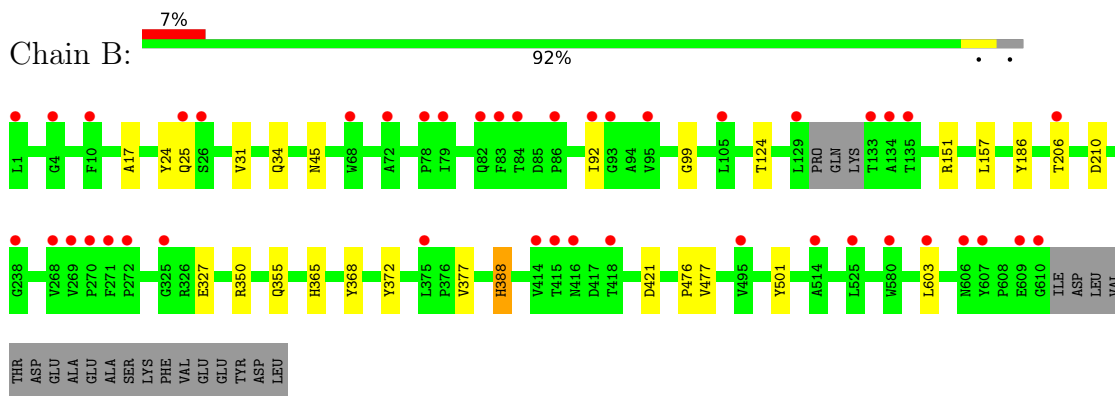
3 Residue-property plots

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.

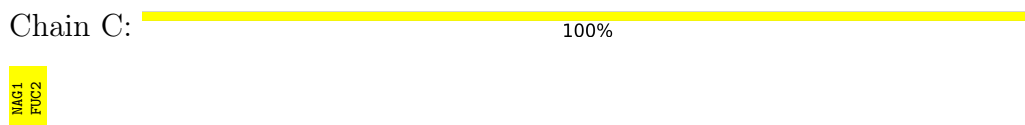
- Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



- Molecule 2: ANGIOTENSIN-CONVERTING ENZYME



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
FUC2

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

Chain D:  100%MAG1
MAG2

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

Chain G:  100%MAG1
MAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%MAG1
MAG2
BMA3
FUC4

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33%  67%MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.03Å 76.47Å 83.16Å 88.78° 64.25° 75.64°	Depositor
Resolution (Å)	74.53 – 1.65 74.53 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.7 (74.53-1.65) 91.7 (74.53-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.208 , 0.242 0.215 , 0.249	Depositor DCC
R_{free} test set	8524 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11113	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: PEG, ZN, CL, PG4, P6G, NIY, NAG, BMA, FUC

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	0.69	0/5133	0.84	1/6991 (0.0%)
2	B	0.67	0/5109	0.83	1/6959 (0.0%)
All	All	0.68	0/10242	0.83	2/13950 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	TRP	N-CA-C	6.67	120.68	112.54
2	B	377	VAL	N-CA-C	6.12	117.60	110.62

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	4969	0	4744	17	0
2	B	4951	0	4724	15	0
3	C	24	0	22	0	0
3	F	24	0	22	0	0
4	D	28	0	25	0	0
4	G	28	0	25	0	0
5	E	49	0	43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	39	0	34	0	0
7	A	4	0	2	0	0
7	B	4	0	2	0	0
8	A	16	0	6	1	0
8	B	16	0	7	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	21	0	30	0	0
11	B	21	0	30	0	0
12	B	10	0	13	0	0
13	B	19	0	26	0	0
14	A	510	0	0	2	0
14	B	376	0	0	0	0
All	All	11113	0	9755	32	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 2.

All (32) 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:365:HIS:HD1	1:A:388:HIS:HD2	1.33	0.74
1:A:365:HIS:HD1	1:A:388:HIS:CD2	2.09	0.71
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.73	0.69
2:B:350:ARG:H	2:B:355:GLN:HE21	1.46	0.64
2:B:124:THR:HG22	2:B:327:GLU:CG	2.32	0.59
2:B:206:THR:HG23	2:B:210:ASP:OD2	2.04	0.56
2:B:365:HIS:HD1	2:B:388:HIS:CD2	2.25	0.55
2:B:124:THR:HG22	2:B:327:GLU:HG2	1.88	0.55
1:A:467:ARG:HH11	1:A:471:GLN:HE22	1.56	0.54
1:A:12:ALA:O	14:A:2006:HOH:O	2.19	0.51
1:A:81:GLN:HB2	1:A:82:GLN:HE22	1.74	0.50
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.93	0.50
2:B:157:LEU:HD11	2:B:477:VAL:HG13	1.94	0.50
1:A:372:TYR:OH	1:A:388:HIS:HE1	1.94	0.49
1:A:206:THR:HG23	1:A:210:ASP:OD2	2.13	0.48
2:B:365:HIS:HD1	2:B:388:HIS:HD2	1.62	0.47
2:B:31:VAL:O	2:B:34:GLN:HG3	2.14	0.47
2:B:99:GLY:HA2	2:B:186:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:CD1	8:A:907:NIY:HB2	2.50	0.46
1:A:270:PRO:HD3	1:A:426:LEU:HD22	1.98	0.45
1:A:270:PRO:HD3	1:A:426:LEU:CD2	2.47	0.45
1:A:32:LEU:HD12	1:A:377:VAL:HG21	2.00	0.44
2:B:17:ALA:HB1	2:B:92:ILE:HD11	1.99	0.44
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.48	0.44
1:A:85:ASP:HB3	1:A:88:LEU:HB3	2.00	0.44
2:B:24:TYR:HD2	2:B:25:GLN:HG3	1.84	0.42
1:A:570:LEU:C	1:A:570:LEU:HD23	2.44	0.42
2:B:477:VAL:HG12	2:B:603:LEU:HD21	2.00	0.42
2:B:501:TYR:CD1	8:B:907:NIY:HB2	2.56	0.41
2:B:157:LEU:HD13	2:B:476:PRO:HB2	2.03	0.41
2:B:124:THR:HG22	2:B:327:GLU:HG3	2.02	0.40
1:A:84:THR:HB	14:A:2007:HOH:O	2.21	0.40

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	606/629 (96%)	594 (98%)	11 (2%)	1 (0%)	43	27
2	B	604/629 (96%)	593 (98%)	10 (2%)	1 (0%)	43	27
All	All	1210/1258 (96%)	1187 (98%)	21 (2%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
2	B	45	ASN

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	523/541 (97%)	519 (99%)	4 (1%)	73	60
2	B	519/541 (96%)	514 (99%)	5 (1%)	68	52
All	All	1042/1082 (96%)	1033 (99%)	9 (1%)	70	56

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	133	THR
1	A	372	TYR
1	A	388	HIS
2	B	151	ARG
2	B	368	TYR
2	B	372	TYR
2	B	388	HIS
2	B	421	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	82	GLN
1	A	87	GLN
1	A	224	ASN
1	A	388	HIS
1	A	471	GLN
1	A	585	ASN
2	B	87	GLN
2	B	203	ASN
2	B	355	GLN
2	B	388	HIS
2	B	527	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 ⓘ

15 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	C	1	1,3	14,14,15	0.78	0	17,19,21	1.50	4 (23%)
3	FUC	C	2	3	10,10,11	0.62	0	14,14,16	1.75	3 (21%)
4	NAG	D	1	1,4	14,14,15	0.39	0	17,19,21	1.03	2 (11%)
4	NAG	D	2	4	14,14,15	0.42	0	17,19,21	1.02	2 (11%)
5	NAG	E	1	1,5	14,14,15	0.44	0	17,19,21	0.70	0
5	NAG	E	2	5	14,14,15	0.33	0	17,19,21	0.71	0
5	BMA	E	3	5	11,11,12	0.31	0	15,15,17	0.73	0
5	FUC	E	4	5	10,10,11	0.43	0	14,14,16	0.37	0
3	NAG	F	1	2,3	14,14,15	0.50	0	17,19,21	1.27	2 (11%)
3	FUC	F	2	3	10,10,11	0.62	0	14,14,16	1.74	3 (21%)
4	NAG	G	1	2,4	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	0.55	0	17,19,21	1.45	2 (11%)
6	NAG	H	1	2,6	14,14,15	0.38	0	17,19,21	1.02	1 (5%)
6	NAG	H	2	6	14,14,15	0.36	0	17,19,21	1.03	0
6	BMA	H	3	6	11,11,12	0.38	0	15,15,17	0.90	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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	FUC	E	4	5	-	-	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
4	NAG	G	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
6	NAG	H	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C1-O5-C5	4.93	118.79	112.19
3	C	2	FUC	C1-C2-C3	4.47	116.15	109.64
3	F	2	FUC	C1-C2-C3	4.31	115.92	109.64
3	C	2	FUC	O5-C1-C2	3.34	118.77	110.79
3	F	1	NAG	C4-C3-C2	3.23	115.76	111.02
4	G	1	NAG	O5-C1-C2	-3.17	106.39	111.29
3	F	2	FUC	C1-O5-C5	3.02	120.09	112.97
3	C	1	NAG	C4-C3-C2	2.87	115.22	111.02
3	C	1	NAG	O5-C5-C6	2.77	113.06	107.66
4	D	1	NAG	C1-O5-C5	2.69	115.79	112.19
4	D	2	NAG	C4-C3-C2	2.59	114.81	111.02
3	C	2	FUC	C1-O5-C5	2.53	118.93	112.97
6	H	1	NAG	O5-C1-C2	-2.50	107.42	111.29
3	C	1	NAG	C1-C2-N2	-2.40	106.65	110.43
3	F	2	FUC	O5-C1-C2	2.26	116.19	110.79
3	C	1	NAG	C2-N2-C7	2.25	125.91	122.90
6	H	3	BMA	C1-C2-C3	2.19	112.84	109.64
4	D	1	NAG	O5-C1-C2	-2.14	107.98	111.29
4	G	2	NAG	C3-C4-C5	2.05	113.95	110.23
3	F	1	NAG	O5-C5-C6	2.04	111.62	107.66
4	D	2	NAG	C3-C4-C5	2.04	113.92	110.23

There are no chirality outliers.

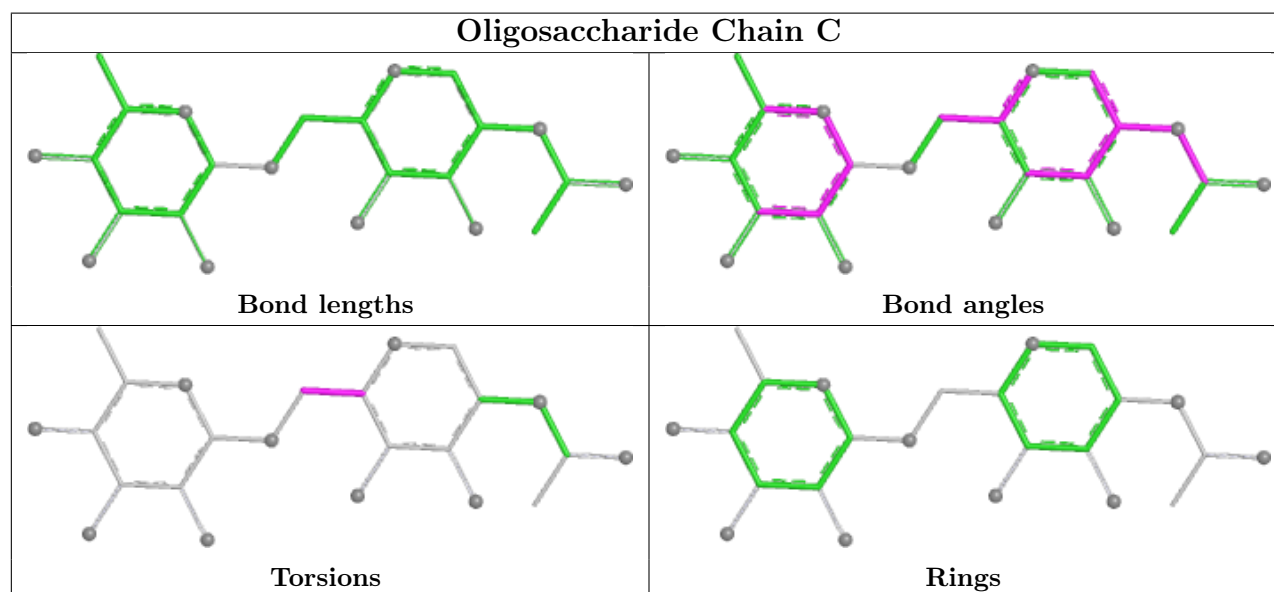
All (8) torsion outliers are listed below:

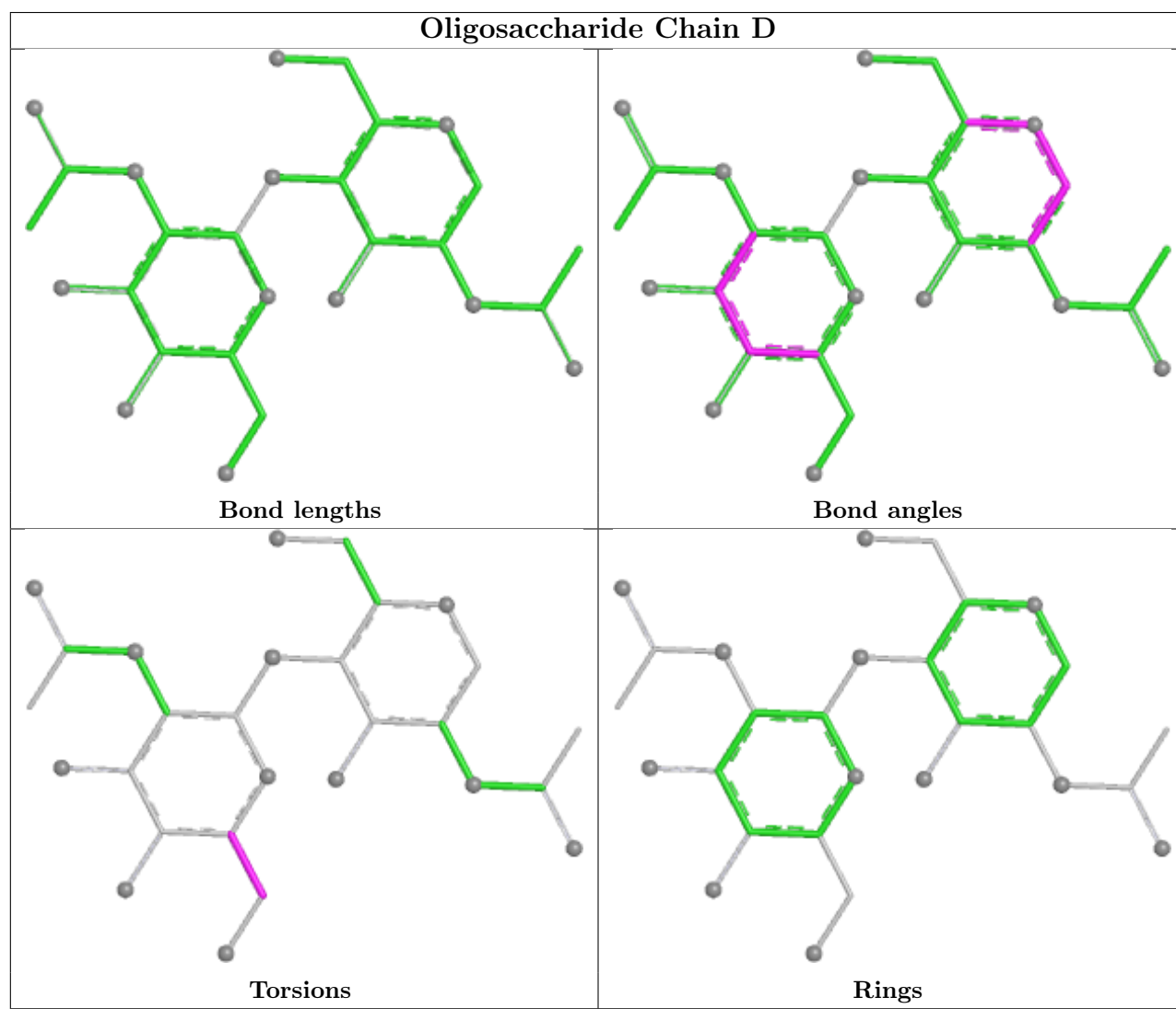
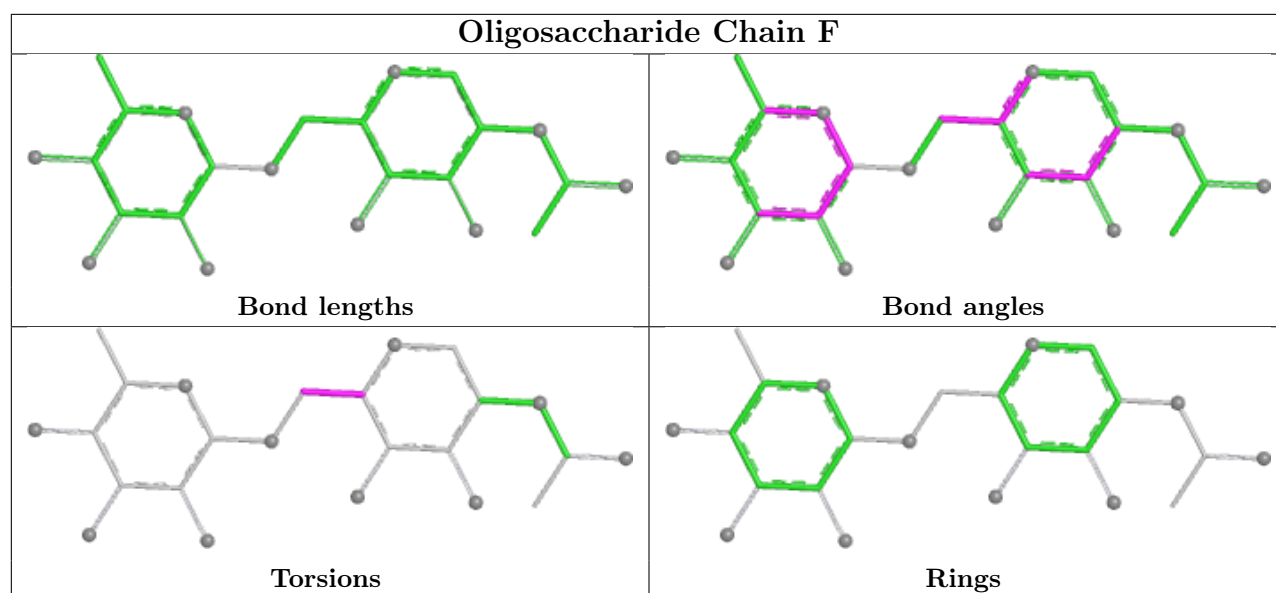
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
6	H	3	BMA	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

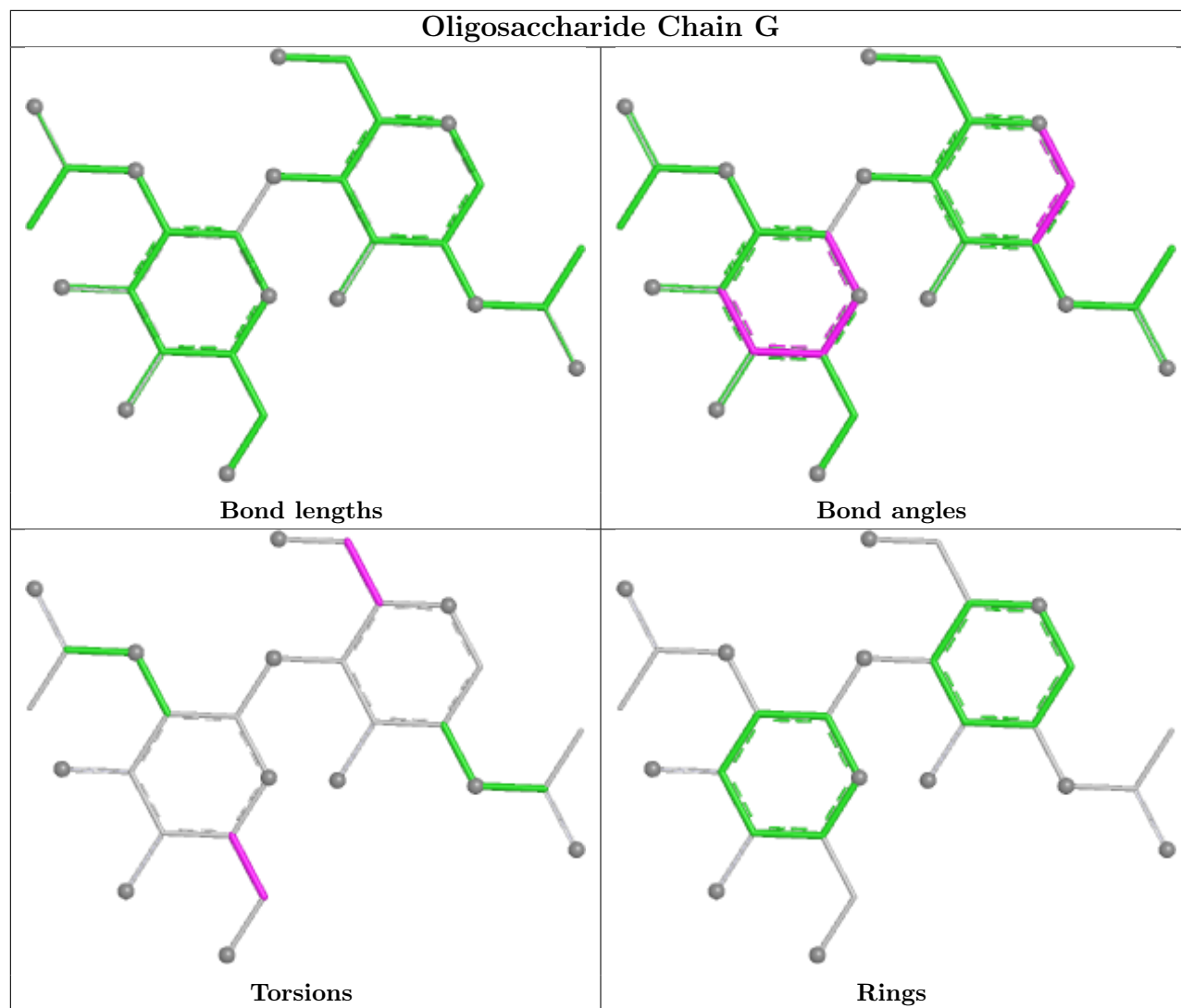
There are no ring outliers.

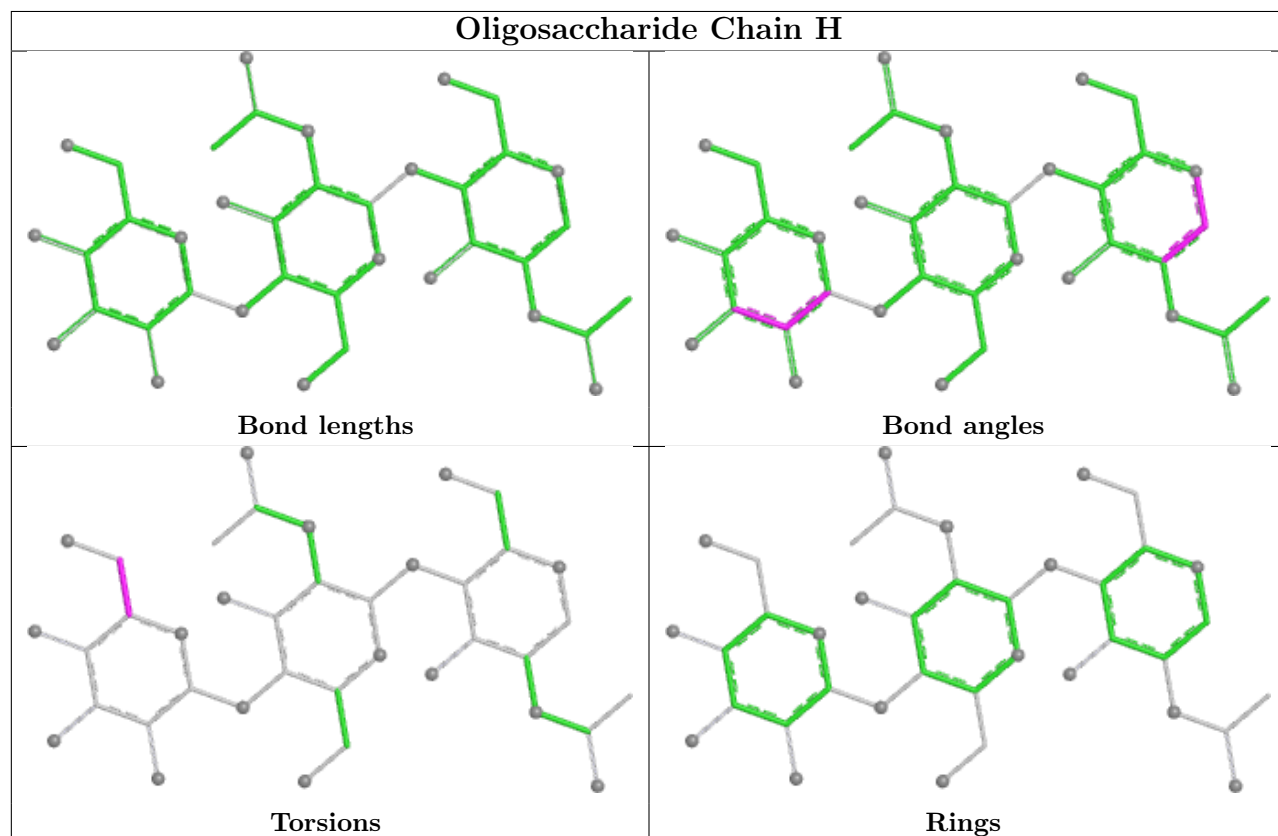
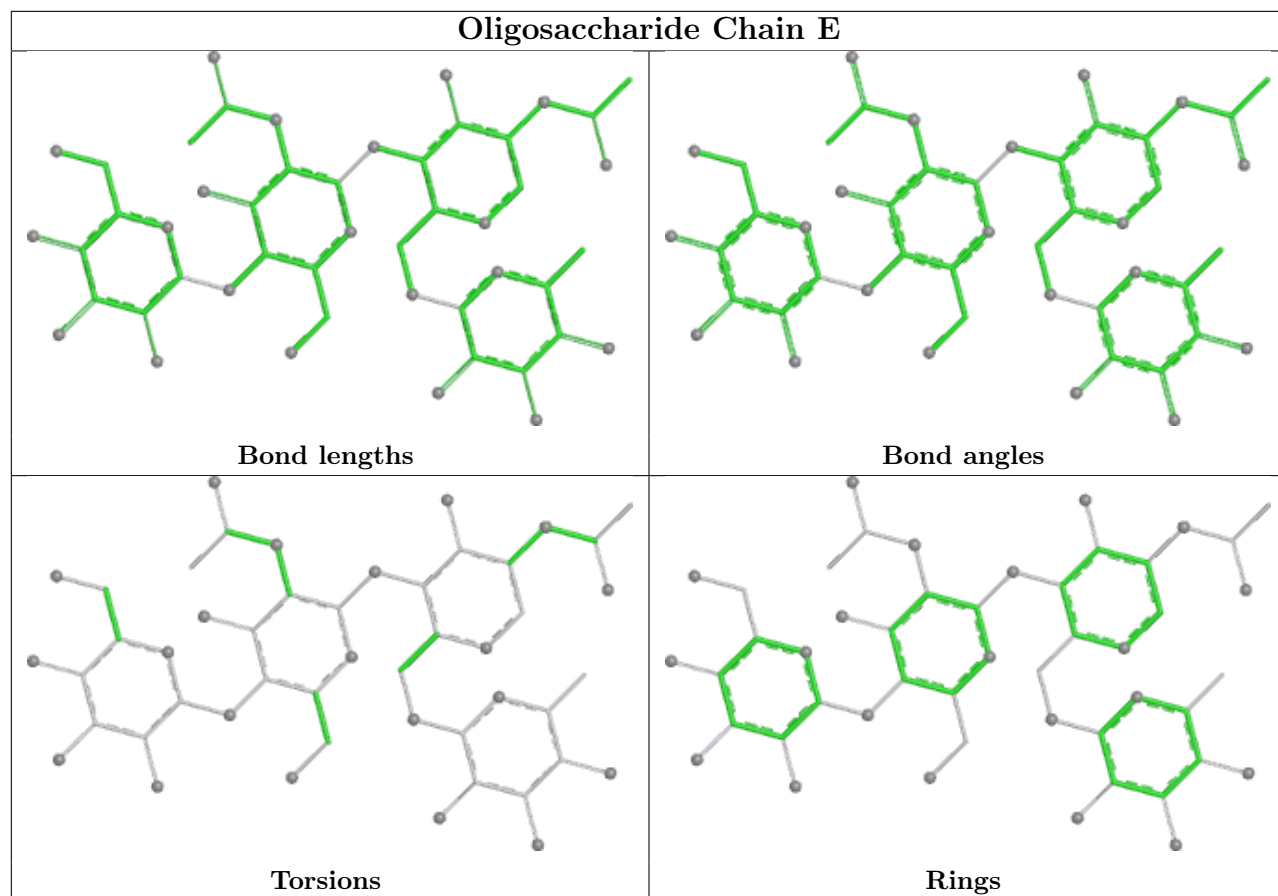
No monomer is involved in short contacts.

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

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	NIY	A	907	7	15,16,16	5.51	5 (33%)	14,22,22	1.18	1 (7%)
11	PEG	A	1622	-	6,6,6	0.48	0	5,5,5	0.40	0
11	PEG	B	1623	-	6,6,6	0.50	0	5,5,5	0.20	0
7	GLY	A	906	8	3,3,4	0.78	0	1,2,4	1.27	0
12	PG4	B	1611	-	9,9,12	0.39	0	8,8,11	0.36	0
13	P6G	B	1621	-	18,18,18	0.71	0	17,17,17	0.64	0
7	GLY	B	906	8	3,3,4	0.75	0	1,2,4	0.75	0
8	NIY	B	907	7	15,16,16	5.54	4 (26%)	14,22,22	1.53	2 (14%)
11	PEG	B	1620	-	6,6,6	0.52	0	5,5,5	0.20	0
11	PEG	A	1621	-	6,6,6	0.47	0	5,5,5	0.27	0
11	PEG	B	1622	-	6,6,6	0.48	0	5,5,5	0.37	0
11	PEG	A	1620	-	6,6,6	0.49	0	5,5,5	0.50	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	NIY	A	907	7	-	2/10/12/12	0/1/1/1
11	PEG	A	1622	-	-	2/4/4/4	-
11	PEG	B	1623	-	-	2/4/4/4	-
7	GLY	A	906	8	-	0/0/1/2	-
12	PG4	B	1611	-	-	2/7/7/10	-
13	P6G	B	1621	-	-	5/16/16/16	-
7	GLY	B	906	8	-	0/0/1/2	-
8	NIY	B	907	7	-	4/10/12/12	0/1/1/1
11	PEG	B	1620	-	-	2/4/4/4	-
11	PEG	A	1621	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PEG	B	1622	-	-	3/4/4/4	-
11	PEG	A	1620	-	-	3/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	907	NIY	O2-NN	19.02	1.55	1.22
8	B	907	NIY	O2-NN	18.74	1.55	1.22
8	B	907	NIY	CE1-NN	-7.46	1.32	1.45
8	A	907	NIY	CE1-NN	-6.54	1.33	1.45
8	B	907	NIY	CB-CG	-5.96	1.37	1.51
8	A	907	NIY	CB-CG	-5.67	1.37	1.51
8	A	907	NIY	O1-NN	3.06	1.55	1.35
8	B	907	NIY	O1-NN	2.18	1.49	1.35
8	A	907	NIY	OXT-C	-2.00	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	907	NIY	CG-CB-CA	-3.14	107.71	114.13
8	B	907	NIY	CB-CG-CD1	-2.56	116.03	120.43
8	A	907	NIY	CG-CB-CA	-2.07	109.89	114.13

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	907	NIY	N-CA-CB-CG
8	B	907	NIY	N-CA-CB-CG
8	B	907	NIY	C-CA-CB-CG
8	B	907	NIY	CZ-CE1-NN-O2
13	B	1621	P6G	O4-C5-C6-O7
11	A	1620	PEG	O1-C1-C2-O2
11	A	1620	PEG	O2-C3-C4-O4
11	B	1622	PEG	O1-C1-C2-O2
11	B	1623	PEG	O2-C3-C4-O4
13	B	1621	P6G	O16-C17-C18-O19
11	B	1622	PEG	O2-C3-C4-O4
12	B	1611	PG4	O1-C1-C2-O2
12	B	1611	PG4	O2-C3-C4-O3
13	B	1621	P6G	C9-C8-O7-C6

Continued on next page...

Continued from previous page...

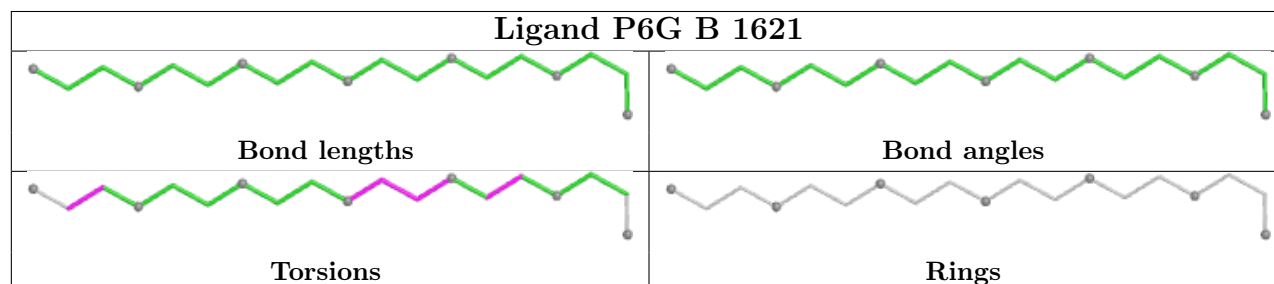
Mol	Chain	Res	Type	Atoms
11	A	1622	PEG	C1-C2-O2-C3
11	B	1622	PEG	C1-C2-O2-C3
11	B	1620	PEG	O2-C3-C4-O4
11	A	1621	PEG	C4-C3-O2-C2
13	B	1621	P6G	O7-C8-C9-O10
8	B	907	NIY	CD1-CE1-NN-O2
8	A	907	NIY	C-CA-CB-CG
11	B	1620	PEG	C4-C3-O2-C2
11	A	1621	PEG	O2-C3-C4-O4
11	A	1620	PEG	C4-C3-O2-C2
13	B	1621	P6G	C8-C9-O10-C11
11	B	1623	PEG	C4-C3-O2-C2
11	A	1621	PEG	O1-C1-C2-O2
11	A	1622	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	907	NIY	1	0
8	B	907	NIY	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	607/629 (96%)	0.32	48 (7%)	18 21	14, 26, 48, 73	3 (0%)
2	B	607/629 (96%)	0.50	43 (7%)	22 25	15, 29, 48, 75	1 (0%)
All	All	1214/1258 (96%)	0.41	91 (7%)	20 23	14, 28, 48, 75	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASP	6.5
1	A	414	VAL	5.9
1	A	80	TRP	5.6
1	A	88	LEU	5.6
1	A	83	PHE	5.2
1	A	78	PRO	4.9
2	B	414	VAL	4.5
1	A	21	ALA	4.5
1	A	79	ILE	4.4
1	A	25	GLN	4.3
1	A	15	ALA	4.2
1	A	17	ALA	4.1
1	A	95	VAL	4.1
2	B	606	ASN	4.0
2	B	269	VAL	4.0
1	A	84	THR	3.9
1	A	129	LEU	3.9
1	A	20	PHE	3.8
2	B	129	LEU	3.8
1	A	94	ALA	3.8
1	A	325	GLY	3.6
2	B	610	GLY	3.6
1	A	19	LEU	3.6
2	B	607	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	606	ASN	3.5
1	A	24	TYR	3.5
2	B	270	PRO	3.4
1	A	81	GLN	3.2
2	B	133	THR	3.1
2	B	135	THR	3.1
1	A	377	VAL	3.0
1	A	16	GLY	3.0
2	B	105	LEU	3.0
2	B	325	GLY	2.9
2	B	25	GLN	2.9
1	A	13	GLU	2.9
1	A	413	ARG	2.9
2	B	415	THR	2.8
2	B	418	THR	2.8
1	A	10	PHE	2.7
2	B	82	GLN	2.7
1	A	86	PRO	2.7
2	B	92	ILE	2.7
2	B	83	PHE	2.7
1	A	133	THR	2.7
1	A	72	ALA	2.7
2	B	134	ALA	2.7
1	A	64	PHE	2.7
1	A	31	VAL	2.6
1	A	91	ILE	2.6
1	A	75	LEU	2.6
2	B	609	GLU	2.6
1	A	92	ILE	2.6
2	B	78	PRO	2.6
1	A	206	THR	2.5
1	A	11	SER	2.5
1	A	18	GLN	2.5
2	B	1	LEU	2.5
1	A	607	TYR	2.5
2	B	4	GLY	2.5
2	B	206	THR	2.5
2	B	271	PHE	2.4
2	B	272	PRO	2.4
2	B	68	TRP	2.4
1	A	378	SER	2.3
1	A	608	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	2.3
2	B	525	LEU	2.3
2	B	10	PHE	2.3
1	A	93	GLY	2.3
2	B	72	ALA	2.3
1	A	135	THR	2.3
1	A	415	THR	2.3
2	B	416	ASN	2.2
1	A	76	TYR	2.2
2	B	86	PRO	2.2
2	B	603	LEU	2.2
2	B	95	VAL	2.2
2	B	580	TRP	2.2
2	B	84	THR	2.2
1	A	134	ALA	2.1
2	B	93	GLY	2.1
2	B	26	SER	2.1
2	B	79	ILE	2.1
2	B	375	LEU	2.1
1	A	82	GLN	2.1
1	A	52	ARG	2.0
2	B	238	GLY	2.0
2	B	514	ALA	2.0
2	B	268	VAL	2.0
2	B	495	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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.

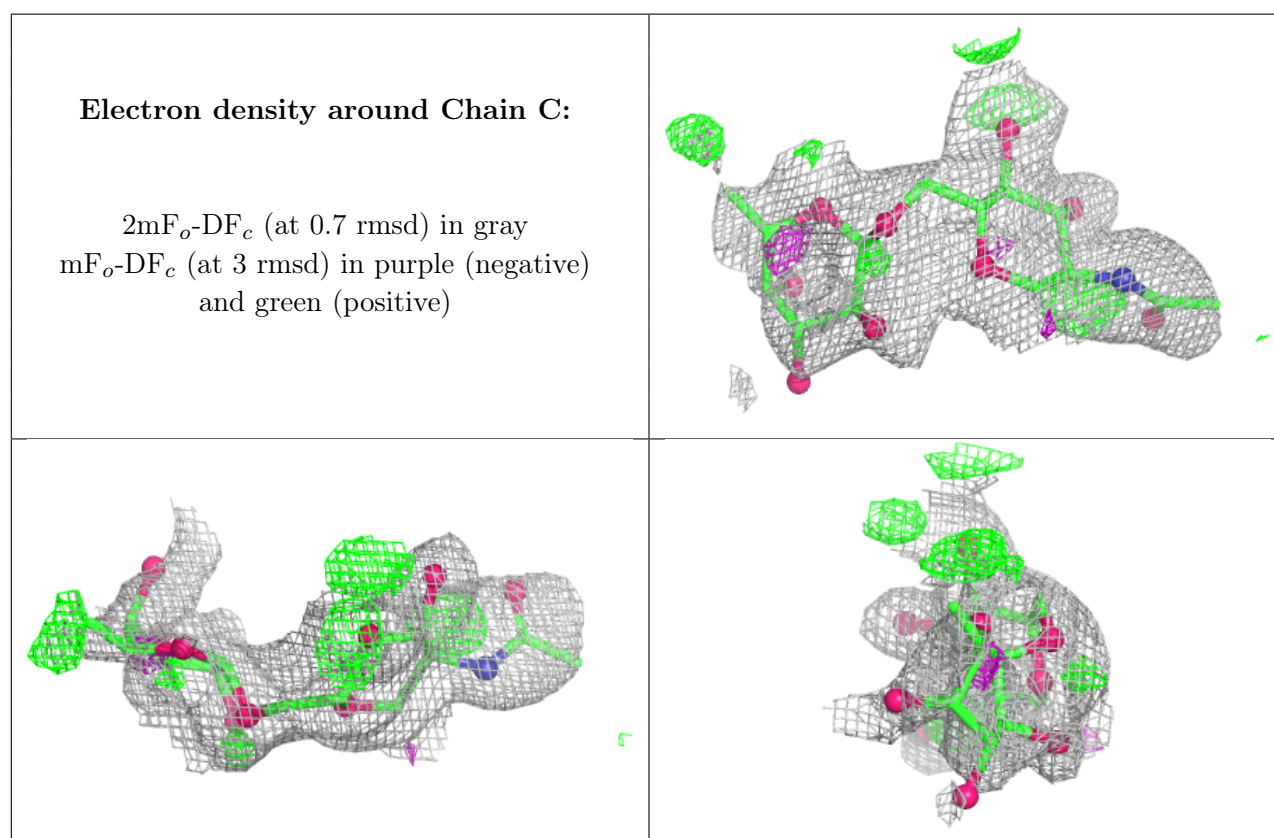
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	C	2	10/11	0.62	0.17	60,66,68,69	0
3	FUC	F	2	10/11	0.65	0.21	61,66,70,71	0
4	NAG	D	2	14/15	0.72	0.14	55,67,72,73	0

Continued on next page...

Continued from previous page...

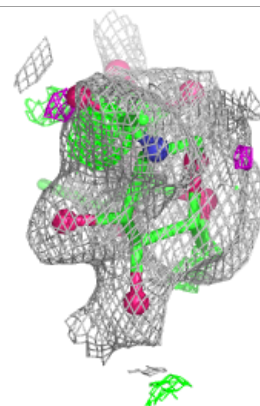
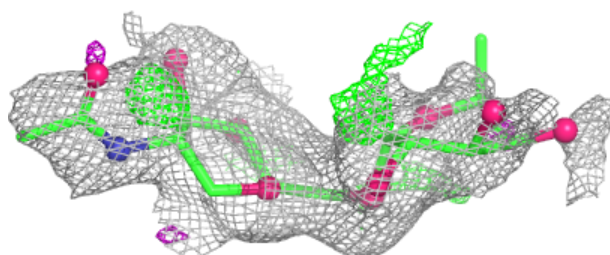
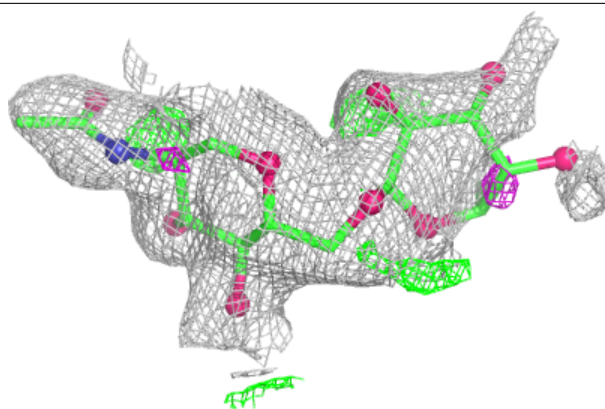
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	H	3	11/12	0.72	0.13	82,83,85,87	0
4	NAG	G	2	14/15	0.73	0.12	63,66,70,71	0
4	NAG	D	1	14/15	0.73	0.15	48,51,56,59	0
6	NAG	H	2	14/15	0.79	0.13	73,77,79,81	0
6	NAG	H	1	14/15	0.79	0.14	63,65,69,70	0
3	NAG	F	1	14/15	0.82	0.13	42,48,54,60	0
5	BMA	E	3	11/12	0.83	0.11	59,61,63,63	0
5	FUC	E	4	10/11	0.85	0.14	45,47,49,52	0
5	NAG	E	2	14/15	0.88	0.10	42,48,54,56	0
4	NAG	G	1	14/15	0.88	0.10	42,44,49,56	0
3	NAG	C	1	14/15	0.88	0.12	34,41,50,50	0
5	NAG	E	1	14/15	0.92	0.08	35,37,46,48	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.



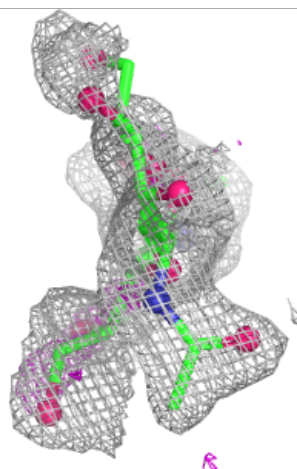
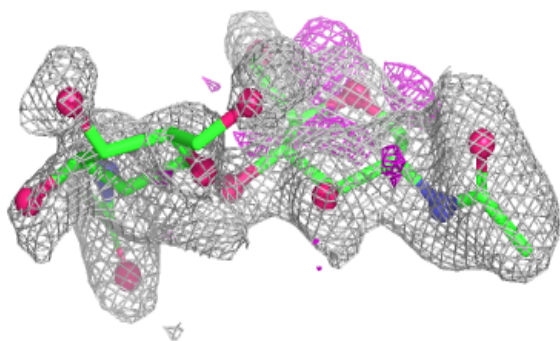
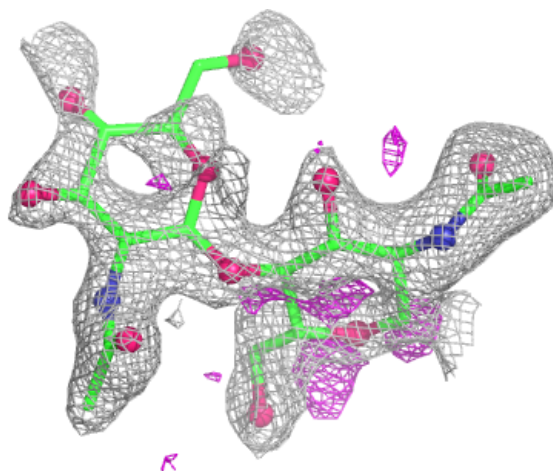
Electron density around Chain F:

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



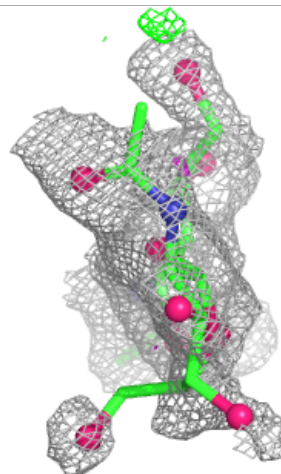
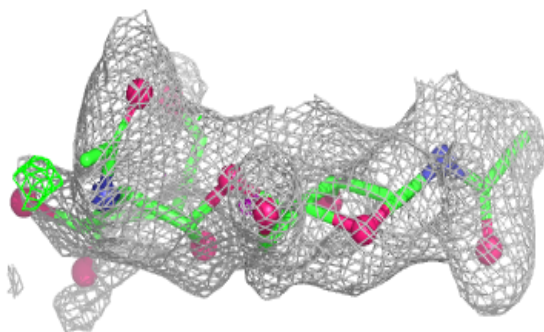
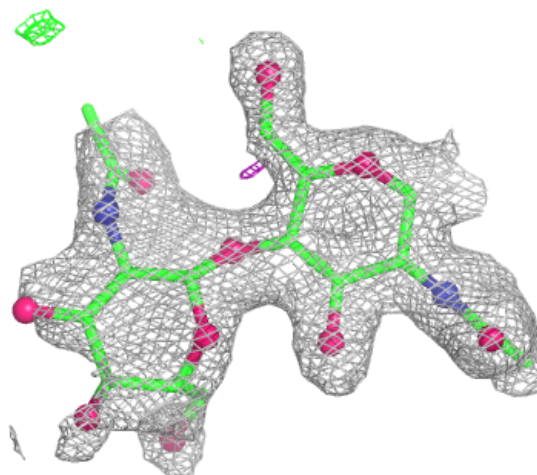
Electron density around Chain D:

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



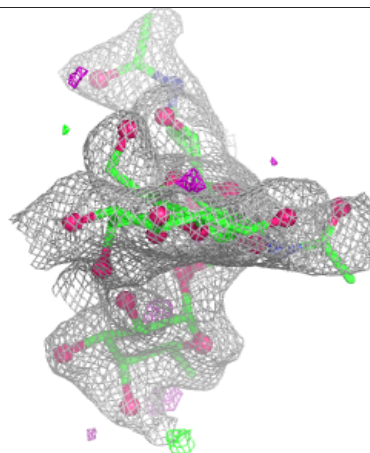
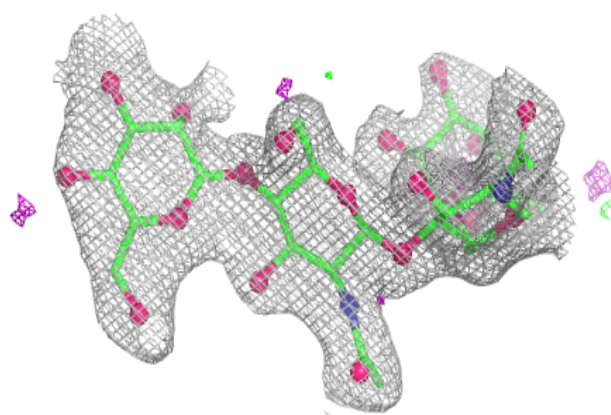
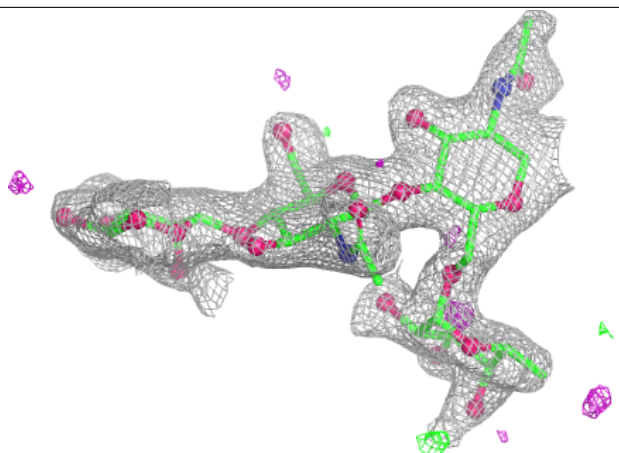
Electron density around Chain G:

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

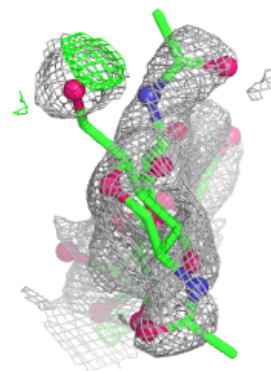
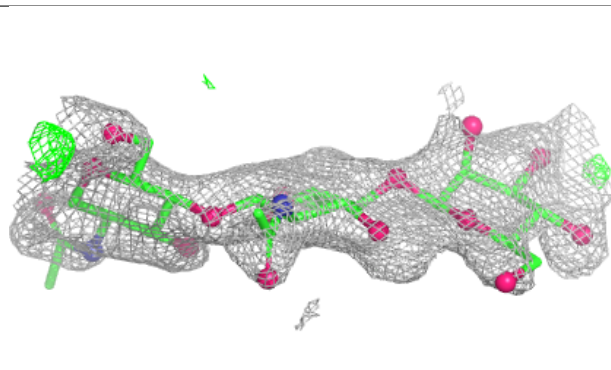
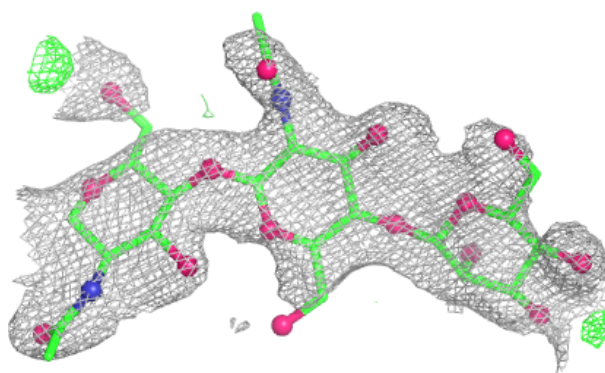


Electron density around Chain E:

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

**Electron density around Chain H:**

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

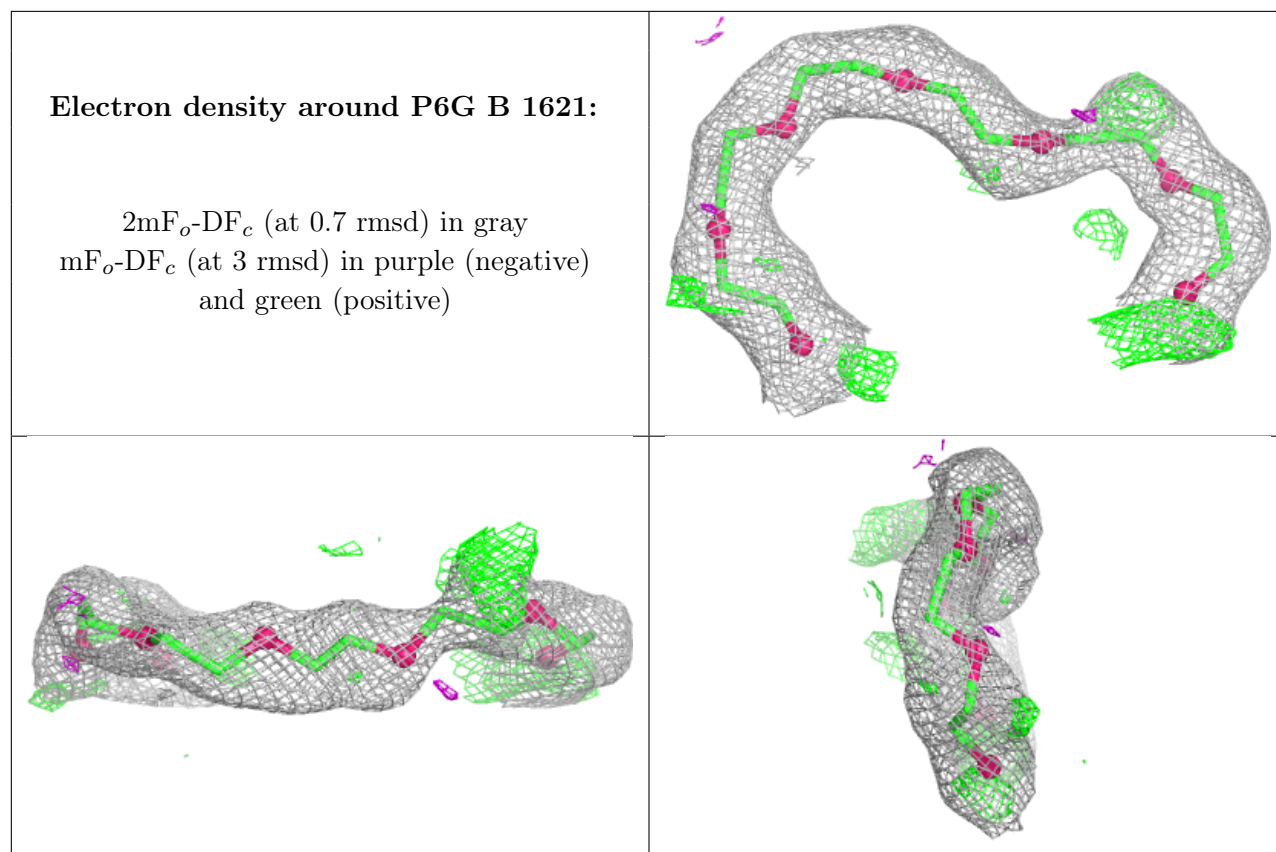


6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
7	GLY	A	906	4/5	0.70	0.18	42,43,44,44	0
7	GLY	B	906	4/5	0.74	0.17	44,44,45,47	0
8	NIY	A	907	16/16	0.79	0.16	23,41,48,49	0
13	P6G	B	1621	19/19	0.80	0.15	35,45,49,50	0
11	PEG	B	1623	7/7	0.81	0.17	61,62,65,66	0
11	PEG	A	1622	7/7	0.82	0.14	40,42,45,46	0
11	PEG	B	1622	7/7	0.83	0.16	56,57,58,58	0
8	NIY	B	907	16/16	0.84	0.14	25,45,52,59	0
11	PEG	A	1621	7/7	0.84	0.14	51,51,55,58	0
12	PG4	B	1611	10/13	0.88	0.12	40,45,47,47	0
11	PEG	A	1620	7/7	0.88	0.14	51,52,54,55	0
11	PEG	B	1620	7/7	0.89	0.11	39,40,43,47	0
10	CL	B	1612	1/1	0.98	0.04	23,23,23,23	0
10	CL	A	1611	1/1	0.99	0.02	19,19,19,19	0
9	ZN	B	1001	1/1	0.99	0.02	20,20,20,20	0
9	ZN	A	1001	1/1	1.00	0.01	19,19,19,19	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.