



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:38 PM UTC

PDB ID : 5AMB / pdb_00005amb
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 35-42
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2015-03-10
Resolution : 1.55 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

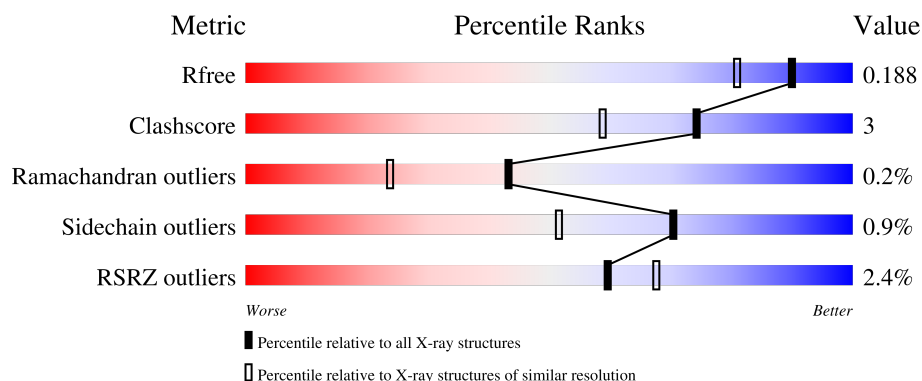
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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.



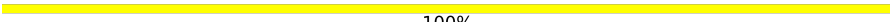
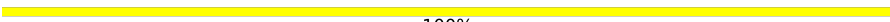
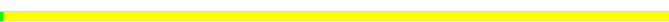
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	
1	B	629	
2	P	8	
2	Q	8	
3	C	2	

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	D	2	 100%
4	G	2	 100%
5	E	4	 25%  75%
6	H	3	 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11095 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	2	0
			4964	3187	852	906	19			
1	B	607	Total	C	N	O	S	0	0	0
			4940	3174	848	899	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	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
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
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 2 is a protein called AMYLOID BETA A4 PROTEIN.

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

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

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



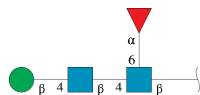
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



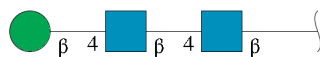
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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			

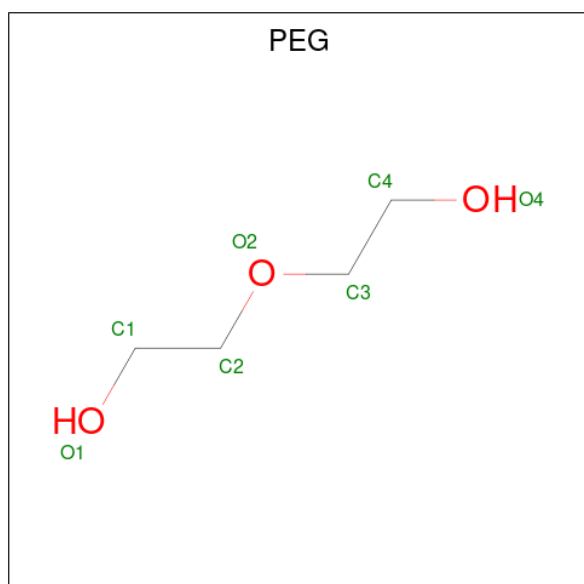
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

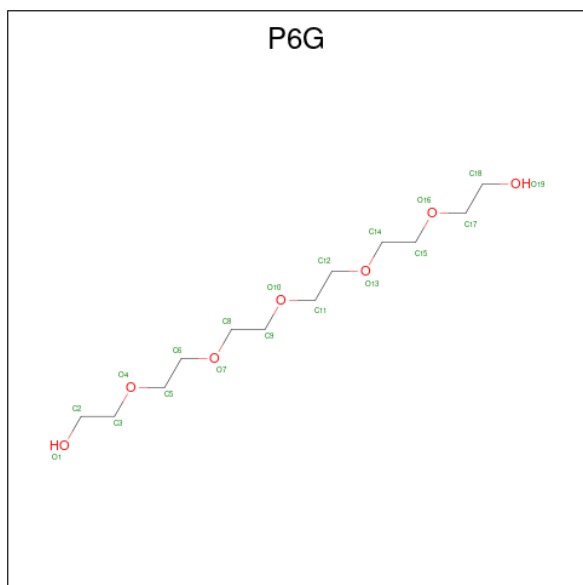
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	B	1	Total	Cl	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



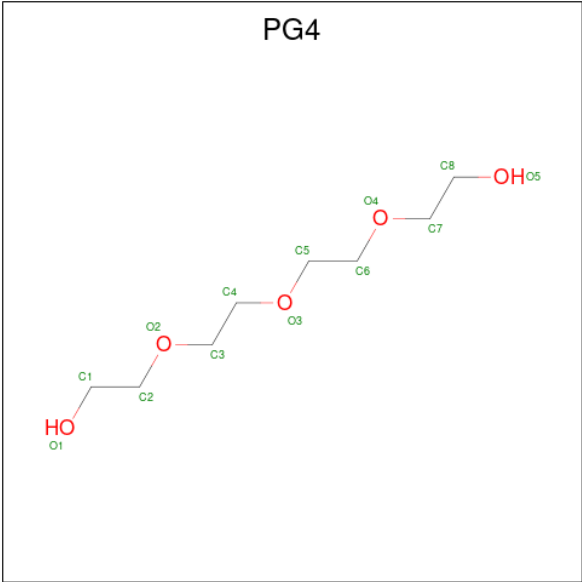
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

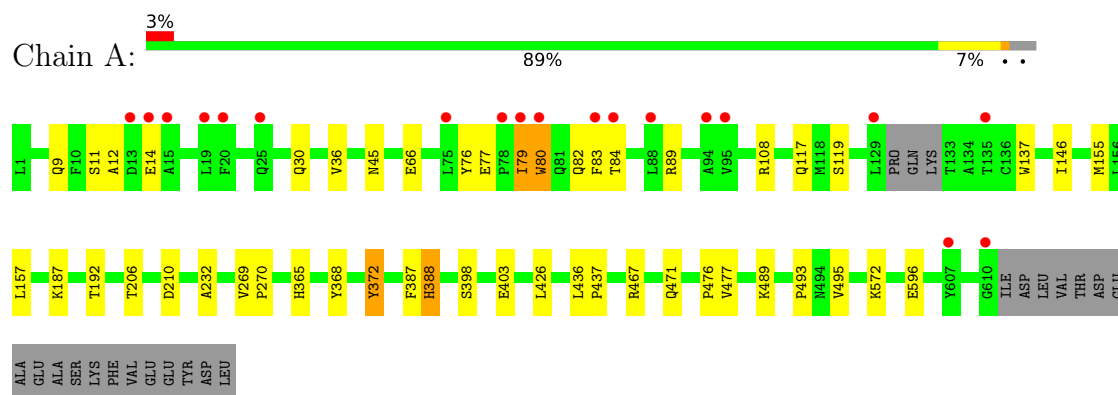
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	501	Total	O	0	0
			501	501		
12	B	367	Total	O	0	0
			367	367		
12	P	2	Total	O	0	0
			2	2		
12	Q	2	Total	O	0	0
			2	2		

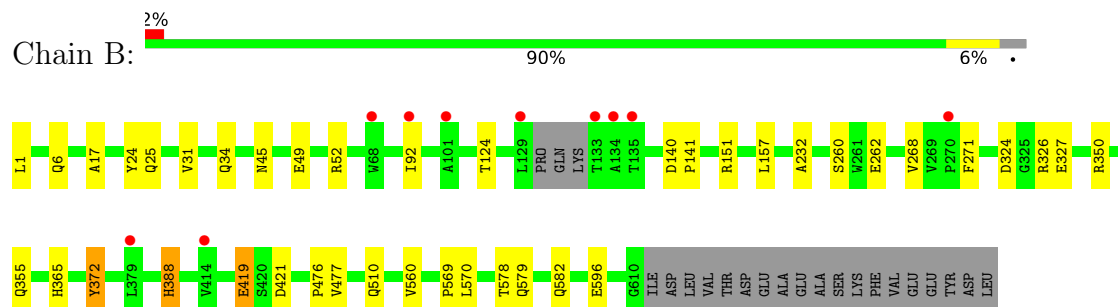
3 Residue-property plots

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 1: ANGIOTENSIN-CONVERTING ENZYME



• Molecule 2: AMYLOID BETA A4 PROTEIN



• Molecule 2: AMYLOID BETA A4 PROTEIN

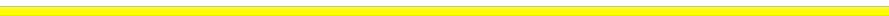


• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%

NAG1
FUC2

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

Chain F:  100%

NAG1
FUC2

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

Chain D:  100%

NAG1
NAG2

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

Chain G:  100%

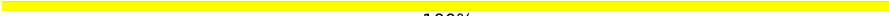
NAG1
NAG2

- 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:  25% 75%

NAG1
NAG2
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:  100%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.98Å 76.95Å 83.22Å 88.63° 64.14° 75.22°	Depositor
Resolution (Å)	74.51 – 1.55 74.51 – 1.55	Depositor EDS
% Data completeness (in resolution range)	87.8 (74.51-1.55) 87.9 (74.51-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.158 , 0.181 0.167 , 0.188	Depositor DCC
R_{free} test set	9798 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11095	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, P6G, BMA, ZN, PG4, CL, PEG, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	4/5125 (0.1%)	0.88	1/6980 (0.0%)
1	B	0.83	1/5095 (0.0%)	0.85	1/6940 (0.0%)
2	P	0.93	0/13	0.64	0/15
2	Q	0.79	0/13	0.51	0/15
All	All	0.86	5/10246 (0.0%)	0.87	2/13950 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	SER	N-CA	5.83	1.53	1.46
1	B	579	GLN	C-O	5.54	1.30	1.24
1	A	387	PHE	N-CA	5.40	1.52	1.46
1	A	80	TRP	N-CA	5.33	1.53	1.46
1	A	119	SER	N-CA	5.13	1.52	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	TRP	N-CA-C	11.13	126.37	113.01
1	B	419	GLU	N-CA-C	-5.68	103.14	110.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ILE	Peptide

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	4964	0	4741	33	0
1	B	4940	0	4707	27	0
2	P	14	0	15	0	0
2	Q	14	0	15	0	0
3	C	24	0	22	1	0
3	F	24	0	22	1	0
4	D	28	0	25	0	0
4	G	28	0	25	0	0
5	E	49	0	43	0	0
6	H	39	0	34	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	21	0	30	2	0
9	B	7	0	10	0	0
10	A	19	0	26	3	0
10	B	38	0	52	0	0
11	B	10	0	13	0	0
12	A	501	0	0	6	0
12	B	367	0	0	2	0
12	P	2	0	0	0	0
12	Q	2	0	0	0	0
All	All	11095	0	9780	62	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 3.

All (62) 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:B:260:SER:OG	1:B:262:GLU:OE1	1.87	0.93
1:A:365:HIS:HD1	1:A:388:HIS:HD2	1.26	0.84
1:B:124:THR:HG22	1:B:327:GLU:HG2	1.60	0.81
1:A:365:HIS:HD1	1:A:388:HIS:CD2	2.00	0.80
1:B:365:HIS:HD1	1:B:388:HIS:HD2	1.30	0.78
1:A:270:PRO:HD3	1:A:426:LEU:HD23	1.68	0.73
1:B:365:HIS:HD1	1:B:388:HIS:CD2	2.05	0.73
1:A:467:ARG:HH11	1:A:471:GLN:HE22	1.38	0.72
1:A:137:TRP:CH2	1:A:155:MET:HE1	2.29	0.68
1:A:12:ALA:O	12:A:1101:HOH:O	2.12	0.68
1:A:14:GLU:HG2	1:A:83:PHE:CD1	2.30	0.66
1:B:350:ARG:H	1:B:355:GLN:HE21	1.43	0.64
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.79	0.64
1:A:596:GLU:OE2	3:F:1:NAG:O7	2.16	0.63
1:A:187:LYS:HE2	1:A:192:THR:O	1.98	0.63
1:A:206:THR:HG23	1:A:210:ASP:OD2	1.99	0.62
1:A:137:TRP:CZ3	1:A:155:MET:HE1	2.36	0.61
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.83	0.59
1:A:14:GLU:OE2	1:A:83:PHE:HA	2.03	0.58
1:A:372:TYR:OH	1:A:388:HIS:HE1	1.87	0.57
1:B:24:TYR:HD2	1:B:25:GLN:HG3	1.69	0.57
1:B:419:GLU:O	1:B:421:ASP:N	2.36	0.56
1:A:79:ILE:HD12	1:A:80:TRP:HA	1.87	0.56
1:B:124:THR:HG22	1:B:327:GLU:CG	2.34	0.56
1:B:49:GLU:OE2	1:B:52:ARG:NH2	2.39	0.53
1:A:467:ARG:NH1	1:A:471:GLN:HE22	2.07	0.53
10:A:1006:P6G:H31	12:A:1539:HOH:O	2.09	0.51
1:A:84:THR:HB	12:A:1523:HOH:O	2.09	0.51
10:A:1006:P6G:H81	12:A:1279:HOH:O	2.11	0.50
1:B:596:GLU:OE2	3:C:1:NAG:O7	2.29	0.50
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.93	0.49
1:B:1:LEU:N	12:B:805:HOH:O	2.45	0.49
1:B:271:PHE:CE2	1:B:419:GLU:HG2	2.47	0.49
1:B:560:VAL:CG2	12:B:938:HOH:O	2.61	0.49
1:A:572:LYS:HD2	9:A:1003:PEG:H11	1.94	0.48
1:A:76:TYR:HB3	1:A:80:TRP:HB3	1.95	0.48
1:A:436:LEU:N	1:A:437:PRO:HD2	2.29	0.48
1:B:17:ALA:HB1	1:B:92:ILE:HD11	1.94	0.48
1:B:31:VAL:O	1:B:34:GLN:HG3	2.14	0.47
1:B:1:LEU:HD23	1:B:6:GLN:HG2	1.97	0.47
1:A:232:ALA:HB2	9:A:1005:PEG:H22	1.96	0.45
1:B:578:THR:O	1:B:582:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.98	0.45
1:A:117[A]:GLN:NE2	12:A:1106:HOH:O	2.40	0.45
1:A:66:GLU:CD	1:A:108:ARG:HH22	2.24	0.44
1:B:124:THR:CG2	1:B:327:GLU:HG2	2.41	0.44
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.01	0.43
1:B:232:ALA:CB	1:B:268:VAL:HG12	2.49	0.43
1:A:30:GLN:NE2	12:A:1121:HOH:O	2.52	0.43
1:A:76:TYR:O	1:A:77:GLU:C	2.62	0.43
1:B:372:TYR:OH	1:B:388:HIS:HE1	2.01	0.43
1:A:83:PHE:HB2	1:A:89:ARG:CG	2.50	0.42
1:A:269:VAL:HA	1:A:270:PRO:HD3	1.91	0.42
1:B:324:ASP:OD1	1:B:326:ARG:HB2	2.20	0.41
1:A:79:ILE:O	1:A:82:GLN:OE1	2.38	0.41
1:A:489:LYS:O	1:A:493:PRO:HD2	2.20	0.41
1:B:140:ASP:HA	1:B:141:PRO:HA	1.88	0.41
1:A:495:VAL:HG12	1:A:495:VAL:O	2.21	0.41
1:B:419:GLU:C	1:B:421:ASP:N	2.79	0.41
1:B:570:LEU:C	1:B:570:LEU:HD23	2.46	0.41
1:A:146:ILE:HD13	1:A:155:MET:CE	2.51	0.41
1:A:36:VAL:HA	10:A:1006:P6G:H172	2.03	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	605/629 (96%)	593 (98%)	11 (2%)	1 (0%)	43	24
1	B	603/629 (96%)	591 (98%)	11 (2%)	1 (0%)	43	24
All	All	1208/1258 (96%)	1184 (98%)	22 (2%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/541 (96%)	516 (99%)	6 (1%)	65	43
1	B	516/541 (95%)	513 (99%)	3 (1%)	78	64
2	P	1/5 (20%)	1 (100%)	0	100	100
2	Q	1/5 (20%)	1 (100%)	0	100	100
All	All	1040/1092 (95%)	1031 (99%)	9 (1%)	70	51

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	SER
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	403	GLU
1	B	151	ARG
1	B	372	TYR
1	B	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	224	ASN
1	A	388	HIS
1	A	471	GLN
1	A	527	GLN
1	A	585	ASN

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Mol	Chain	Res	Type
1	B	355	GLN
1	B	388	HIS
1	B	423	ASN
1	B	579	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	3,1	14,14,15	0.64	0	17,19,21	0.80	0
3	FUC	C	2	3	10,10,11	0.36	0	14,14,16	0.69	0
4	NAG	D	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	D	2	4	14,14,15	0.49	0	17,19,21	1.39	2 (11%)
5	NAG	E	1	5	14,14,15	0.96	1 (7%)	17,19,21	1.08	0
5	NAG	E	2	5	14,14,15	0.37	0	17,19,21	1.04	0
5	BMA	E	3	5	11,11,12	0.60	0	15,15,17	2.06	3 (20%)
5	FUC	E	4	5	10,10,11	0.69	0	14,14,16	1.65	1 (7%)
3	NAG	F	1	3,1	14,14,15	0.57	0	17,19,21	1.05	0
3	FUC	F	2	3	10,10,11	0.56	0	14,14,16	1.61	3 (21%)
4	NAG	G	1	4,1	14,14,15	0.38	0	17,19,21	0.96	1 (5%)
4	NAG	G	2	4	14,14,15	0.48	0	17,19,21	1.63	2 (11%)
6	NAG	H	1	6,1	14,14,15	0.38	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	H	2	6	14,14,15	0.38	0	17,19,21	1.15	2 (11%)
6	BMA	H	3	6	11,11,12	0.72	0	15,15,17	1.84	3 (20%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	2.57	1.48	1.43
5	E	1	NAG	O5-C1	-2.38	1.39	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	4	FUC	O2-C2-C1	5.49	121.79	109.22
5	E	3	BMA	O3-C3-C2	5.22	120.72	110.05
5	E	3	BMA	C1-O5-C5	4.81	118.64	112.19
6	H	3	BMA	O3-C3-C2	4.57	119.38	110.05
4	G	2	NAG	O4-C4-C3	4.35	120.63	110.38
4	G	2	NAG	C3-C4-C5	4.21	117.86	110.23
4	D	2	NAG	C3-C4-C5	3.52	116.61	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	FUC	C3-C4-C5	3.45	115.05	109.81
6	H	3	BMA	C1-O5-C5	3.43	116.78	112.19
6	H	3	BMA	C2-C3-C4	3.35	116.76	110.86
4	D	2	NAG	O4-C4-C3	3.22	117.96	110.38
5	E	3	BMA	C2-C3-C4	2.99	116.11	110.86
3	F	2	FUC	C1-O5-C5	2.83	119.64	112.97
4	D	1	NAG	O5-C5-C4	2.73	117.46	110.83
6	H	2	NAG	C3-C4-C5	2.40	114.59	110.23
3	F	2	FUC	C1-C2-C3	2.35	113.06	109.64
6	H	2	NAG	C4-C3-C2	2.21	114.25	111.02
4	G	1	NAG	O3-C3-C2	-2.04	105.16	109.40
6	H	1	NAG	C2-N2-C7	2.04	125.64	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

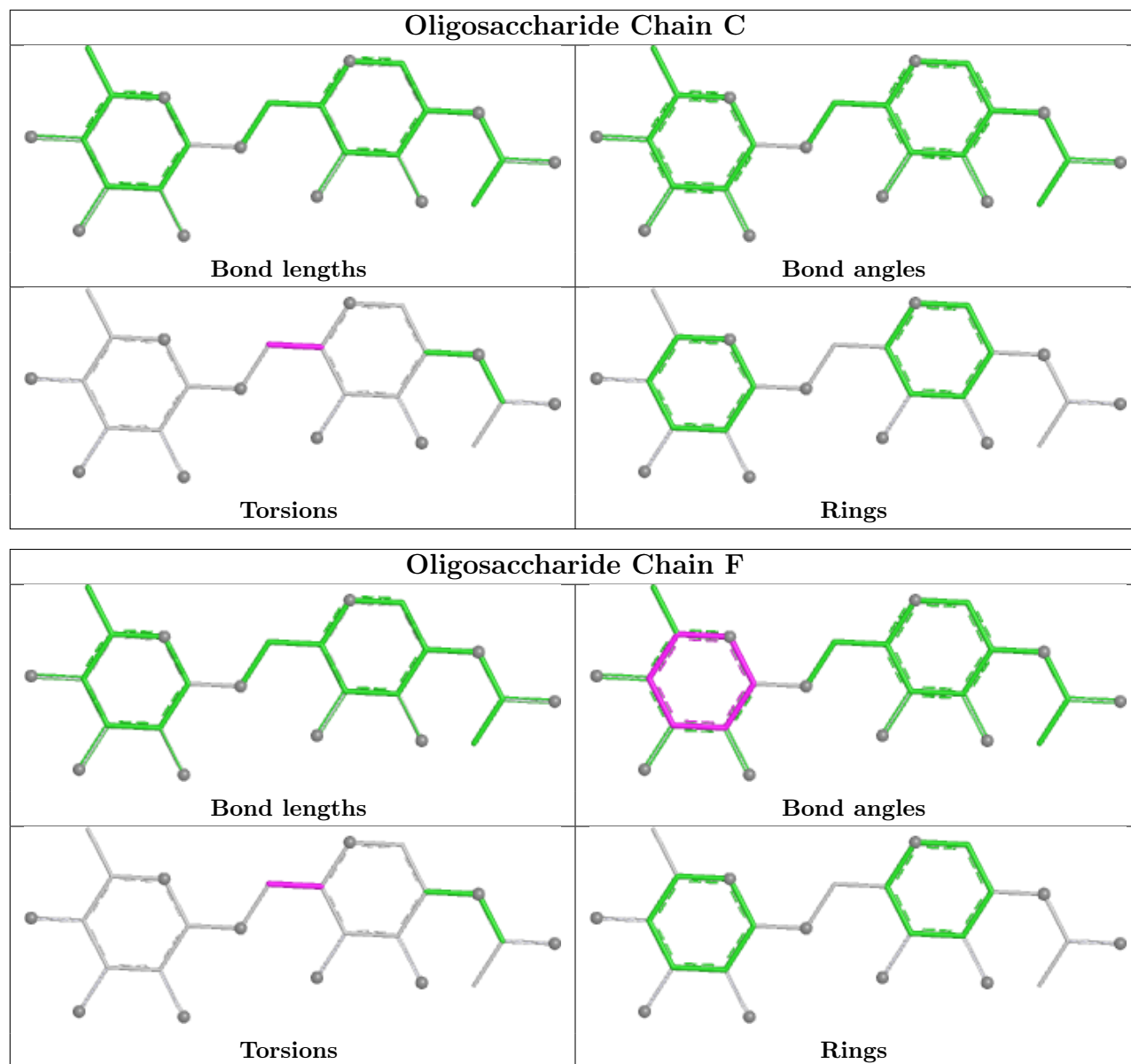
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	C1-C2-N2-C7
5	E	1	NAG	C1-C2-N2-C7

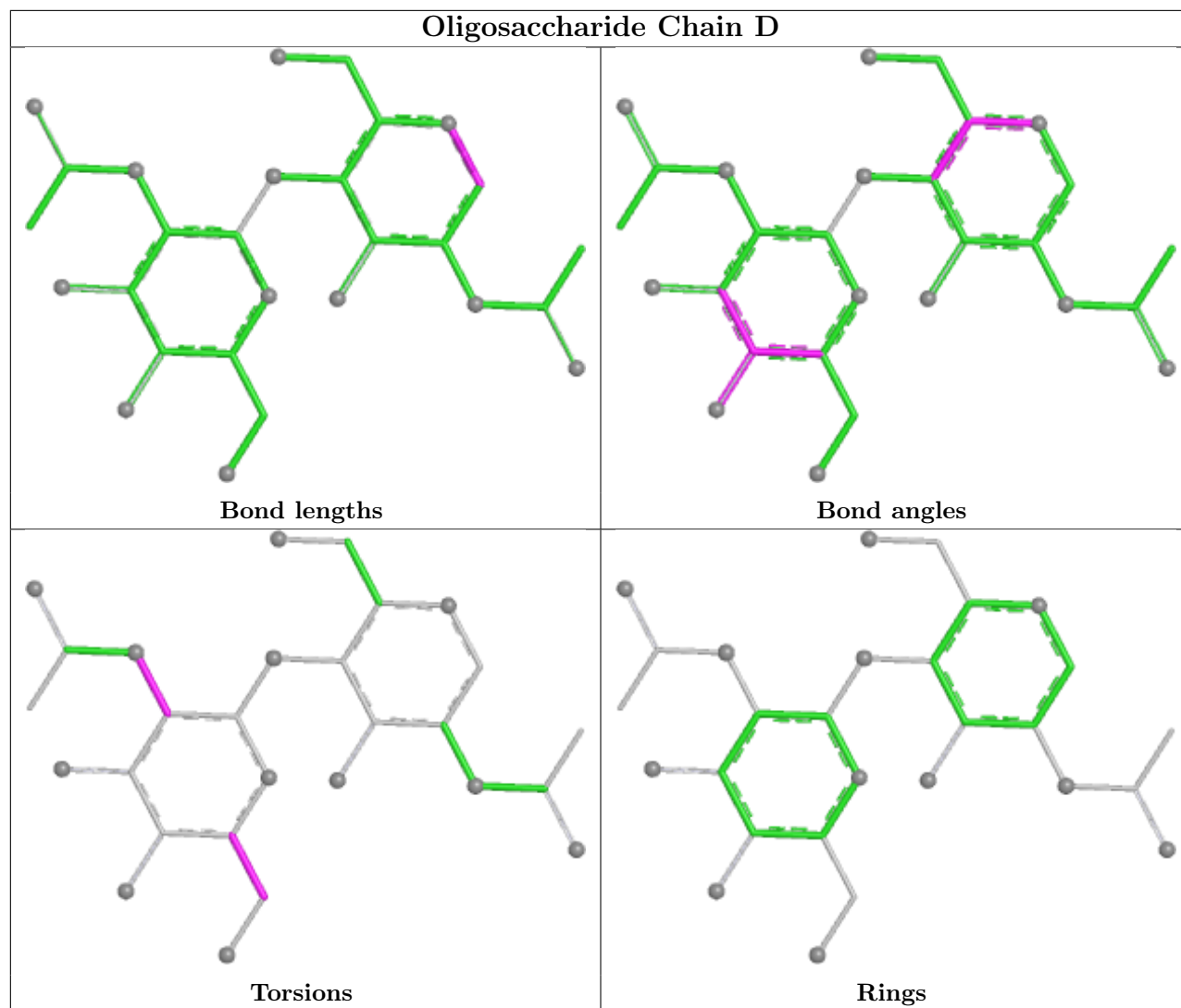
There are no ring outliers.

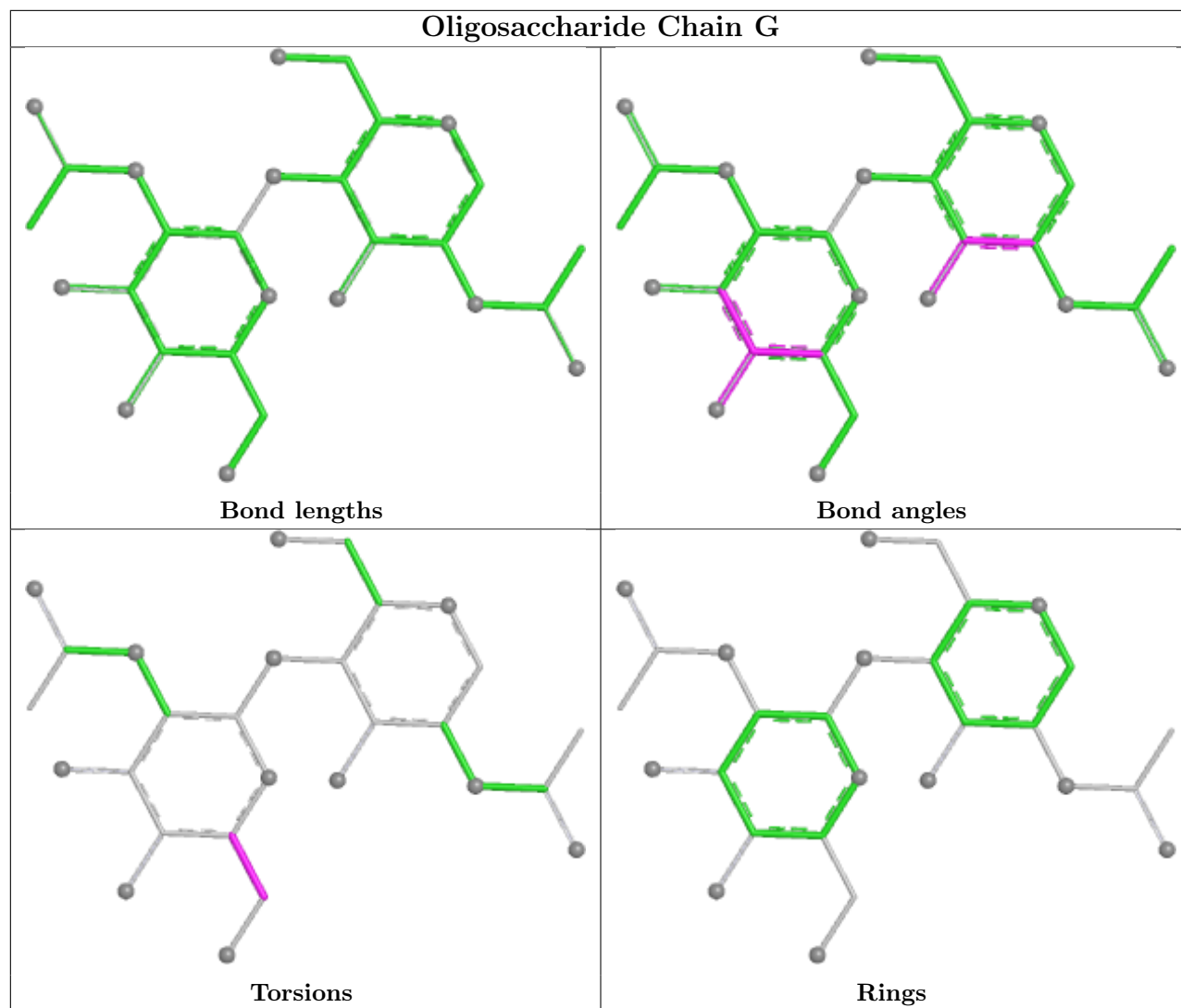
2 monomers are involved in 2 short contacts:

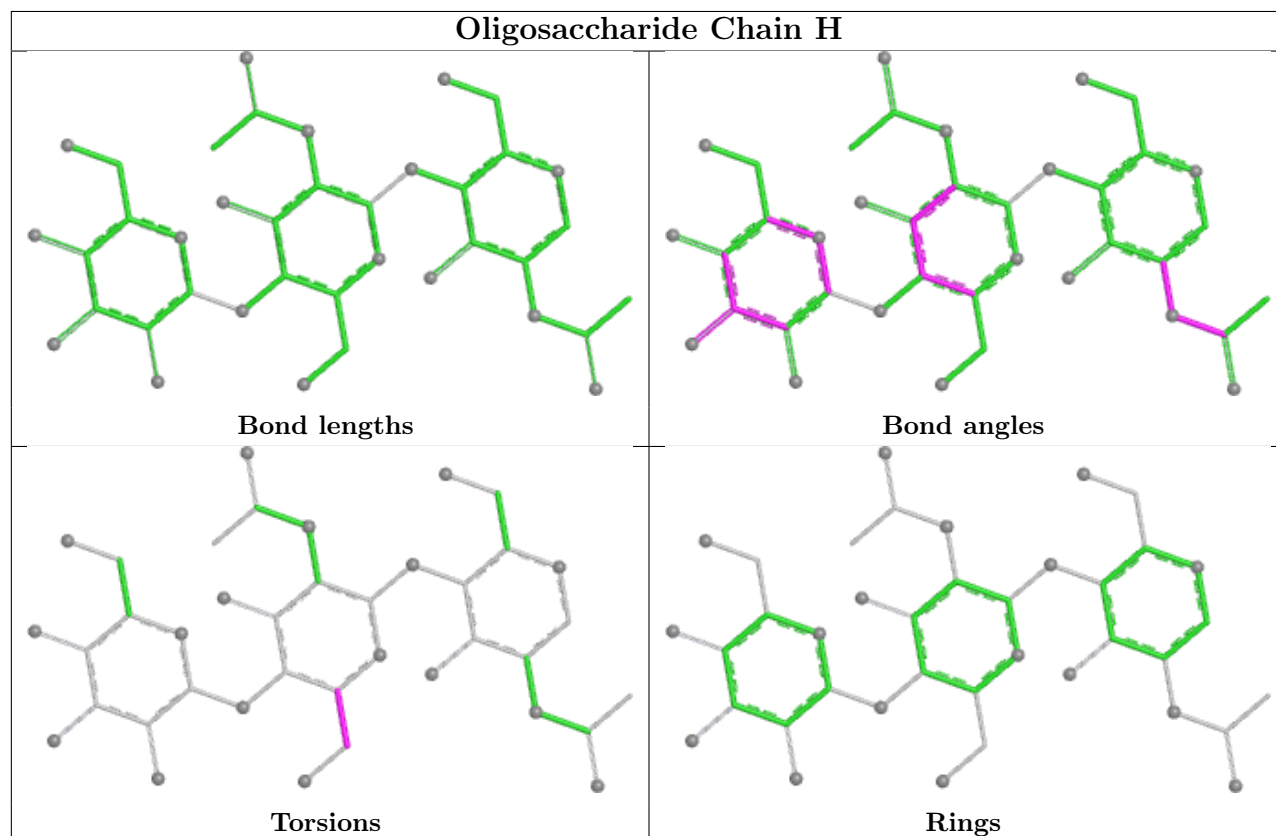
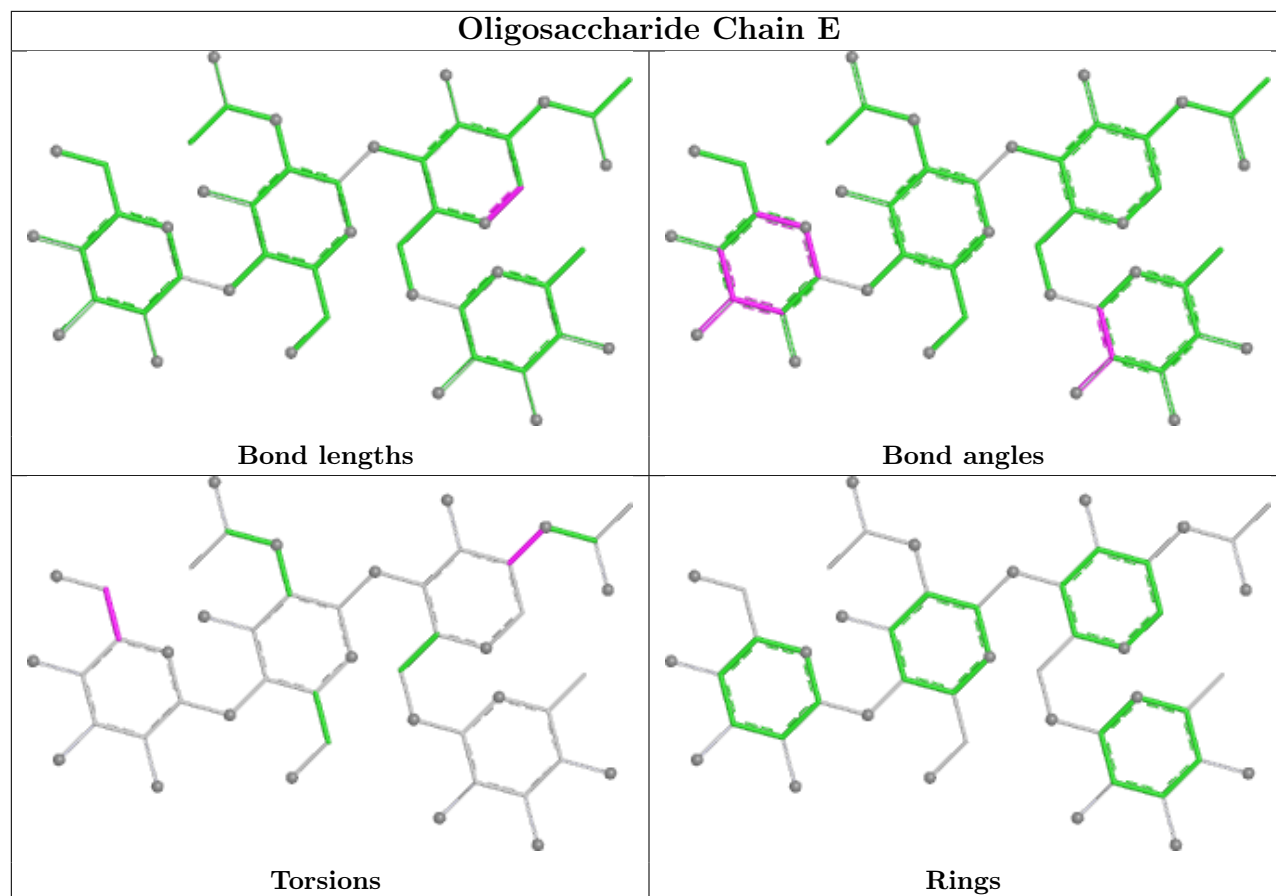
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	C	1	NAG	1	0

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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
10	P6G	B	706	-	18,18,18	0.52	0	17,17,17	0.24	0
11	PG4	B	701	-	9,9,12	0.54	0	8,8,11	0.49	0
9	PEG	A	1003	-	6,6,6	0.50	0	5,5,5	0.61	0
9	PEG	A	1004	-	6,6,6	0.48	0	5,5,5	0.34	0
10	P6G	A	1006	-	18,18,18	0.45	0	17,17,17	0.51	0
9	PEG	A	1005	-	6,6,6	0.59	0	5,5,5	0.37	0
9	PEG	B	704	-	6,6,6	0.55	0	5,5,5	0.23	0
10	P6G	B	705	-	18,18,18	0.67	0	17,17,17	0.38	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
10	P6G	B	706	-	-	11/16/16/16	-
11	PG4	B	701	-	-	5/7/7/10	-
9	PEG	A	1003	-	-	4/4/4/4	-
9	PEG	A	1004	-	-	2/4/4/4	-
10	P6G	A	1006	-	-	11/16/16/16	-
9	PEG	A	1005	-	-	1/4/4/4	-
9	PEG	B	704	-	-	1/4/4/4	-
10	P6G	B	705	-	-	6/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

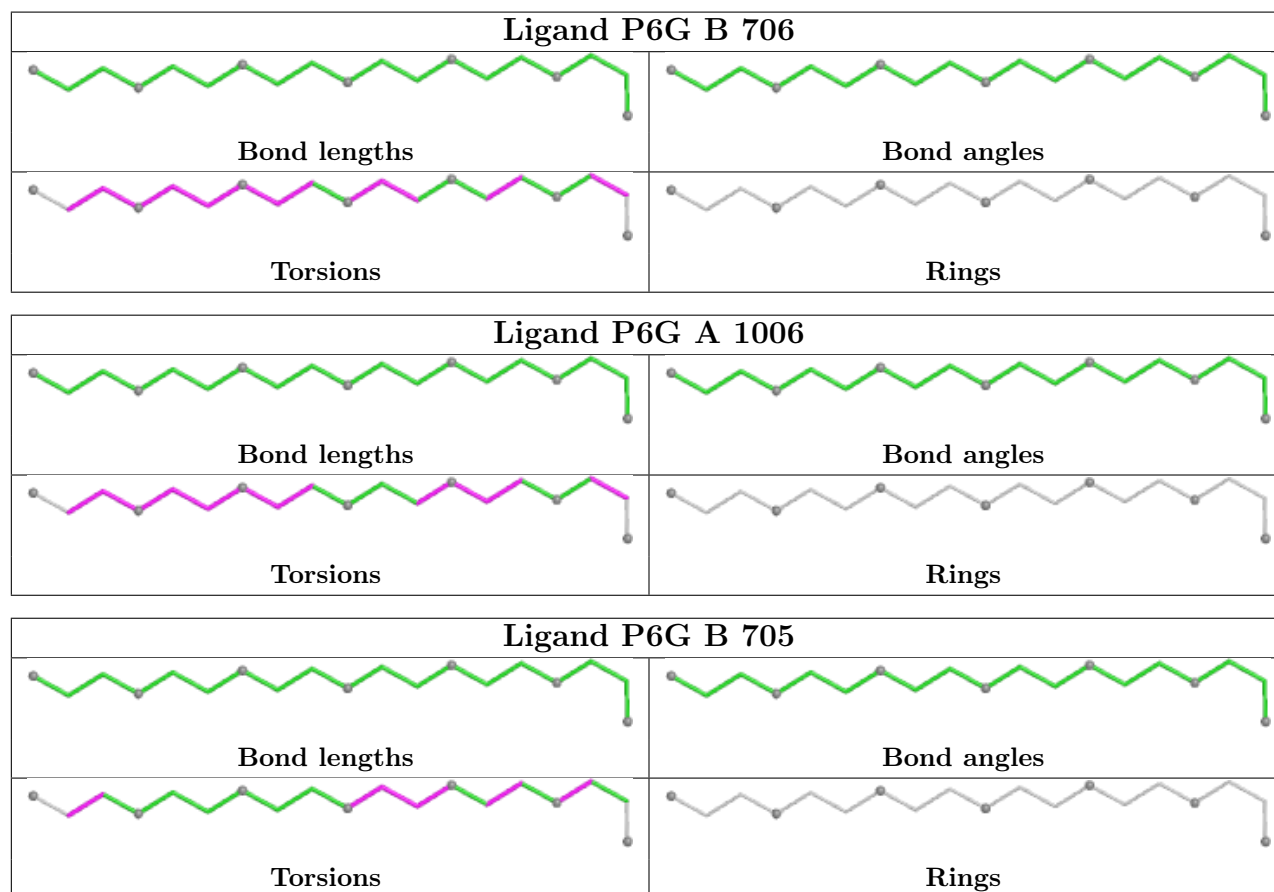
Mol	Chain	Res	Type	Atoms
10	A	1006	P6G	O13-C14-C15-O16
10	B	705	P6G	O4-C5-C6-O7
10	A	1006	P6G	O10-C11-C12-O13
11	B	701	PG4	O2-C3-C4-O3
10	B	706	P6G	O10-C11-C12-O13
10	B	706	P6G	O7-C8-C9-O10
9	A	1003	PEG	O2-C3-C4-O4
9	B	704	PEG	O2-C3-C4-O4
10	A	1006	P6G	O16-C17-C18-O19
10	B	705	P6G	O16-C17-C18-O19
10	B	706	P6G	O16-C17-C18-O19
11	B	701	PG4	O1-C1-C2-O2
9	A	1003	PEG	O1-C1-C2-O2
11	B	701	PG4	O3-C5-C6-O4
10	B	706	P6G	O1-C2-C3-O4
10	A	1006	P6G	O4-C5-C6-O7
10	A	1006	P6G	O1-C2-C3-O4
10	B	706	P6G	O4-C5-C6-O7
9	A	1005	PEG	C1-C2-O2-C3
10	A	1006	P6G	C18-C17-O16-C15
10	A	1006	P6G	C15-C14-O13-C12
9	A	1003	PEG	C4-C3-O2-C2
10	B	705	P6G	O7-C8-C9-O10
9	A	1003	PEG	C1-C2-O2-C3
9	A	1004	PEG	C4-C3-O2-C2
10	A	1006	P6G	C11-C12-O13-C14
10	B	706	P6G	C11-C12-O13-C14
10	B	706	P6G	C8-C9-O10-C11
10	B	706	P6G	C15-C14-O13-C12
10	A	1006	P6G	C9-C8-O7-C6
10	B	705	P6G	C9-C8-O7-C6
10	B	706	P6G	C14-C15-O16-C17
11	B	701	PG4	C4-C3-O2-C2
11	B	701	PG4	C3-C4-O3-C5
10	B	706	P6G	C18-C17-O16-C15
10	B	705	P6G	C2-C3-O4-C5
10	A	1006	P6G	C5-C6-O7-C8
10	A	1006	P6G	C14-C15-O16-C17
10	B	706	P6G	O13-C14-C15-O16
9	A	1004	PEG	O2-C3-C4-O4
10	B	705	P6G	C8-C9-O10-C11

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1003	PEG	1	0
10	A	1006	P6G	3	0
9	A	1005	PEG	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%)	-0.23	19 (3%)	51	60	18, 30, 52, 87	2 (0%)
1	B	607/629 (96%)	-0.02	10 (1%)	70	78	21, 36, 58, 87	0
2	P	2/8 (25%)	-0.38	0	100	100	26, 26, 26, 30	0
2	Q	2/8 (25%)	-0.13	0	100	100	27, 27, 27, 31	0
All	All	1218/1274 (95%)	-0.13	29 (2%)	59	67	18, 33, 56, 87	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	TRP	5.4
1	A	14	GLU	4.6
1	A	78	PRO	3.4
1	B	129	LEU	3.3
1	A	88	LEU	3.0
1	B	133	THR	3.0
1	A	94	ALA	2.9
1	B	92	ILE	2.9
1	A	129	LEU	2.9
1	A	83	PHE	2.8
1	A	19	LEU	2.8
1	B	101	ALA	2.7
1	B	414	VAL	2.7
1	A	610	GLY	2.7
1	A	84	THR	2.7
1	B	270	PRO	2.7
1	A	95	VAL	2.6
1	A	15	ALA	2.6
1	A	607	TYR	2.6
1	A	25	GLN	2.6
1	B	68	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	2.3
1	B	379	LEU	2.3
1	A	75	LEU	2.2
1	B	134	ALA	2.2
1	A	20	PHE	2.1
1	A	135	THR	2.1
1	B	135	THR	2.1
1	A	13	ASP	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 ⓘ

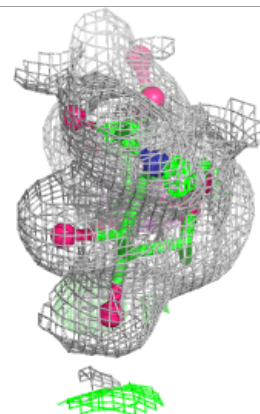
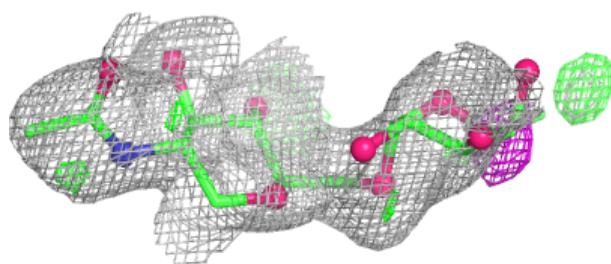
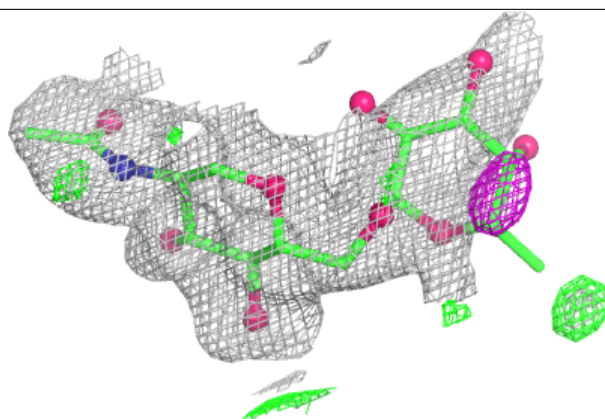
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	36,46,55,69	0
3	FUC	C	2	10/11	-	-	64,75,79,93	0
6	NAG	H	1	14/15	0.87	0.10	56,63,75,88	0
3	FUC	F	2	10/11	-	-	65,81,88,91	0
4	NAG	D	1	14/15	-	-	50,57,64,71	0
4	NAG	D	2	14/15	-	-	58,71,85,92	0
3	NAG	F	1	14/15	0.92	0.09	44,51,60,75	0
5	NAG	E	1	14/15	0.93	0.09	34,40,45,50	0
4	NAG	G	2	14/15	0.94	0.07	84,92,109,116	0
5	NAG	E	2	14/15	-	-	44,56,66,66	0
5	BMA	E	3	11/12	-	-	63,66,79,84	0
5	FUC	E	4	10/11	-	-	46,57,66,68	0
4	NAG	G	1	14/15	0.98	0.05	47,55,73,74	0
6	NAG	H	2	14/15	-	-	78,81,96,106	0
6	BMA	H	3	11/12	-	-	91,99,101,103	0

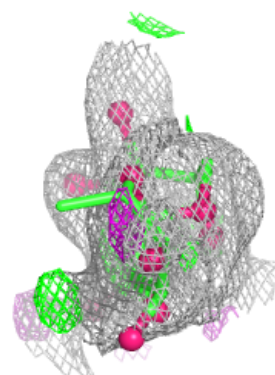
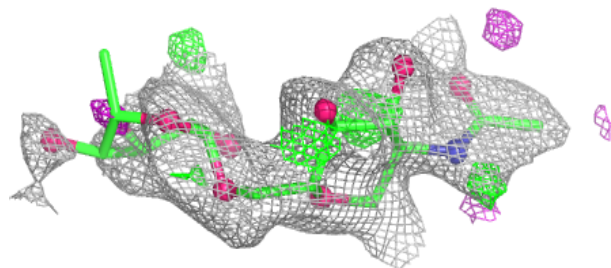
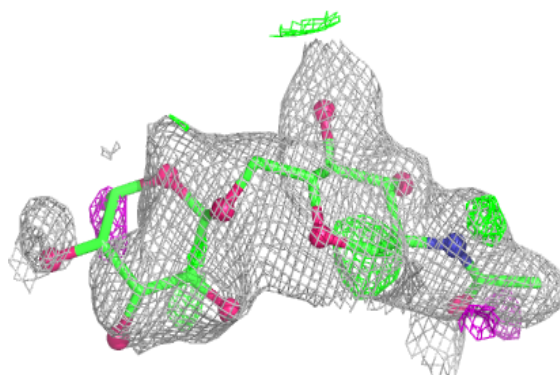
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

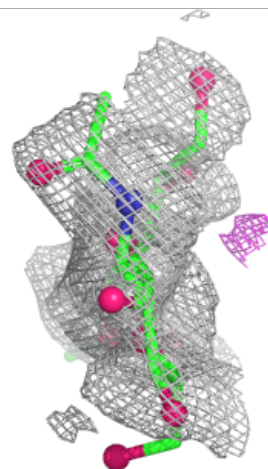
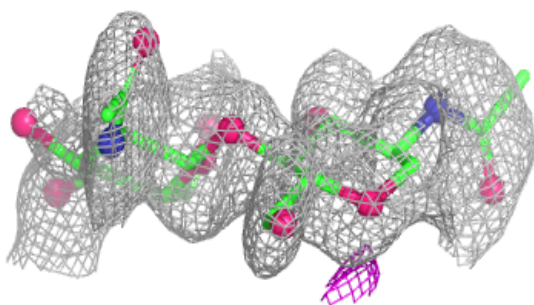
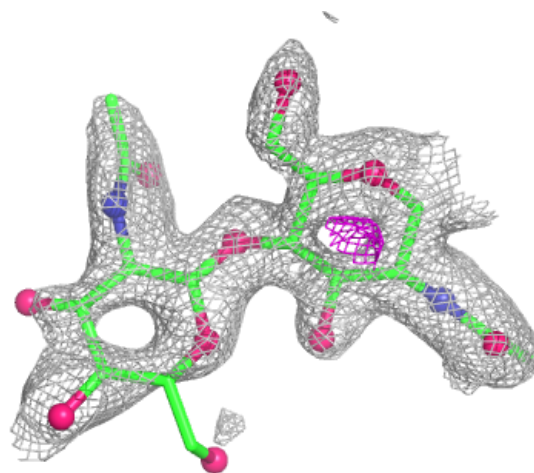
**Electron density around Chain F:**

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



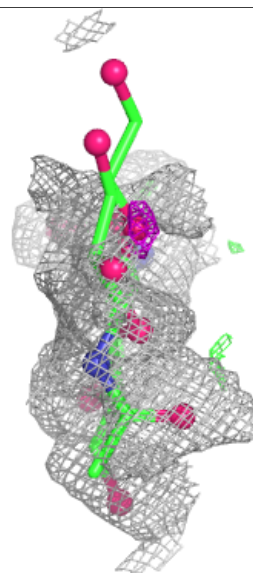
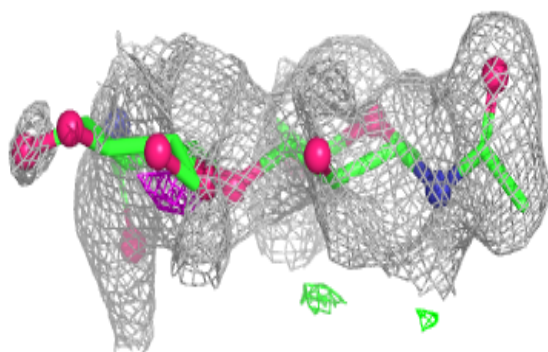
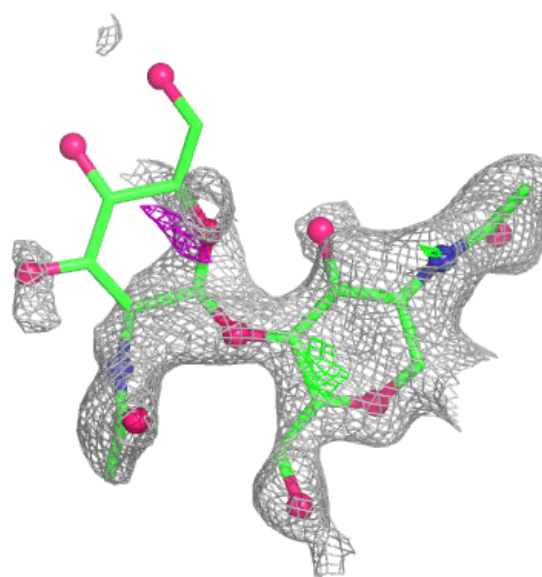
Electron density around Chain D:

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



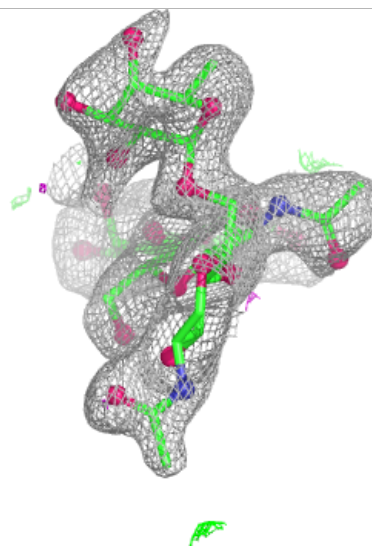
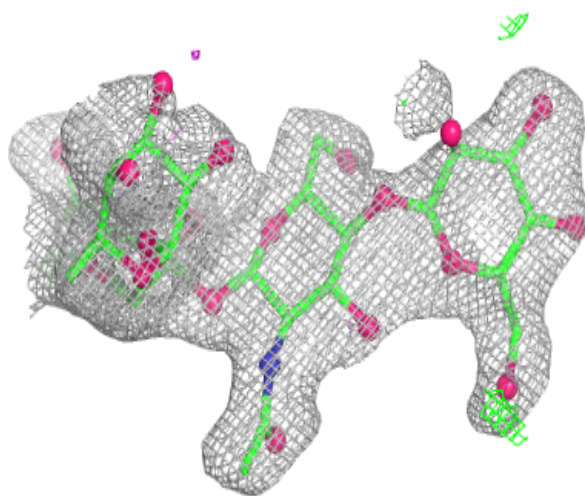
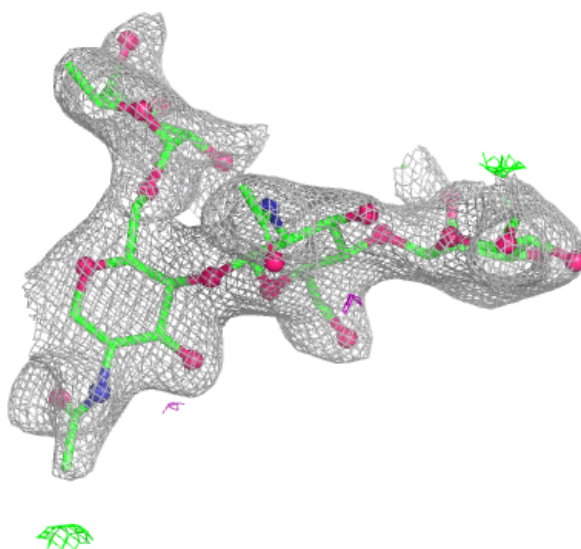
Electron density around Chain G:

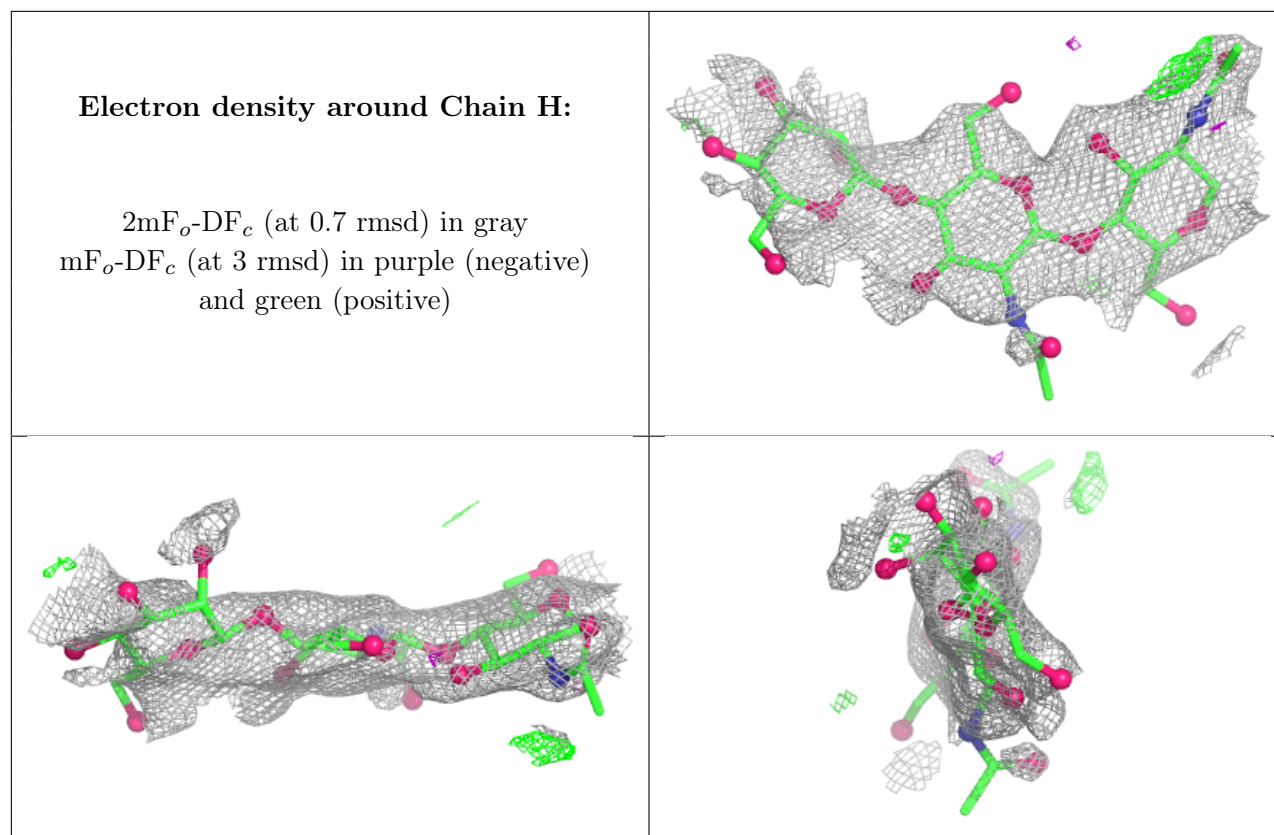
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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.

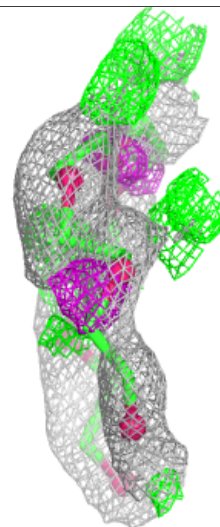
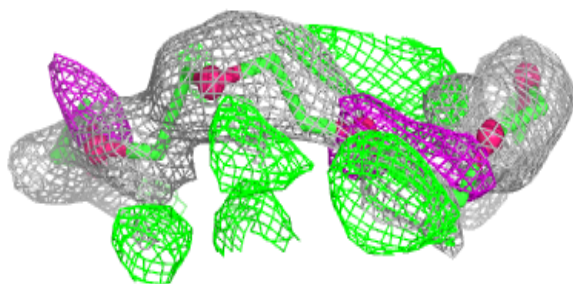
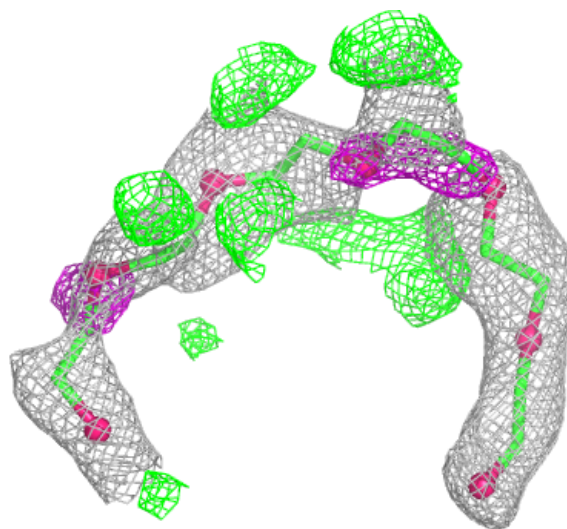
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	P6G	A	1006	19/19	0.75	0.17	46,52,56,56	0
10	P6G	B	706	19/19	0.76	0.17	47,52,58,59	0
9	PEG	A	1005	7/7	0.88	0.11	31,40,46,72	0
10	P6G	B	705	19/19	0.89	0.11	44,55,62,63	0
9	PEG	A	1003	7/7	0.90	0.10	50,52,62,68	0
9	PEG	A	1004	7/7	0.94	0.08	50,52,65,77	0
9	PEG	B	704	7/7	0.95	0.06	38,44,50,55	0
11	PG4	B	701	10/13	0.95	0.09	43,54,56,60	0
8	CL	B	703	1/1	0.99	0.02	29,29,29,29	0
7	ZN	A	1001	1/1	1.00	0.01	25,25,25,25	0
7	ZN	B	702	1/1	1.00	0.01	25,25,25,25	0
8	CL	A	1002	1/1	1.00	0.02	23,23,23,23	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.

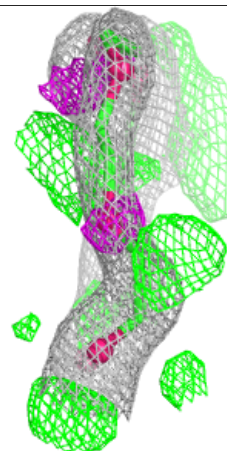
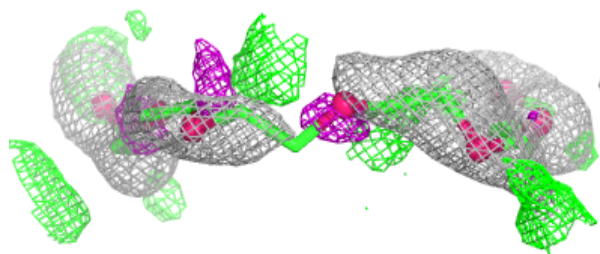
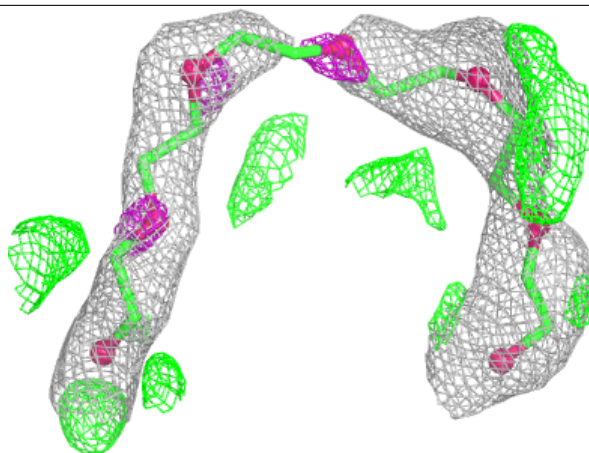
Electron density around P6G A 1006:

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



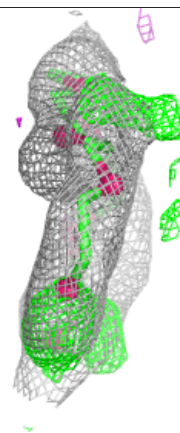
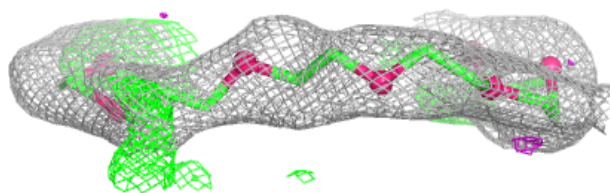
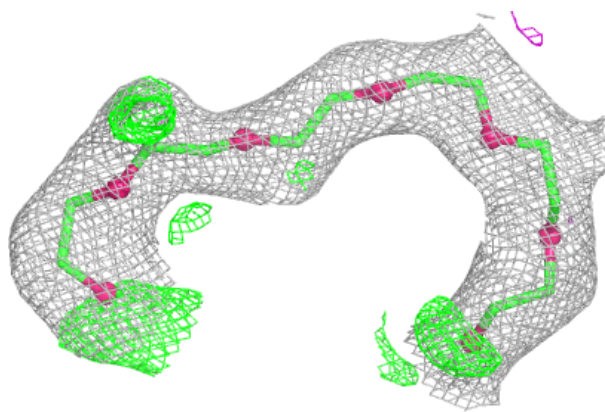
Electron density around P6G B 706:

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



Electron density around P6G B 705:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.