



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:54 PM UTC

PDB ID : 5AM8 / pdb_00005am8
Title : Crystal structure of the Angiotensin-1 converting enzyme N-domain in complex with amyloid-beta 4-10
Authors : Masuyer, G.; Larmuth, K.M.; Douglas, R.G.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2015-03-10
Resolution : 1.90 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

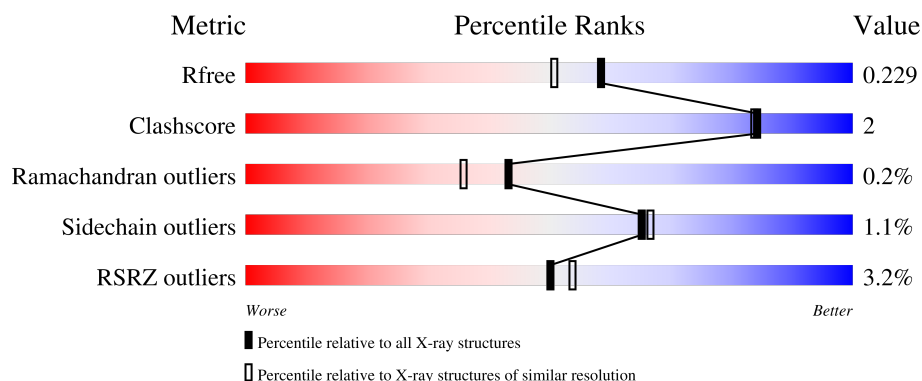
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 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	 2% 90% 6% .
1	B	629	 3% 90% 5% .
1	C	629	 2% 90% 6% .
1	D	629	 4% 91% 6% .
2	P	7	 14% 29% 57%

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Mol	Chain	Length	Quality of chain
2	Q	7	
2	R	7	
2	S	7	
3	E	2	
3	F	2	
3	H	2	
3	K	2	
4	G	2	
4	J	2	
5	I	3	
6	L	4	
7	M	4	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22316 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	604	Total	C	N	O	S	0	1	0
			4939	3173	849	898	19			
1	B	606	Total	C	N	O	S	0	1	0
			4950	3179	852	900	19			
1	C	606	Total	C	N	O	S	0	1	0
			4959	3186	852	902	19			
1	D	612	Total	C	N	O	S	0	5	0
			5029	3229	867	914	19			

There are 32 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	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	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
C	9	GLN	ASN	engineered mutation	UNP P12821
C	25	GLN	ASN	engineered mutation	UNP P12821
C	82	GLN	ASN	engineered mutation	UNP P12821
C	117	GLN	ASN	engineered mutation	UNP P12821
C	289	GLN	ASN	engineered mutation	UNP P12821

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Chain	Residue	Modelled	Actual	Comment	Reference
C	545	ARG	GLN	engineered mutation	UNP P12821
C	576	LEU	PRO	engineered mutation	UNP P12821
C	629	LEU	ARG	engineered mutation	UNP P12821
D	9	GLN	ASN	engineered mutation	UNP P12821
D	25	GLN	ASN	engineered mutation	UNP P12821
D	82	GLN	ASN	engineered mutation	UNP P12821
D	117	GLN	ASN	engineered mutation	UNP P12821
D	289	GLN	ASN	engineered mutation	UNP P12821
D	545	ARG	GLN	engineered mutation	UNP P12821
D	576	LEU	PRO	engineered mutation	UNP P12821
D	629	LEU	ARG	engineered mutation	UNP P12821

- Molecule 2 is a protein called BETA-AMYLOID PROTEIN 42.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	P	3	Total C N O 15 7 3 5	0	0	1
2	Q	3	Total C N O 15 7 3 5	0	0	1
2	R	3	Total C N O 15 7 3 5	0	0	1
2	S	3	Total C N O 15 7 3 5	0	0	1

- Molecule 3 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
3	E	2	Total C N O 28 16 2 10	0	0	0
3	F	2	Total C N O 28 16 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0
3	K	2	Total C N O 28 16 2 10	0	0	0

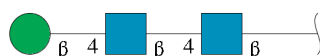
- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta

a-D-glucopyranose.



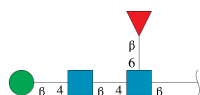
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	J	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 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.



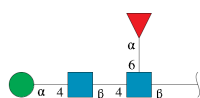
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 7 is an oligosaccharide called alpha-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
7	M	4	Total	C	N	O	0	0	0
			49	28	2	19			

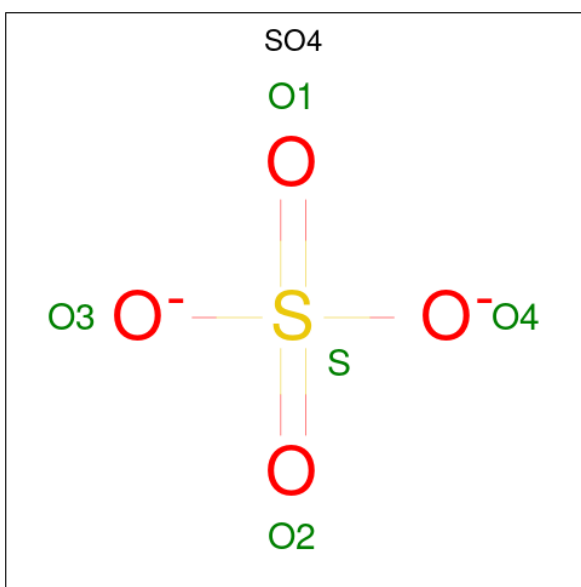
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		
8	B	1	Total	Zn	0	0
			1	1		
8	C	1	Total	Zn	0	0
			1	1		
8	D	1	Total	Zn	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

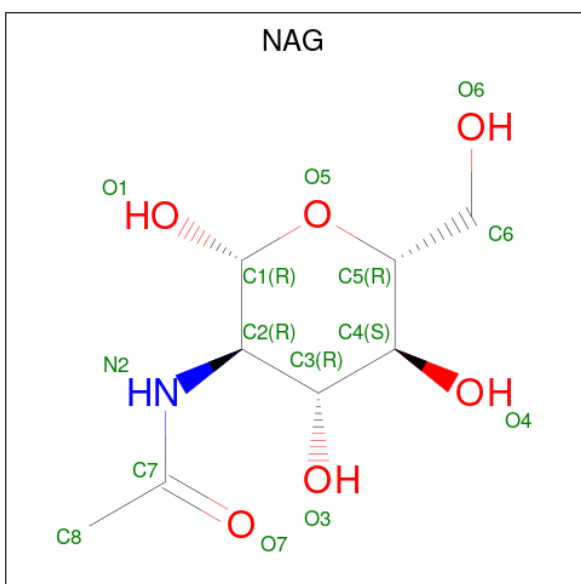
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	1	Total	Cl	0	0
			1	1		
9	C	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



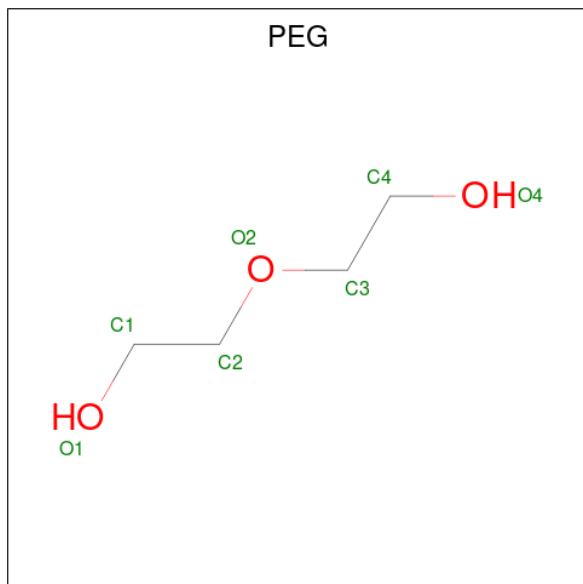
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



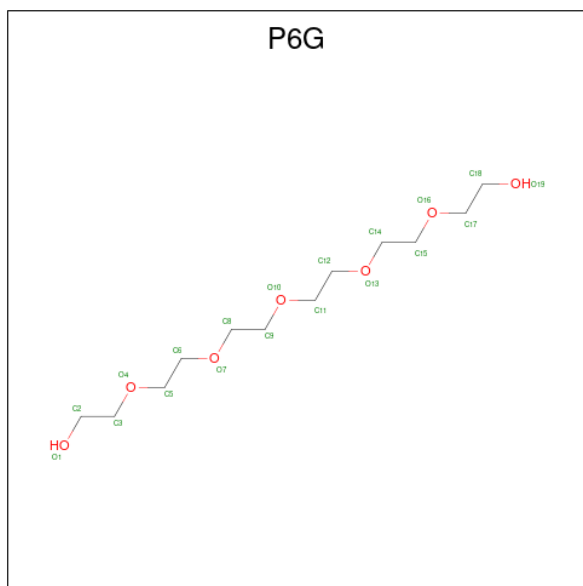
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	A	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		
12	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		
12	C	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		
12	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



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

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

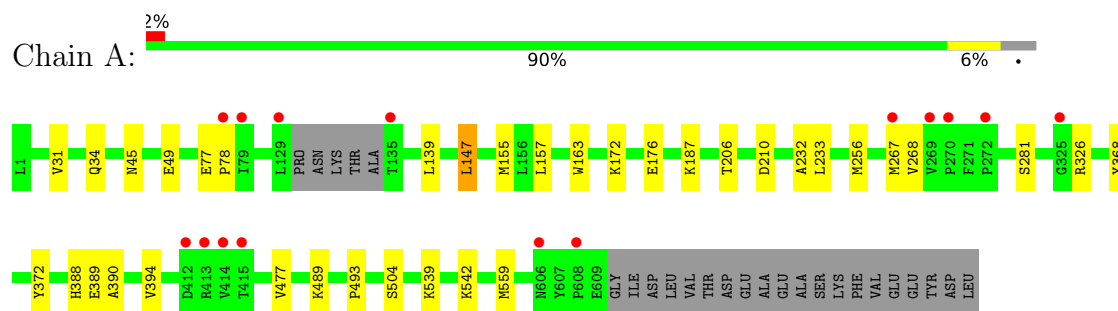
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	391	Total	O	0	0
			391	391		
14	B	458	Total	O	0	0
			458	458		
14	C	513	Total	O	0	0
			513	513		
14	D	464	Total	O	0	0
			464	464		
14	R	1	Total	O	0	0
			1	1		
14	S	2	Total	O	0	0
			2	2		

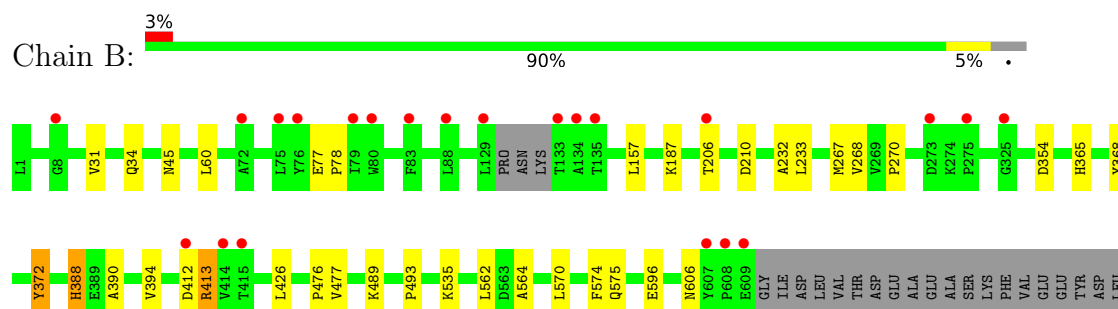
3 Residue-property plots

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.

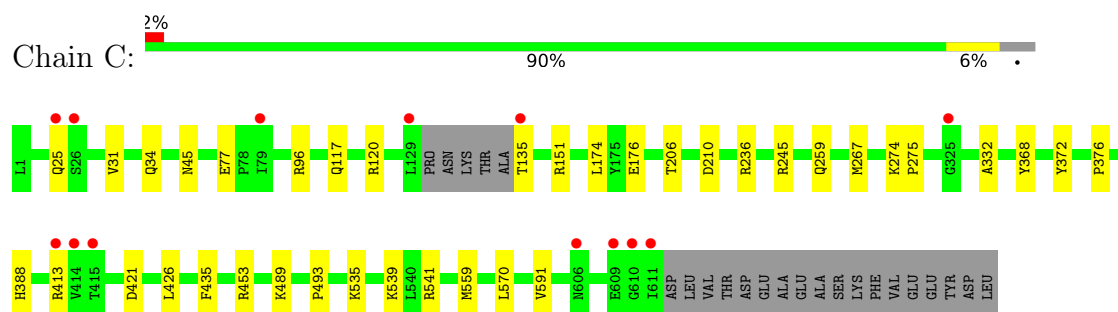
• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



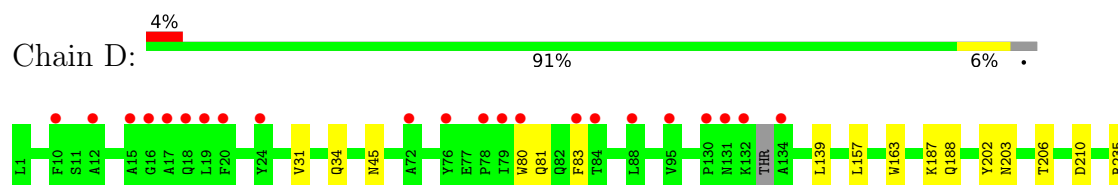
• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

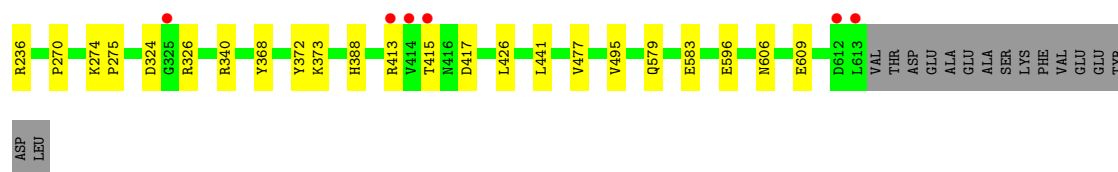


• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME



• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

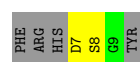




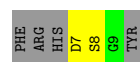
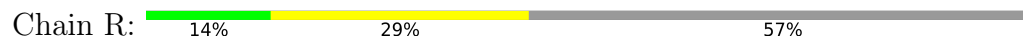
- Molecule 2: BETA-AMYLOID PROTEIN 42



- Molecule 2: BETA-AMYLOID PROTEIN 42



- Molecule 2: BETA-AMYLOID PROTEIN 42



- Molecule 2: BETA-AMYLOID PROTEIN 42



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



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



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





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

Chain K: 100%



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

Chain G: 50% 50%



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

Chain J: 50% 50%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



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

Chain L: 25% 75%



- Molecule 7: alpha-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 M: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.45Å 101.76Å 114.36Å 85.23° 86.07° 81.45°	Depositor
Resolution (Å)	113.78 – 1.90 113.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (113.78-1.90) 93.2 (113.78-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.185 , 0.224 0.193 , 0.229	Depositor DCC
R_{free} test set	12020 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	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	22316	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0333e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BMA, FUC, SO4, MAN, CL, NAG, FUL, PEG, P6G, ZN

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	0.65	0/5098	0.80	0/6944
1	B	0.66	0/5108	0.81	0/6957
1	C	0.69	0/5117	0.81	0/6968
1	D	0.68	0/5195	0.80	0/7075
2	P	1.76	1/14 (7.1%)	1.13	0/18
2	Q	2.05	1/14 (7.1%)	0.93	0/18
2	R	1.72	1/14 (7.1%)	1.26	0/18
2	S	1.80	1/14 (7.1%)	0.81	0/18
All	All	0.68	4/20574 (0.0%)	0.81	0/28016

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	8	SER	C-N	-7.26	1.23	1.33
2	S	8	SER	C-N	-6.23	1.24	1.33
2	P	8	SER	C-N	-6.19	1.24	1.33
2	R	8	SER	C-N	-6.05	1.24	1.33

There are no bond angle outliers.

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	4939	0	4712	16	0
1	B	4950	0	4725	23	0
1	C	4959	0	4745	22	0
1	D	5029	0	4808	23	0
2	P	15	0	8	1	0
2	Q	15	0	8	1	0
2	R	15	0	8	1	0
2	S	15	0	8	0	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	H	28	0	25	0	0
3	K	28	0	25	0	0
4	G	24	0	22	1	0
4	J	24	0	22	1	0
5	I	39	0	34	0	0
6	L	49	0	43	0	0
7	M	49	0	43	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
10	C	5	0	0	0	0
10	D	5	0	0	0	0
11	A	14	0	13	0	0
11	D	28	0	26	1	0
12	A	28	0	40	3	0
12	B	35	0	50	0	0
12	C	28	0	40	0	0
12	D	35	0	50	0	0
13	A	19	0	26	1	0
13	B	19	0	26	0	0
13	D	19	0	26	3	0
14	A	391	0	0	4	0
14	B	458	0	0	3	0
14	C	513	0	0	5	0
14	D	464	0	0	2	0
14	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	S	2	0	0	0	0
All	All	22316	0	19583	90	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 (90) 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:233:LEU:HD23	1:B:267:MET:HE1	1.63	0.80
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.67	0.75
1:A:233:LEU:HD23	1:A:267:MET:HE1	1.69	0.75
1:A:147:LEU:HD22	1:A:256:MET:HA	1.68	0.74
1:C:206:THR:HG23	1:C:210:ASP:OD2	1.89	0.73
1:A:206:THR:HG23	1:A:210:ASP:OD2	1.91	0.71
1:B:365:HIS:HD1	1:B:388:HIS:CD2	2.09	0.70
1:D:206:THR:HG23	1:D:210:ASP:OD2	1.93	0.69
1:C:453:ARG:NH1	14:C:2414:HOH:O	2.23	0.69
1:C:413:ARG:NH2	14:C:2379:HOH:O	2.27	0.66
1:A:539:LYS:HE3	1:A:559:MET:O	1.96	0.65
1:C:176:GLU:OE1	14:C:2196:HOH:O	2.13	0.65
1:B:354:ASP:OD2	14:B:2315:HOH:O	2.15	0.63
1:B:206:THR:HG23	1:B:210:ASP:OD2	1.99	0.62
12:A:1201:PEG:O4	13:A:1202:P6G:O19	2.19	0.60
1:B:365:HIS:HD1	1:B:388:HIS:HD2	1.49	0.60
1:C:245:ARG:HG2	1:C:591:VAL:HG11	1.83	0.59
1:B:596:GLU:OE2	11:D:1100:NAG:O7	2.19	0.59
14:C:2505:HOH:O	4:J:2:FUC:H4	2.03	0.58
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.86	0.58
1:C:236:ARG:HD2	1:C:267:MET:HE3	1.86	0.57
1:D:235:ARG:HH11	13:D:1201:P6G:H172	1.68	0.57
1:C:426:LEU:O	1:C:426:LEU:HG	1.99	0.56
1:D:157:LEU:HD11	1:D:477:VAL:HG13	1.88	0.55
1:C:274:LYS:HB3	1:C:275:PRO:CD	2.37	0.54
1:B:412:ASP:O	1:B:413:ARG:CB	2.56	0.53
1:D:188:GLN:HG2	14:D:2186:HOH:O	2.08	0.53
1:D:275:PRO:HG3	1:D:413:ARG:HG2	1.91	0.52
1:D:235:ARG:HH12	13:D:1201:P6G:H112	1.75	0.52
1:A:172:LYS:O	1:A:176:GLU:HG3	2.11	0.51
1:D:596:GLU:OE2	4:G:1:NAG:O7	2.29	0.50
1:A:187:LYS:HE3	14:A:2178:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:LYS:HB3	1:D:275:PRO:CD	2.42	0.50
1:B:232:ALA:CB	1:B:268:VAL:HG12	2.42	0.50
1:D:579:GLN:NE2	1:D:583:GLU:OE2	2.34	0.50
1:C:539:LYS:HE3	1:C:559:MET:O	2.12	0.49
1:A:389:GLU:HB2	1:A:504:SER:HB2	1.94	0.49
1:A:77:GLU:N	1:A:78:PRO:HD2	2.28	0.49
1:C:151:ARG:HD2	1:C:267:MET:SD	2.53	0.49
12:A:1201:PEG:H22	14:A:2389:HOH:O	2.11	0.49
1:B:412:ASP:O	1:B:413:ARG:HB3	2.13	0.49
1:C:570:LEU:C	1:C:570:LEU:HD23	2.37	0.48
1:B:489:LYS:O	1:B:493:PRO:HD2	2.14	0.48
1:D:340[B]:ARG:HG2	1:D:373:LYS:O	2.13	0.48
1:A:155:MET:HE3	1:A:155:MET:HA	1.96	0.48
1:D:270:PRO:HD3	1:D:426:LEU:HD22	1.95	0.48
1:A:489:LYS:O	1:A:493:PRO:HD2	2.14	0.48
1:D:83:PHE:HA	14:D:2006:HOH:O	2.15	0.47
1:B:31:VAL:O	1:B:34:GLN:HG3	2.15	0.46
1:D:441:LEU:C	1:D:441:LEU:HD12	2.40	0.46
1:D:31:VAL:O	1:D:34:GLN:HG3	2.15	0.45
1:D:495:VAL:O	1:D:495:VAL:HG12	2.16	0.45
1:C:77:GLU:OE2	1:C:96:ARG:NH2	2.49	0.45
1:D:235:ARG:NH1	13:D:1201:P6G:H172	2.31	0.45
1:C:135:THR:HG23	1:C:135:THR:O	2.17	0.45
1:B:372:TYR:OH	1:B:388:HIS:HE1	1.99	0.44
1:D:80:TRP:CE2	1:D:81:GLN:HG3	2.53	0.44
1:A:232:ALA:CB	1:A:268:VAL:HG12	2.48	0.44
1:C:245:ARG:HG2	1:C:591:VAL:CG1	2.47	0.44
1:C:25:GLN:OE1	1:C:376:PRO:HA	2.17	0.44
1:A:31:VAL:O	1:A:34:GLN:HG3	2.18	0.44
1:C:541[B]:ARG:NH1	14:C:2316:HOH:O	2.51	0.43
1:D:139:LEU:HD22	1:D:163:TRP:CZ2	2.53	0.43
1:A:49:GLU:HG2	3:E:2:NAG:H82	2.00	0.43
1:C:259:GLN:O	1:C:435:PHE:HA	2.18	0.43
1:B:570:LEU:C	1:B:570:LEU:HD23	2.43	0.43
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.00	0.43
1:B:60:LEU:HD11	14:B:2001:HOH:O	2.18	0.42
1:B:574:PHE:O	1:B:575:GLN:C	2.62	0.42
1:D:606:ASN:O	1:D:609:GLU:N	2.52	0.42
1:C:332:ALA:HB3	2:R:7:ASP:HB2	2.00	0.42
1:C:117:GLN:HE22	1:C:120:ARG:HE	1.66	0.42
1:D:270:PRO:HD3	1:D:426:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:2323:HOH:O	2:Q:7:ASP:N	2.52	0.42
14:A:2288:HOH:O	2:P:7:ASP:N	2.53	0.42
1:A:157:LEU:HD11	1:A:477:VAL:HG13	2.02	0.41
1:B:77:GLU:HB3	1:B:78:PRO:HD3	2.02	0.41
1:D:324:ASP:OD1	1:D:326:ARG:HB2	2.21	0.41
1:B:426:LEU:O	1:B:426:LEU:HG	2.15	0.41
1:C:489:LYS:O	1:C:493:PRO:HD2	2.20	0.41
1:D:415:THR:OG1	1:D:417:ASP:OD2	2.38	0.41
1:C:31:VAL:O	1:C:34:GLN:HG3	2.20	0.41
1:A:390:ALA:O	1:A:394:VAL:HG23	2.21	0.41
1:A:139:LEU:HD22	1:A:163:TRP:CZ2	2.56	0.41
1:C:77:GLU:HA	1:C:77:GLU:OE1	2.20	0.41
1:B:267:MET:HE2	1:B:267:MET:HB3	1.90	0.40
1:B:562:LEU:HD23	1:B:564:ALA:O	2.21	0.40
12:A:1203:PEG:H41	14:A:2127:HOH:O	2.20	0.40
1:B:390:ALA:O	1:B:394:VAL:HG23	2.22	0.40
1:D:202:TYR:O	1:D:203[B]:ASN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	601/629 (96%)	590 (98%)	9 (2%)	2 (0%)	36	29
1	B	603/629 (96%)	593 (98%)	8 (1%)	2 (0%)	36	29
1	C	603/629 (96%)	593 (98%)	9 (2%)	1 (0%)	43	36
1	D	613/629 (98%)	601 (98%)	11 (2%)	1 (0%)	43	36
2	P	1/7 (14%)	1 (100%)	0	0	100	100
2	Q	1/7 (14%)	1 (100%)	0	0	100	100
2	R	1/7 (14%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2424/2544 (95%)	2381 (98%)	37 (2%)	6 (0%)	43	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	413	ARG
1	A	326	ARG
1	D	45	ASN
1	B	45	ASN
1	A	45	ASN
1	C	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	519/541 (96%)	513 (99%)	6 (1%)	63	63
1	B	519/541 (96%)	513 (99%)	6 (1%)	63	63
1	C	522/541 (96%)	516 (99%)	6 (1%)	65	67
1	D	529/541 (98%)	524 (99%)	5 (1%)	70	73
2	P	2/6 (33%)	2 (100%)	0	100	100
2	Q	2/6 (33%)	2 (100%)	0	100	100
2	R	2/6 (33%)	2 (100%)	0	100	100
2	S	2/6 (33%)	2 (100%)	0	100	100
All	All	2097/2188 (96%)	2074 (99%)	23 (1%)	65	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	281	SER

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Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	A	542	LYS
1	B	187	LYS
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	535	LYS
1	B	606	ASN
1	C	174	LEU
1	C	368	TYR
1	C	372	TYR
1	C	388	HIS
1	C	421	ASP
1	C	535	LYS
1	D	187	LYS
1	D	236	ARG
1	D	368	TYR
1	D	372	TYR
1	D	388	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	82	GLN
1	A	87	GLN
1	A	203	ASN
1	A	263	ASN
1	A	289	GLN
1	A	292	HIS
1	A	494	ASN
1	A	575	GLN
1	B	188	GLN
1	B	216	GLN
1	B	276	ASN
1	B	289	GLN
1	B	388	HIS
1	B	494	ASN
1	C	117	GLN
1	C	494	ASN

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Mol	Chain	Res	Type
1	C	588	ASN
1	D	18	GLN
1	D	224	ASN
1	D	585	ASN

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 ⓘ

23 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	E	1	3,1	14,14,15	0.57	0	17,19,21	1.20	1 (5%)
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.77	0
3	NAG	F	1	3,1	14,14,15	0.70	0	17,19,21	0.94	0
3	NAG	F	2	3	14,14,15	0.55	0	17,19,21	1.08	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.77	0	17,19,21	2.32	3 (17%)
4	FUC	G	2	4	10,10,11	0.71	0	14,14,16	1.17	1 (7%)
3	NAG	H	1	3,1	14,14,15	0.72	0	17,19,21	1.19	1 (5%)
3	NAG	H	2	3	14,14,15	0.51	0	17,19,21	0.90	0
5	NAG	I	1	5,1	14,14,15	0.60	0	17,19,21	0.81	0
5	NAG	I	2	5	14,14,15	0.67	0	17,19,21	0.74	0
5	BMA	I	3	5	11,11,12	0.37	0	15,15,17	0.77	0
4	NAG	J	1	4,1	14,14,15	0.68	0	17,19,21	2.02	5 (29%)
4	FUC	J	2	4	10,10,11	0.78	0	14,14,16	1.84	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	3,1	14,14,15	0.59	0	17,19,21	1.37	2 (11%)
3	NAG	K	2	3	14,14,15	0.55	0	17,19,21	1.27	2 (11%)
6	NAG	L	1	6,1	14,14,15	0.88	1 (7%)	17,19,21	0.94	0
6	NAG	L	2	6	14,14,15	0.68	0	17,19,21	0.93	0
6	BMA	L	3	6	11,11,12	0.66	0	15,15,17	2.35	3 (20%)
6	FUL	L	4	6	10,10,11	0.87	0	14,14,16	1.41	3 (21%)
7	NAG	M	1	7,1	14,14,15	0.85	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	M	2	7	14,14,15	0.64	0	17,19,21	1.15	1 (5%)
7	MAN	M	3	7	11,11,12	0.63	0	15,15,17	2.04	4 (26%)
7	FUC	M	4	7	10,10,11	0.61	0	14,14,16	1.10	1 (7%)

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	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	J	2	4	-	-	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	FUL	L	4	6	-	-	0/1/1/1
7	NAG	M	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	MAN	M	3	7	-	0/2/19/22	0/1/1/1
7	FUC	M	4	7	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1	NAG	O5-C1	-2.10	1.40	1.43
7	M	1	NAG	O5-C1	-2.00	1.40	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	3	BMA	C1-O5-C5	7.28	121.95	112.19
4	G	1	NAG	C2-N2-C7	-6.09	114.74	122.90
4	J	1	NAG	C1-C2-N2	-5.36	101.99	110.43
4	G	1	NAG	C8-C7-N2	4.38	123.38	116.12
7	M	3	MAN	C3-C4-C5	4.21	117.87	110.23
4	G	1	NAG	O7-C7-N2	-4.19	114.58	121.98
6	L	3	BMA	C3-C4-C5	4.15	117.76	110.23
3	E	1	NAG	C1-O5-C5	4.09	117.67	112.19
4	J	1	NAG	C4-C3-C2	3.88	116.70	111.02
7	M	3	MAN	O5-C5-C6	3.87	115.20	107.66
4	J	2	FUC	C3-C4-C5	3.85	115.66	109.81
4	J	2	FUC	C1-C2-C3	3.82	115.21	109.64
7	M	2	NAG	C1-C2-N2	-3.75	104.52	110.43
3	K	1	NAG	C1-O5-C5	3.10	116.34	112.19
7	M	3	MAN	C1-C2-C3	3.07	114.12	109.64
7	M	3	MAN	C2-C3-C4	3.04	116.20	110.86
3	K	1	NAG	O5-C1-C2	-2.96	106.72	111.29
3	H	1	NAG	C1-O5-C5	2.50	115.53	112.19
3	F	2	NAG	O7-C7-C8	-2.49	117.62	122.05
4	J	2	FUC	C2-C3-C4	2.48	115.22	110.86
4	G	2	FUC	O5-C1-C2	-2.41	105.03	110.79
6	L	4	FUL	O5-C5-C6	2.41	112.63	107.40
6	L	3	BMA	O5-C5-C4	2.38	116.61	110.83
7	M	4	FUC	C1-C2-C3	-2.34	106.24	109.64
4	J	1	NAG	C2-N2-C7	2.30	125.98	122.90
3	K	2	NAG	O5-C5-C6	2.30	112.14	107.66
3	K	2	NAG	C3-C4-C5	-2.24	106.17	110.23
4	J	2	FUC	O5-C5-C4	-2.19	105.61	109.55
4	J	1	NAG	O5-C5-C6	2.17	111.88	107.66
7	M	1	NAG	O5-C1-C2	-2.06	108.11	111.29
4	J	1	NAG	O3-C3-C4	-2.04	105.57	110.38
6	L	4	FUL	O3-C3-C2	-2.02	105.94	110.05
6	L	4	FUL	C1-C2-C3	2.01	112.58	109.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

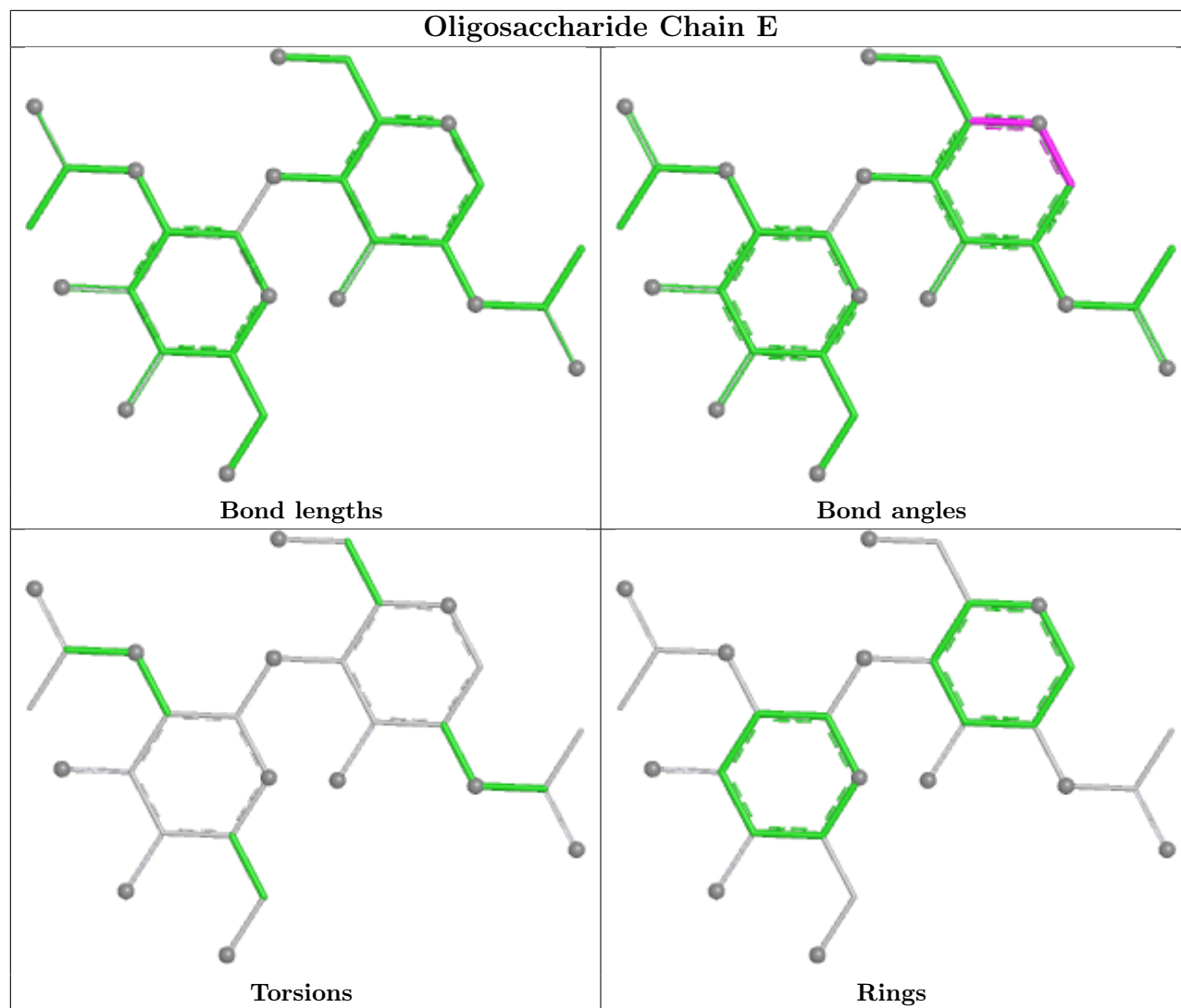
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6

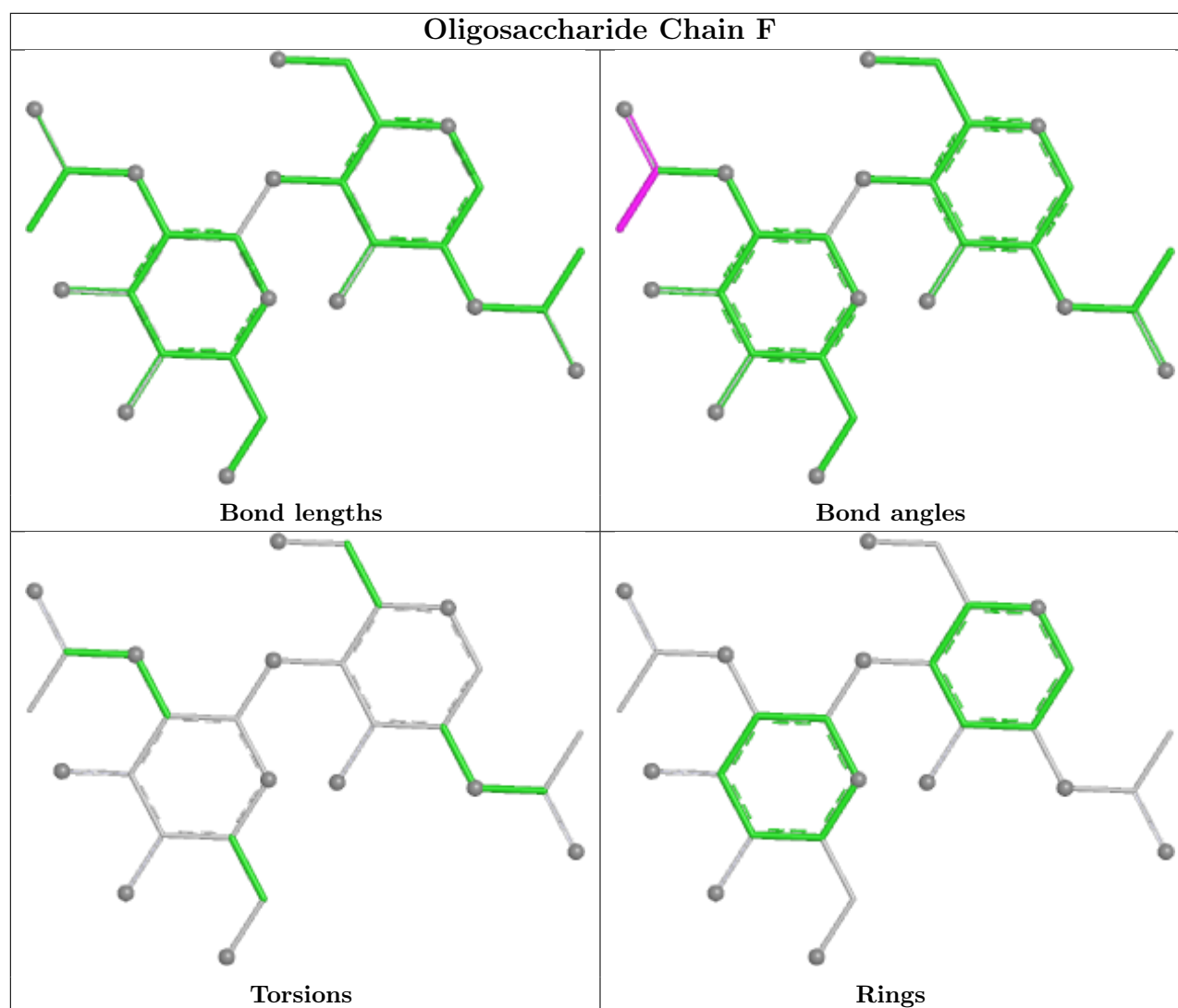
There are no ring outliers.

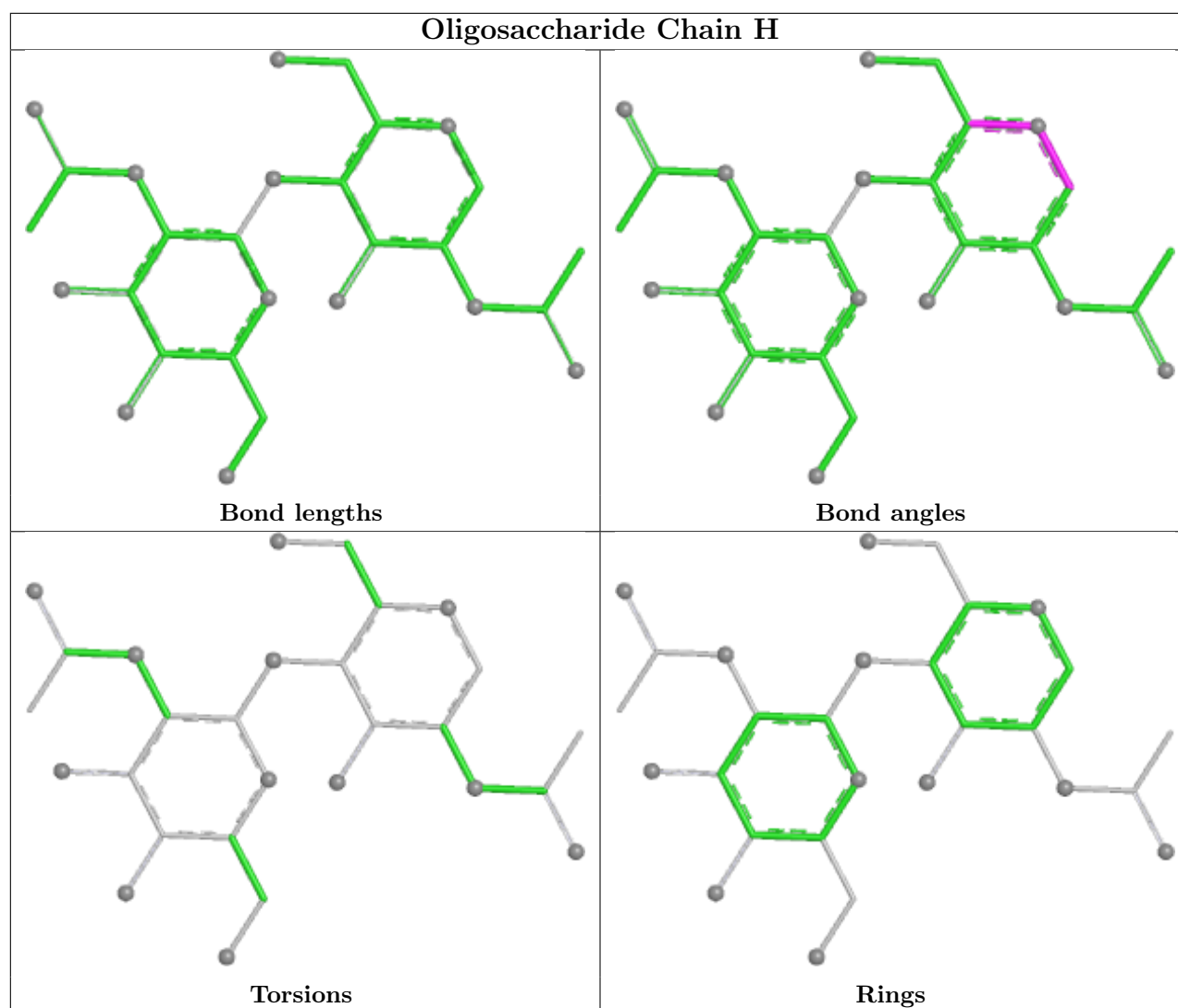
3 monomers are involved in 3 short contacts:

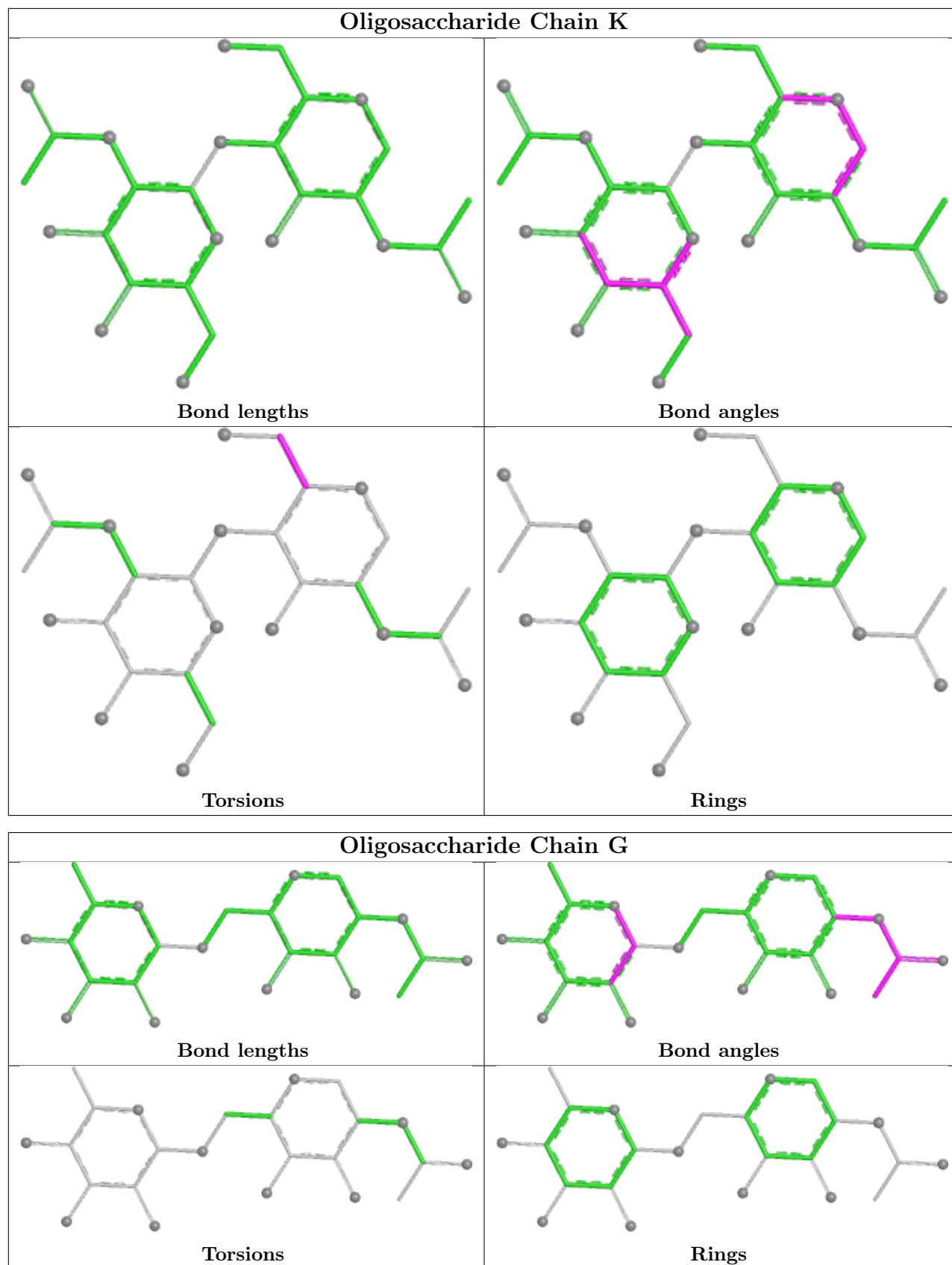
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
4	J	2	FUC	1	0
4	G	1	NAG	1	0

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

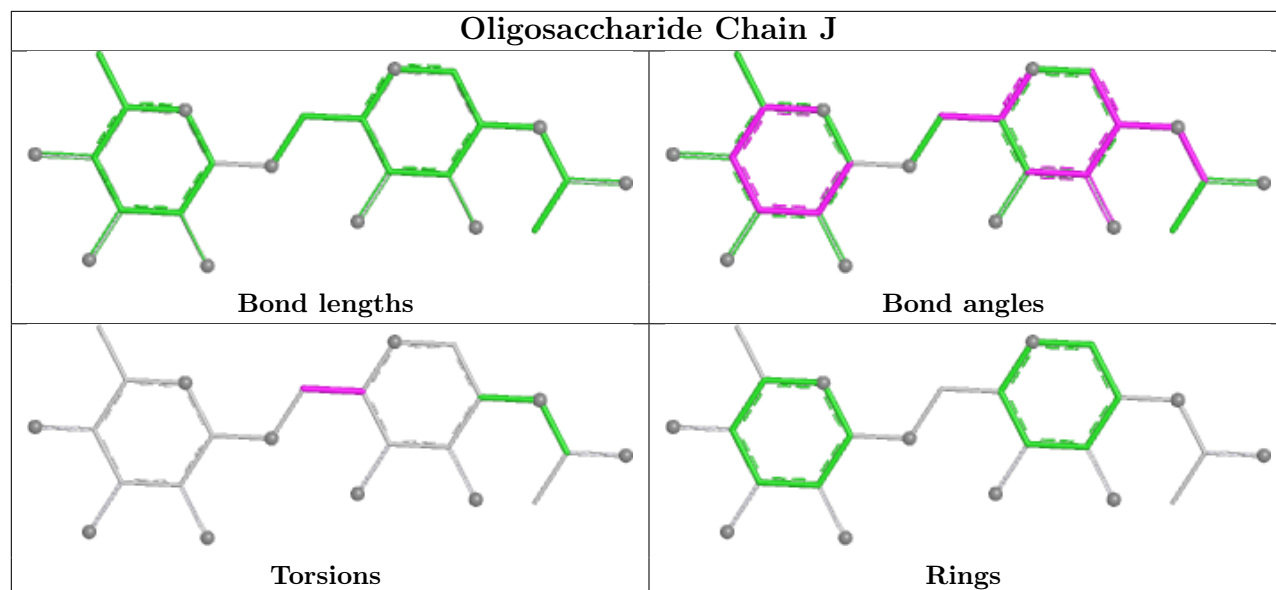




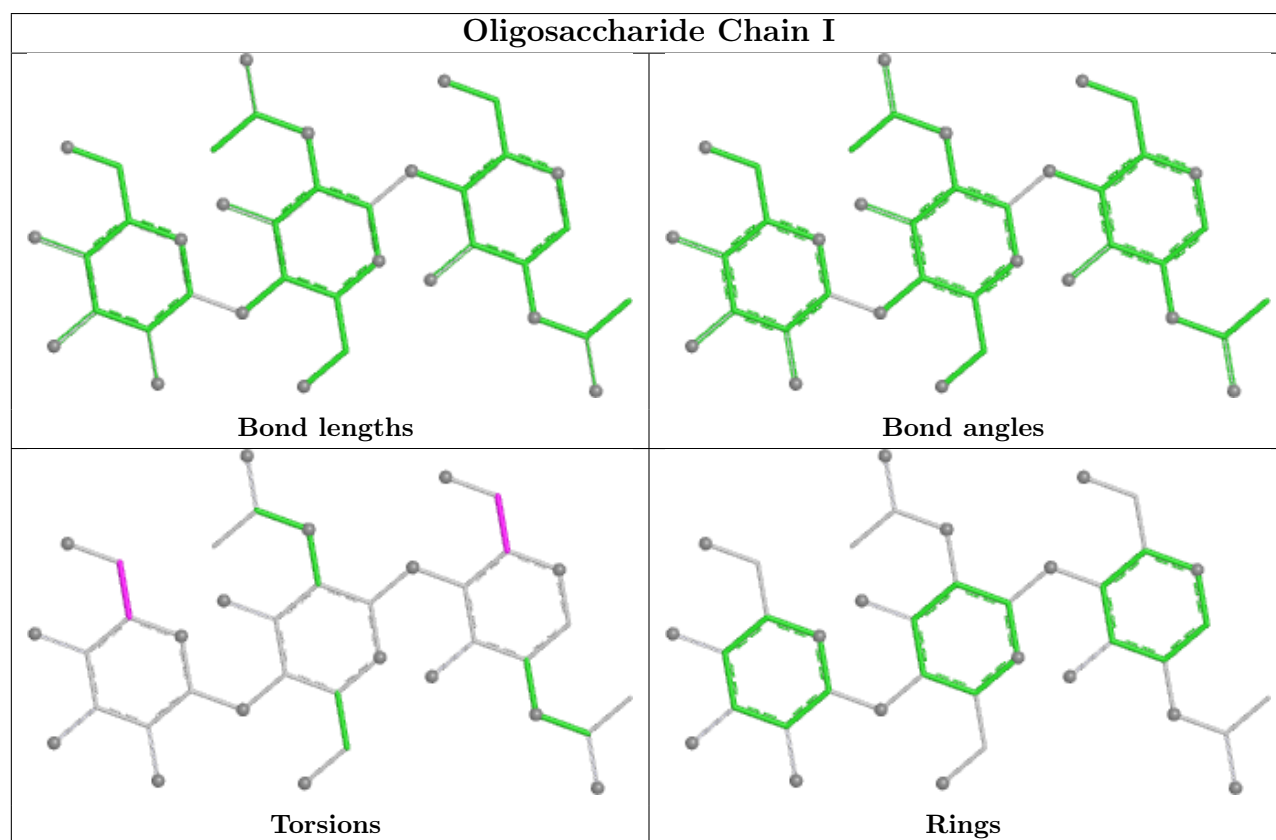


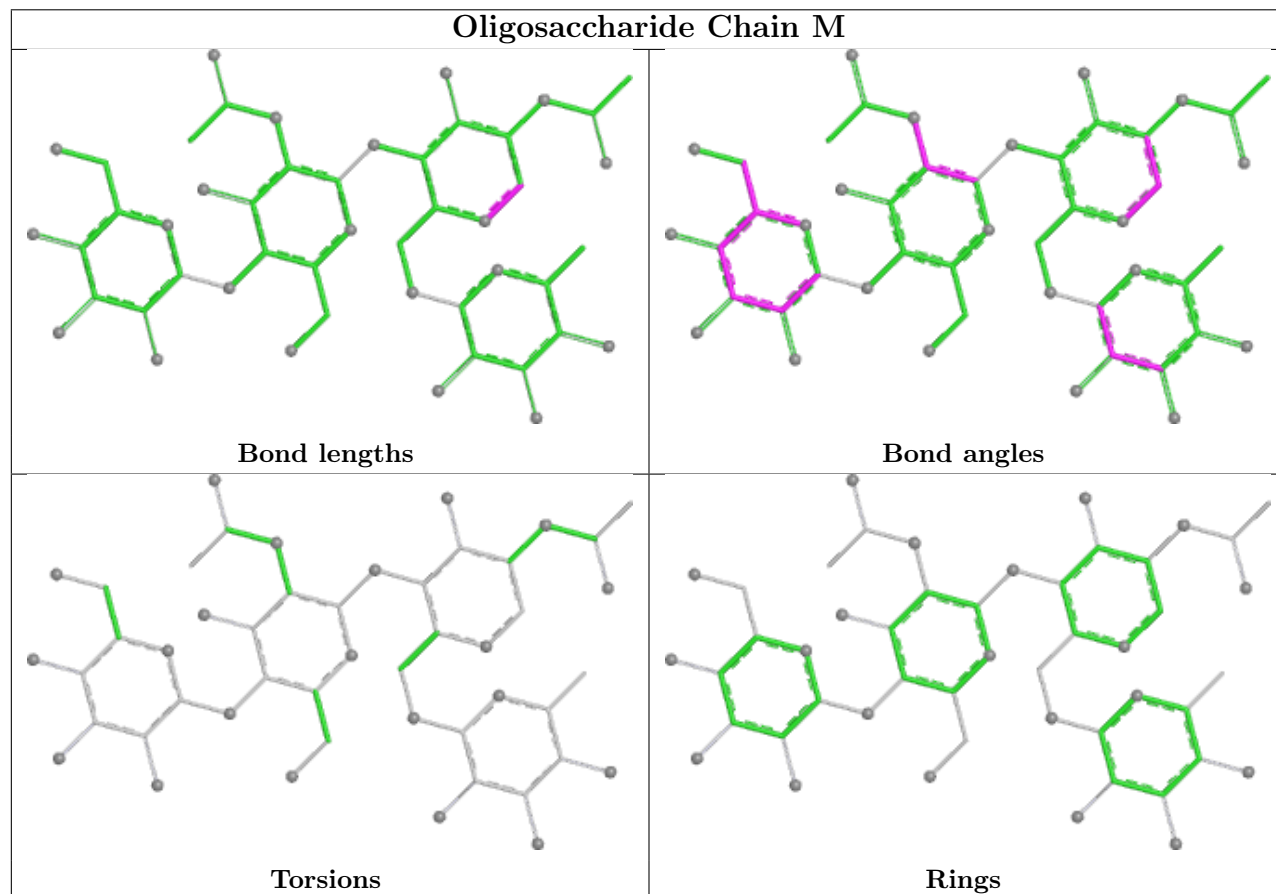
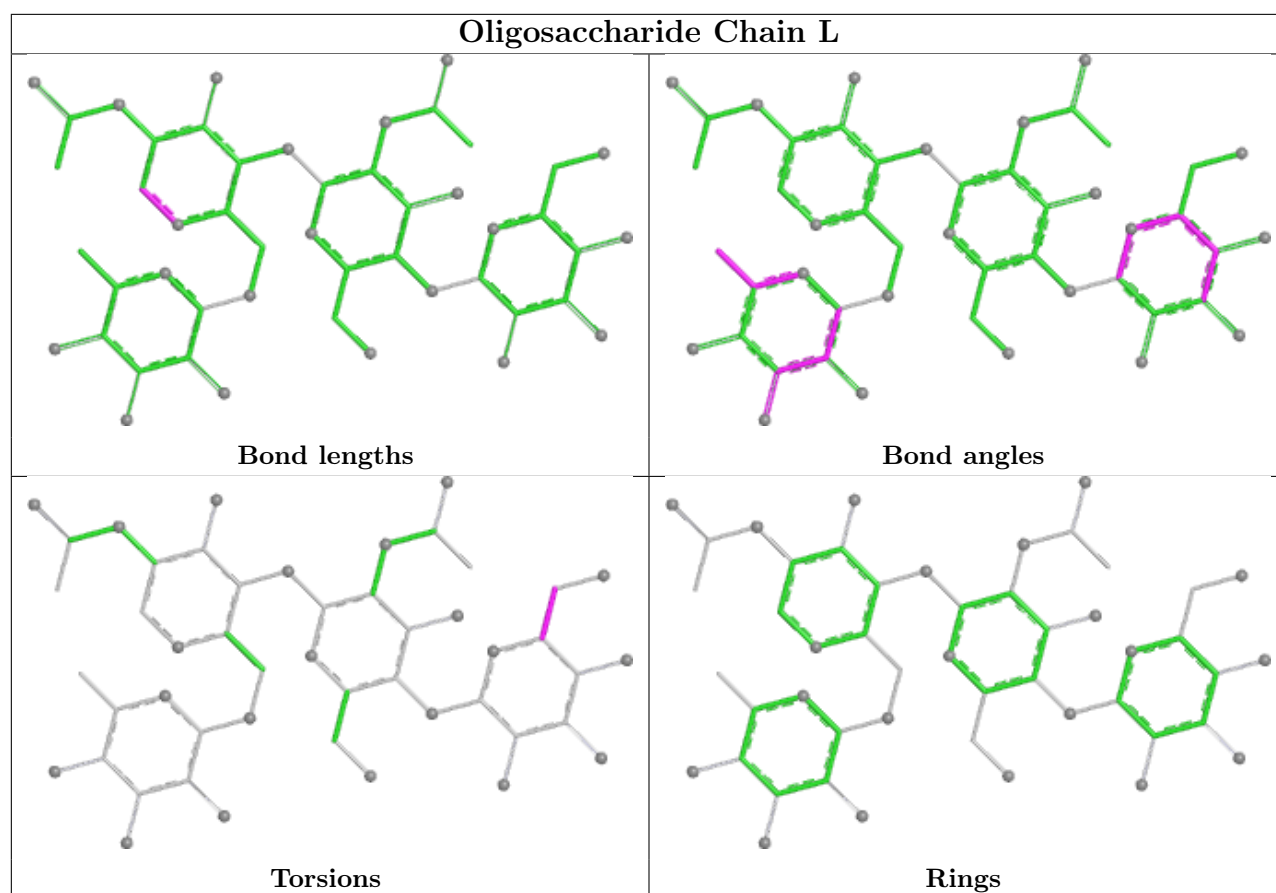


Oligosaccharide Chain J



Oligosaccharide Chain I





5.6 Ligand geometry

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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
12	PEG	D	1203	-	6,6,6	0.50	0	5,5,5	0.16	0
12	PEG	B	1200	-	6,6,6	0.50	0	5,5,5	0.29	0
12	PEG	C	1202	-	6,6,6	0.35	0	5,5,5	0.56	0
10	SO4	A	1003	-	4,4,4	0.48	0	6,6,6	0.23	0
12	PEG	A	1201	-	6,6,6	0.38	0	5,5,5	0.42	0
13	P6G	B	1203	-	18,18,18	0.62	0	17,17,17	0.77	0
11	NAG	D	1100	1	14,14,15	0.30	0	17,19,21	0.56	0
12	PEG	A	1200	-	6,6,6	0.43	0	5,5,5	0.38	0
12	PEG	B	1205	-	6,6,6	0.52	0	5,5,5	0.28	0
12	PEG	B	1204	-	6,6,6	0.62	0	5,5,5	0.24	0
12	PEG	D	1202	-	6,6,6	0.50	0	5,5,5	0.38	0
13	P6G	D	1201	-	18,18,18	0.58	0	17,17,17	0.64	0
10	SO4	B	1003	-	4,4,4	0.46	0	6,6,6	0.32	0
12	PEG	D	1205	-	6,6,6	0.62	0	5,5,5	0.48	0
12	PEG	D	1200	-	6,6,6	0.37	0	5,5,5	0.40	0
12	PEG	B	1201	-	6,6,6	0.60	0	5,5,5	0.50	0
10	SO4	D	1003	-	4,4,4	0.57	0	6,6,6	0.25	0
13	P6G	A	1202	-	18,18,18	0.48	0	17,17,17	0.57	0
12	PEG	C	1201	-	6,6,6	0.44	0	5,5,5	0.31	0
12	PEG	C	1203	-	6,6,6	0.36	0	5,5,5	0.44	0
11	NAG	A	1100	1	14,14,15	0.47	0	17,19,21	1.25	1 (5%)
12	PEG	C	1200	-	6,6,6	0.43	0	5,5,5	0.31	0
11	NAG	D	1101	1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
10	SO4	C	1003	-	4,4,4	0.60	0	6,6,6	0.47	0
12	PEG	A	1203	-	6,6,6	0.50	0	5,5,5	0.30	0
12	PEG	A	1204	-	6,6,6	0.35	0	5,5,5	0.39	0
12	PEG	D	1204	-	6,6,6	0.44	0	5,5,5	0.35	0
12	PEG	B	1202	-	6,6,6	0.47	0	5,5,5	0.41	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
12	PEG	D	1203	-	-	0/4/4/4	-
12	PEG	B	1200	-	-	4/4/4/4	-
12	PEG	C	1202	-	-	1/4/4/4	-
12	PEG	A	1201	-	-	2/4/4/4	-
13	P6G	B	1203	-	-	11/16/16/16	-
11	NAG	D	1100	1	-	2/6/23/26	0/1/1/1
12	PEG	A	1200	-	-	3/4/4/4	-
12	PEG	B	1205	-	-	3/4/4/4	-
12	PEG	B	1204	-	-	4/4/4/4	-
12	PEG	D	1202	-	-	2/4/4/4	-
13	P6G	D	1201	-	-	8/16/16/16	-
12	PEG	D	1205	-	-	2/4/4/4	-
12	PEG	D	1200	-	-	3/4/4/4	-
12	PEG	B	1201	-	-	3/4/4/4	-
13	P6G	A	1202	-	-	10/16/16/16	-
12	PEG	C	1201	-	-	1/4/4/4	-
12	PEG	C	1203	-	-	2/4/4/4	-
11	NAG	A	1100	1	-	0/6/23/26	0/1/1/1
12	PEG	C	1200	-	-	3/4/4/4	-
11	NAG	D	1101	1	-	0/6/23/26	0/1/1/1
12	PEG	A	1203	-	-	1/4/4/4	-
12	PEG	A	1204	-	-	2/4/4/4	-
12	PEG	D	1204	-	-	3/4/4/4	-
12	PEG	B	1202	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1100	NAG	C1-O5-C5	3.36	116.69	112.19
11	D	1101	NAG	C1-O5-C5	2.66	115.75	112.19

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	1100	NAG	O5-C5-C6-O6
13	B	1203	P6G	O7-C8-C9-O10
11	D	1100	NAG	C4-C5-C6-O6
12	C	1202	PEG	O1-C1-C2-O2
12	A	1201	PEG	O2-C3-C4-O4
12	A	1204	PEG	O1-C1-C2-O2
12	C	1200	PEG	O2-C3-C4-O4
12	B	1200	PEG	O1-C1-C2-O2
12	B	1204	PEG	O2-C3-C4-O4
13	A	1202	P6G	O1-C2-C3-O4
13	D	1201	P6G	O10-C11-C12-O13
13	D	1201	P6G	O7-C8-C9-O10
12	C	1200	PEG	O1-C1-C2-O2
13	A	1202	P6G	O16-C17-C18-O19
13	A	1202	P6G	O13-C14-C15-O16
13	A	1202	P6G	O7-C8-C9-O10
13	D	1201	P6G	C8-C9-O10-C11
13	B	1203	P6G	O10-C11-C12-O13
12	A	1200	PEG	O2-C3-C4-O4
12	B	1200	PEG	O2-C3-C4-O4
12	B	1201	PEG	O1-C1-C2-O2
12	D	1205	PEG	O1-C1-C2-O2
13	B	1203	P6G	O1-C2-C3-O4
13	B	1203	P6G	C8-C9-O10-C11
12	B	1201	PEG	O2-C3-C4-O4
12	B	1202	PEG	C1-C2-O2-C3
13	A	1202	P6G	C9-C8-O7-C6
12	B	1200	PEG	C1-C2-O2-C3
12	C	1201	PEG	C4-C3-O2-C2
13	B	1203	P6G	C6-C5-O4-C3
12	D	1202	PEG	C4-C3-O2-C2
12	D	1204	PEG	C1-C2-O2-C3
12	A	1204	PEG	O2-C3-C4-O4
12	B	1205	PEG	O2-C3-C4-O4
13	B	1203	P6G	C2-C3-O4-C5
12	C	1203	PEG	C4-C3-O2-C2
12	A	1201	PEG	C1-C2-O2-C3
12	C	1200	PEG	C1-C2-O2-C3
13	A	1202	P6G	C2-C3-O4-C5
12	D	1200	PEG	O2-C3-C4-O4
13	B	1203	P6G	O16-C17-C18-O19
12	B	1201	PEG	C4-C3-O2-C2
13	B	1203	P6G	C11-C12-O13-C14

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Mol	Chain	Res	Type	Atoms
13	D	1201	P6G	O13-C14-C15-O16
12	B	1204	PEG	O1-C1-C2-O2
12	D	1200	PEG	O1-C1-C2-O2
13	A	1202	P6G	O4-C5-C6-O7
13	A	1202	P6G	C5-C6-O7-C8
12	D	1205	PEG	C4-C3-O2-C2
12	A	1203	PEG	C1-C2-O2-C3
13	A	1202	P6G	C12-C11-O10-C9
13	B	1203	P6G	C5-C6-O7-C8
12	D	1200	PEG	C4-C3-O2-C2
12	A	1200	PEG	C1-C2-O2-C3
13	A	1202	P6G	O10-C11-C12-O13
12	B	1204	PEG	C1-C2-O2-C3
12	B	1204	PEG	C4-C3-O2-C2
12	D	1204	PEG	C4-C3-O2-C2
12	D	1204	PEG	O2-C3-C4-O4
13	D	1201	P6G	C11-C12-O13-C14
12	C	1203	PEG	O1-C1-C2-O2
13	D	1201	P6G	C12-C11-O10-C9
12	A	1200	PEG	O1-C1-C2-O2
12	D	1202	PEG	C1-C2-O2-C3
12	B	1205	PEG	C4-C3-O2-C2
13	B	1203	P6G	O4-C5-C6-O7
13	D	1201	P6G	C9-C8-O7-C6
12	B	1205	PEG	O1-C1-C2-O2
12	B	1200	PEG	C4-C3-O2-C2
13	B	1203	P6G	O13-C14-C15-O16
13	D	1201	P6G	O16-C17-C18-O19

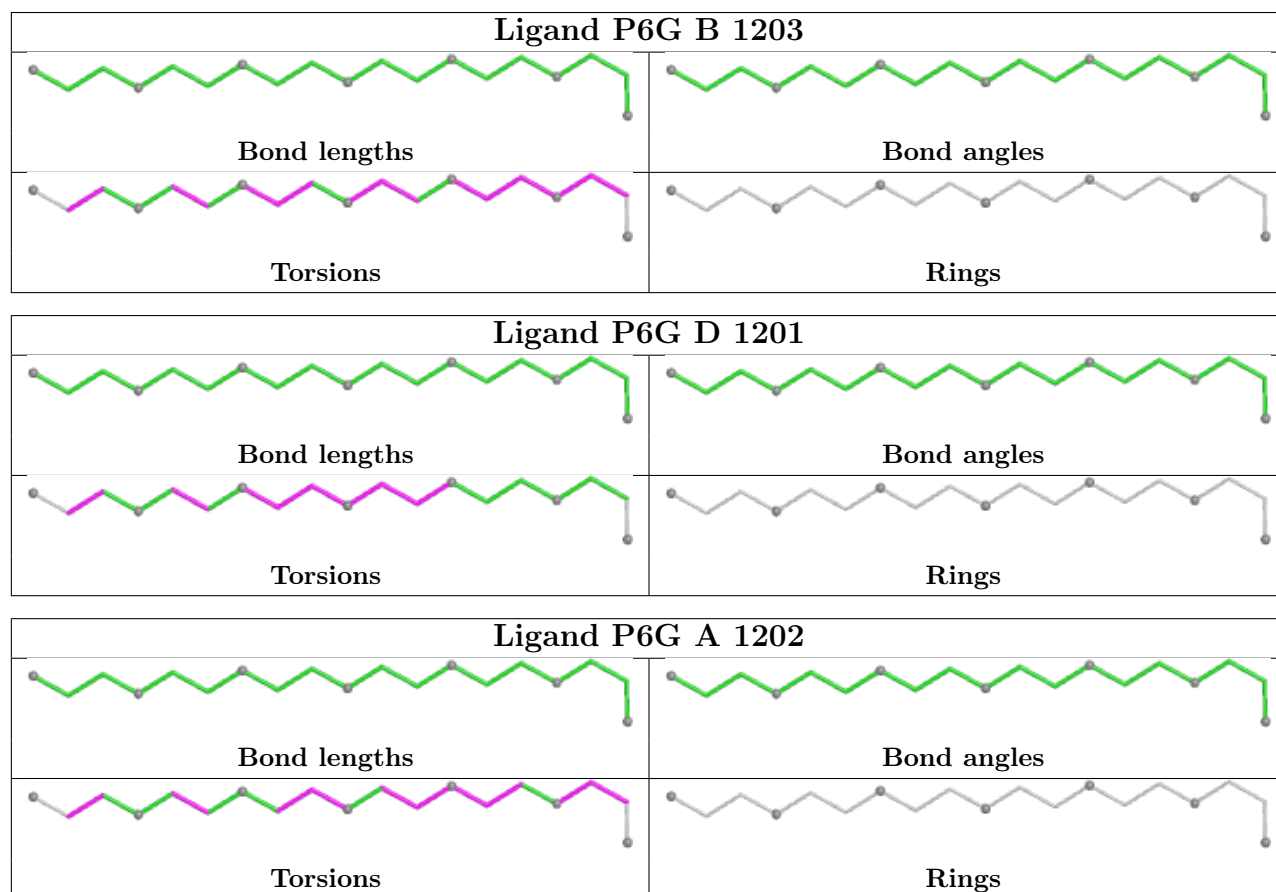
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1201	PEG	2	0
11	D	1100	NAG	1	0
13	D	1201	P6G	3	0
13	A	1202	P6G	1	0
12	A	1203	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	604/629 (96%)	0.09	15 (2%) 58 62	15, 25, 46, 73	1 (0%)
1	B	606/629 (96%)	-0.02	22 (3%) 46 49	13, 23, 43, 68	1 (0%)
1	C	606/629 (96%)	-0.17	13 (2%) 63 67	12, 20, 36, 69	1 (0%)
1	D	612/629 (97%)	-0.05	28 (4%) 37 40	11, 20, 42, 81	5 (0%)
2	P	3/7 (42%)	0.13	0 100 100	23, 23, 23, 29	0
2	Q	3/7 (42%)	0.35	0 100 100	19, 19, 19, 28	0
2	R	3/7 (42%)	-0.15	0 100 100	20, 20, 22, 29	0
2	S	3/7 (42%)	0.21	0 100 100	18, 18, 19, 27	0
All	All	2440/2544 (95%)	-0.04	78 (3%) 50 54	11, 22, 42, 81	8 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	613	LEU	6.6
1	C	611	ILE	5.6
1	D	79	ILE	5.5
1	A	415	THR	5.3
1	D	325	GLY	4.9
1	B	325	GLY	4.9
1	B	135	THR	4.7
1	B	134	ALA	4.7
1	A	78	PRO	4.3
1	C	135	THR	4.2
1	B	80	TRP	4.2
1	A	414	VAL	4.1
1	D	134	ALA	4.0
1	C	413	ARG	3.9
1	D	414	VAL	3.9
1	D	80	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	610	GLY	3.8
1	D	415	THR	3.7
1	A	135	THR	3.6
1	A	269	VAL	3.5
1	D	612	ASP	3.3
1	D	72	ALA	3.3
1	B	133	THR	3.2
1	D	88	LEU	3.2
1	B	79	ILE	3.1
1	A	270	PRO	3.1
1	A	129	LEU	3.1
1	D	95	VAL	3.0
1	D	78	PRO	3.0
1	C	606	ASN	3.0
1	D	131	ASN	3.0
1	B	206	THR	2.9
1	B	83	PHE	2.9
1	D	76	TYR	2.9
1	A	608	PRO	2.9
1	D	12	ALA	2.9
1	B	275	PRO	2.9
1	A	412	ASP	2.8
1	D	130	PRO	2.8
1	A	413	ARG	2.6
1	D	18	GLN	2.6
1	B	129	LEU	2.6
1	B	609	GLU	2.6
1	D	17	ALA	2.6
1	D	413	ARG	2.6
1	C	414	VAL	2.6
1	D	132	LYS	2.5
1	D	15	ALA	2.5
1	B	415	THR	2.5
1	D	83	PHE	2.5
1	D	24	TYR	2.5
1	B	607	TYR	2.4
1	D	20	PHE	2.4
1	C	129	LEU	2.4
1	C	415	THR	2.3
1	C	609	GLU	2.3
1	D	19	LEU	2.3
1	D	10	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	412	ASP	2.3
1	B	414	VAL	2.3
1	A	272	PRO	2.2
1	A	267	MET	2.2
1	D	84	THR	2.2
1	C	325	GLY	2.2
1	D	16	GLY	2.2
1	C	79	ILE	2.1
1	B	75	LEU	2.1
1	C	25	GLN	2.1
1	B	273	ASP	2.1
1	B	88	LEU	2.1
1	B	608	PRO	2.1
1	A	325	GLY	2.1
1	B	8	GLY	2.1
1	B	72	ALA	2.1
1	B	76	TYR	2.0
1	C	26	SER	2.0
1	A	79	ILE	2.0
1	A	606	ASN	2.0

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(Å ²)	Q<0.9
3	NAG	E	1	14/15	-	-	36,38,44,51	0
3	NAG	E	2	14/15	-	-	57,62,64,65	0
3	NAG	F	1	14/15	-	-	62,64,68,70	0
3	NAG	F	2	14/15	-	-	66,67,70,75	0
3	NAG	H	1	14/15	-	-	38,42,49,58	0
3	NAG	H	2	14/15	-	-	62,69,75,79	0
5	NAG	I	2	14/15	0.68	0.14	51,54,57,62	0
3	NAG	K	2	14/15	-	-	43,47,54,57	0

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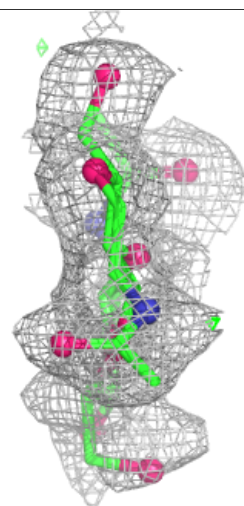
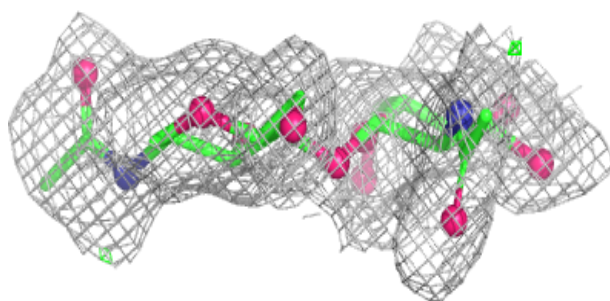
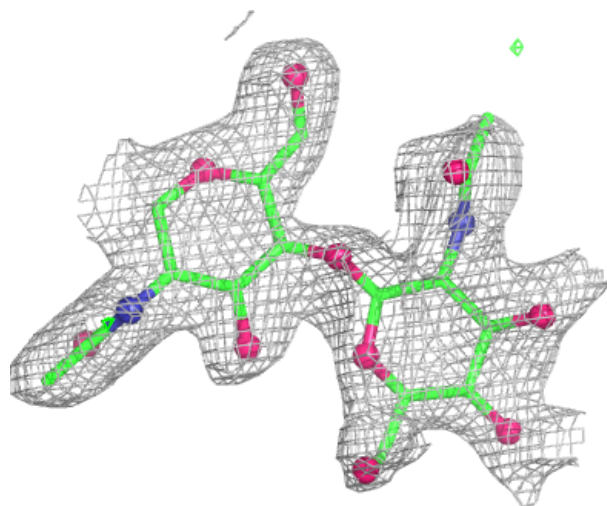
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	G	1	14/15	-	-	33,36,43,44	0
4	FUC	G	2	10/11	-	-	46,50,52,53	0
6	NAG	L	2	14/15	0.70	0.14	36,40,46,46	0
4	FUC	J	2	10/11	-	-	54,61,65,69	0
3	NAG	K	1	14/15	0.74	0.15	27,31,35,38	0
4	NAG	J	1	14/15	0.82	0.13	34,40,48,50	0
5	BMA	I	3	11/12	-	-	64,67,69,70	0
6	NAG	L	1	14/15	0.83	0.12	29,30,34,38	0
7	NAG	M	2	14/15	0.84	0.13	39,45,49,54	0
6	BMA	L	3	11/12	-	-	45,48,53,54	0
6	FUL	L	4	10/11	-	-	43,47,49,51	0
5	NAG	I	1	14/15	0.89	0.09	46,48,51,52	0
7	NAG	M	1	14/15	0.90	0.10	30,33,35,36	0
7	MAN	M	3	11/12	-	-	55,59,60,61	0
7	FUC	M	4	10/11	-	-	37,40,44,44	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.

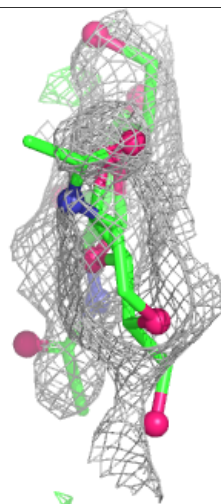
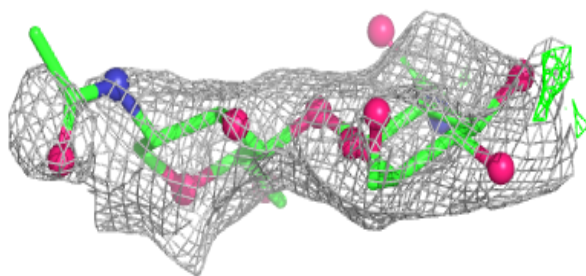
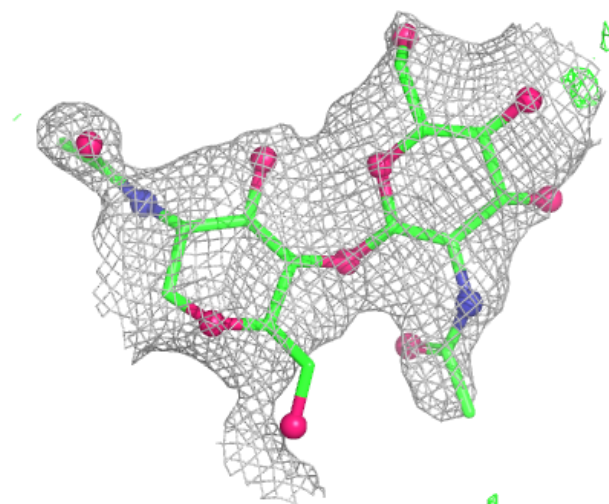
Electron density around Chain E:

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



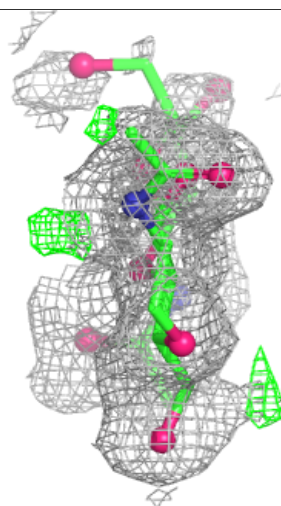
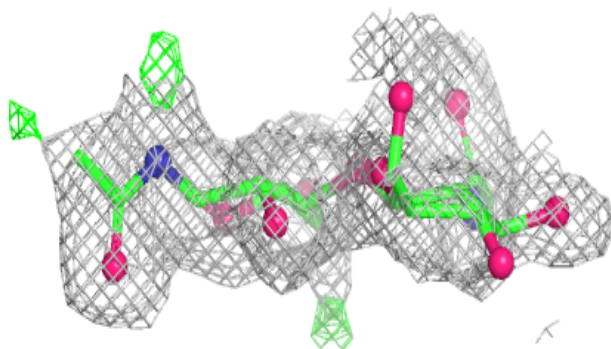
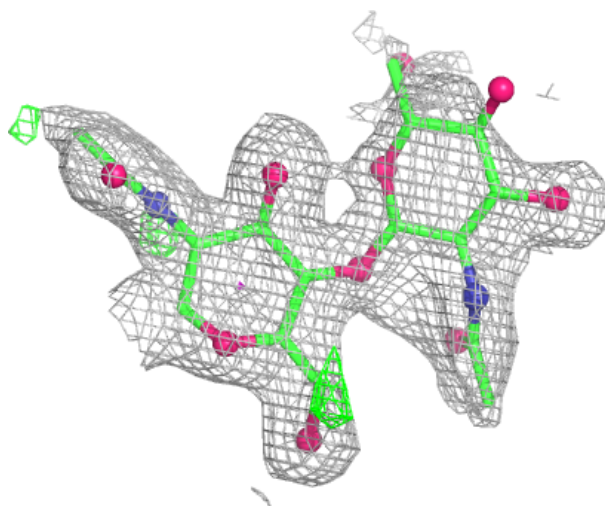
Electron density around Chain F:

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



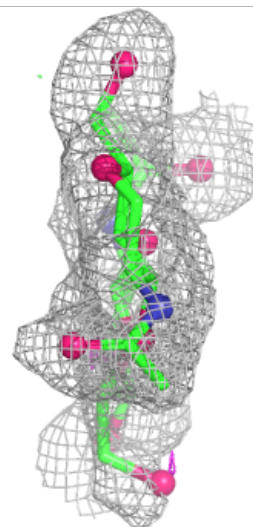
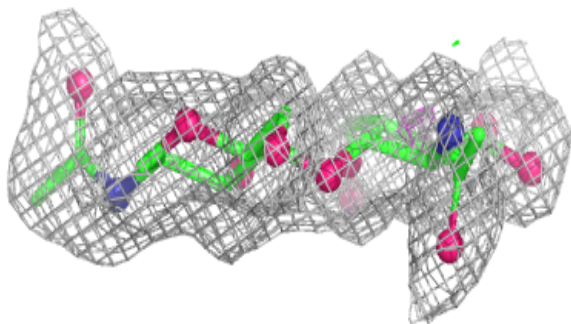
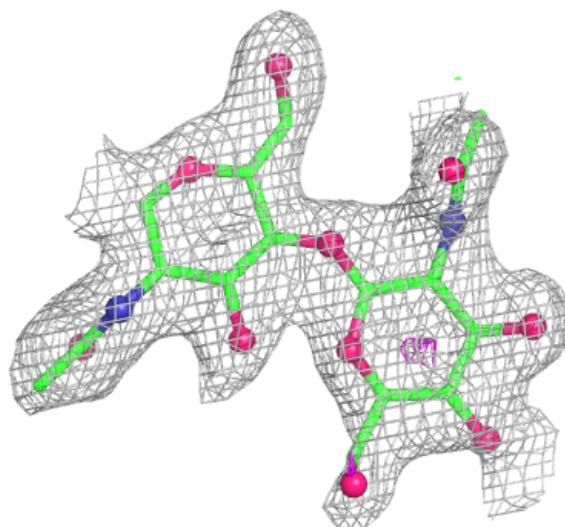
Electron density around Chain H:

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



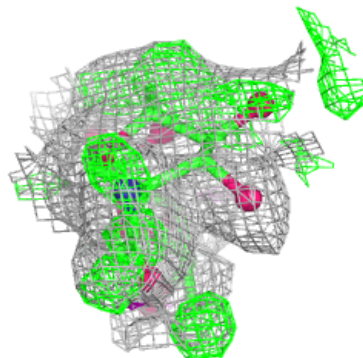
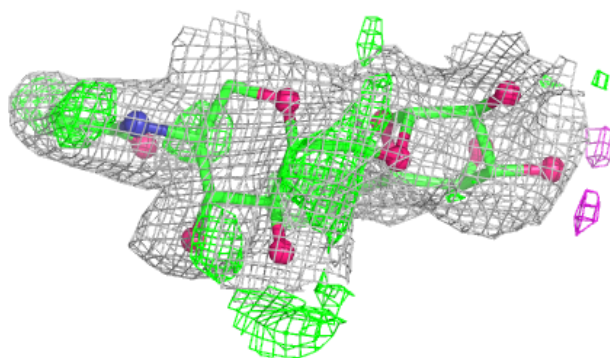
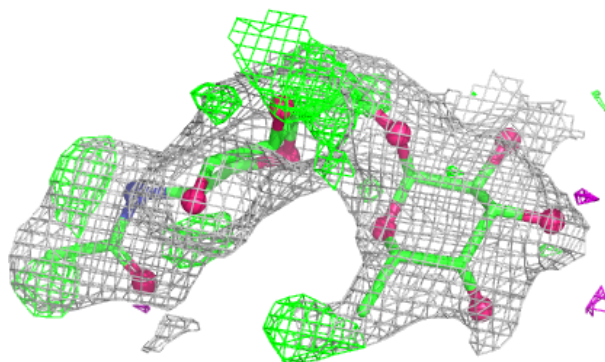
Electron density around Chain K:

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

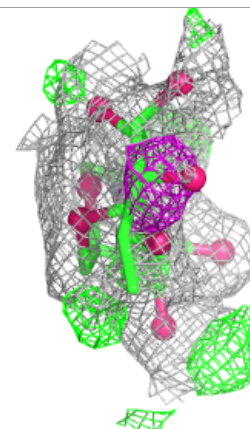
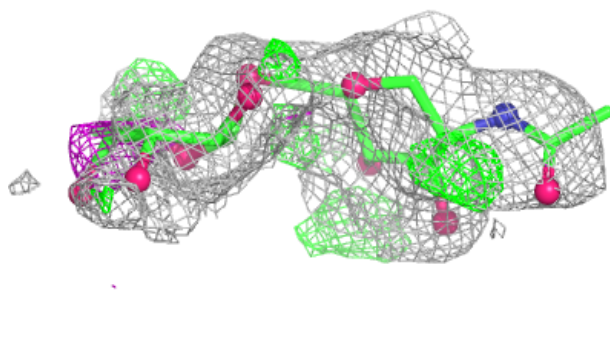
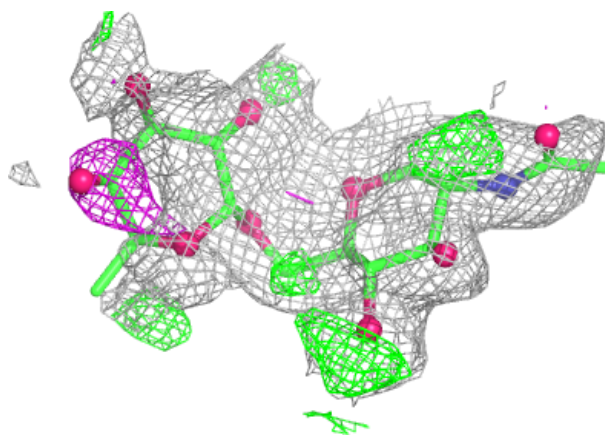


Electron density around Chain G:

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

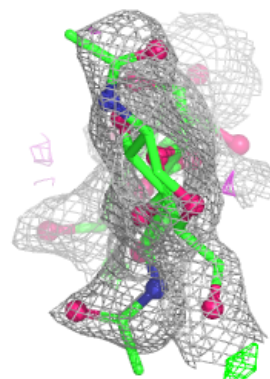
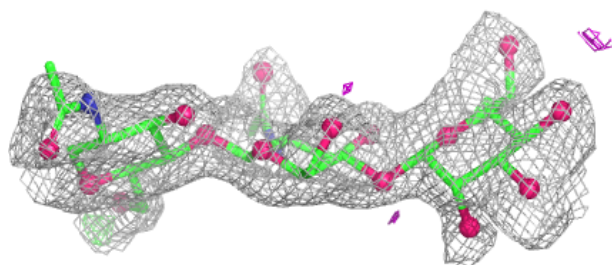
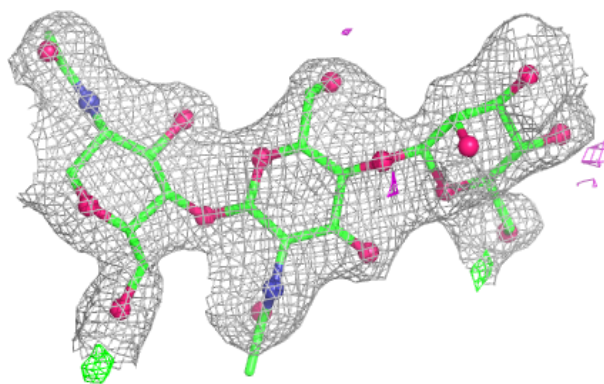
**Electron density around Chain J:**

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



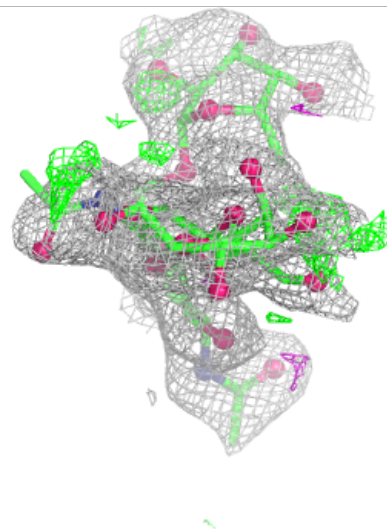
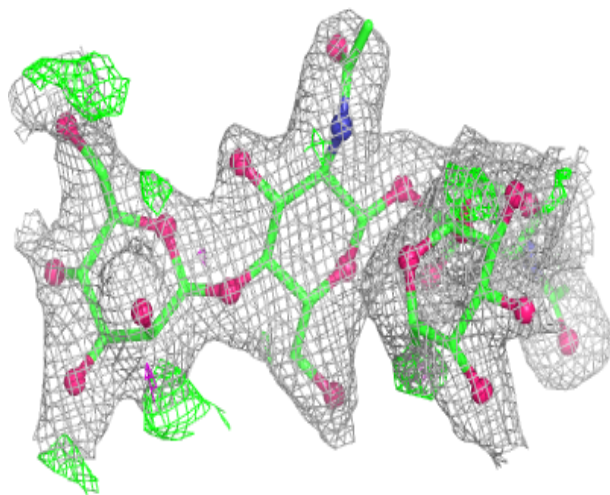
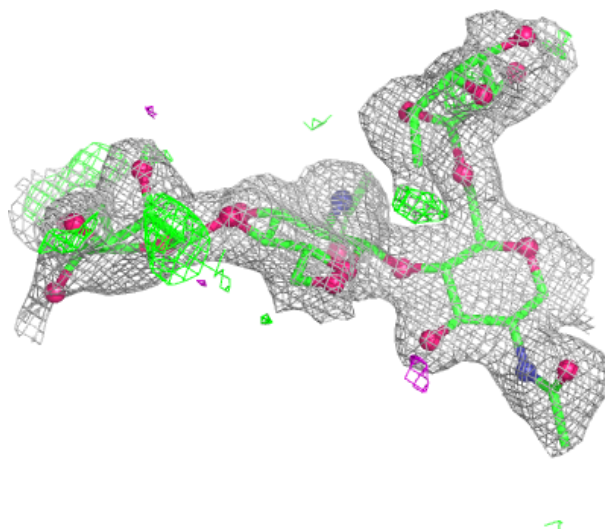
Electron density around Chain I:

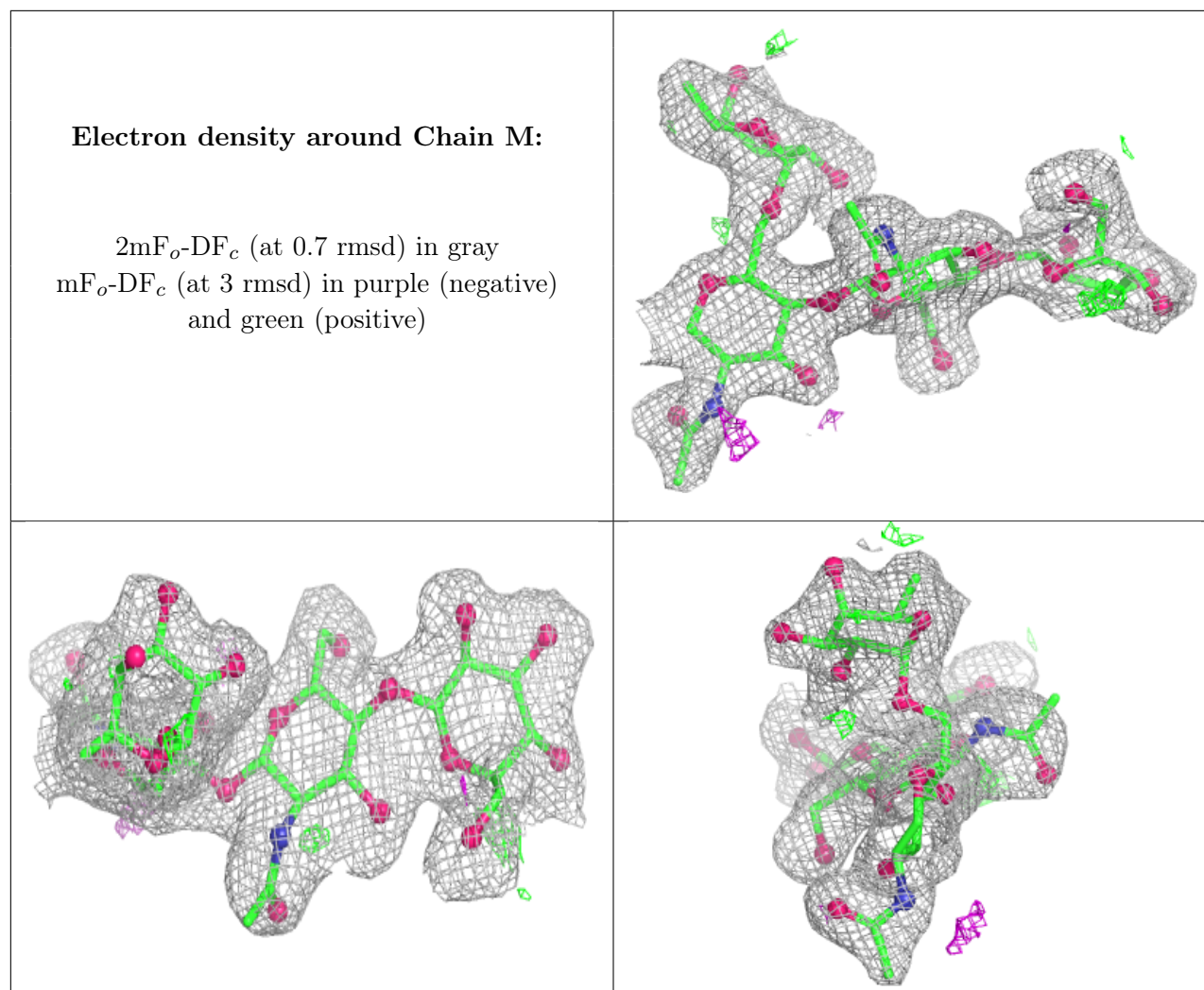
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands [i](#)

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
11	NAG	A	1100	14/15	0.65	0.19	42,47,52,60	0
10	SO4	D	1003	5/5	0.71	0.23	69,69,79,84	0
10	SO4	A	1003	5/5	0.71	0.17	74,80,84,88	0
10	SO4	B	1003	5/5	0.73	0.16	71,73,75,77	0
10	SO4	C	1003	5/5	0.76	0.20	60,62,65,74	0
12	PEG	B	1200	7/7	0.76	0.18	59,61,62,63	0
12	PEG	B	1201	7/7	0.79	0.20	41,43,46,47	0
11	NAG	D	1100	14/15	0.80	0.15	30,36,40,42	0
12	PEG	B	1204	7/7	0.80	0.21	49,51,53,53	0

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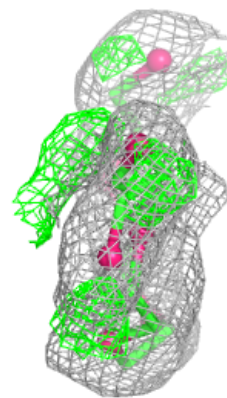
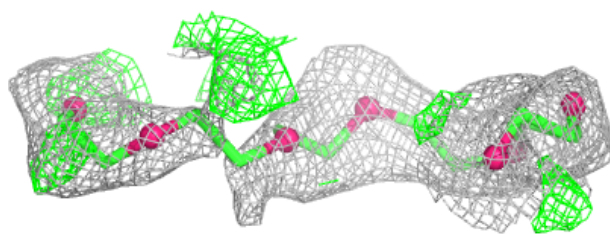
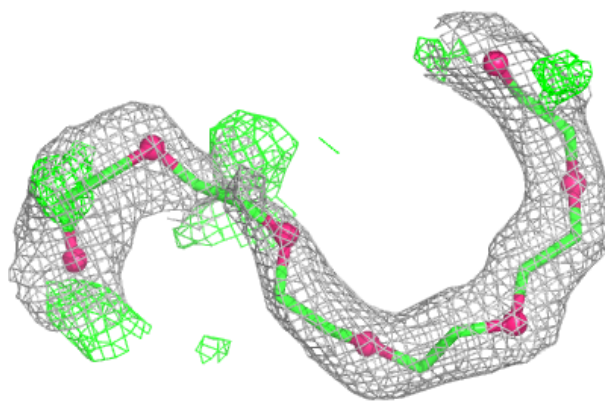
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	PEG	C	1202	7/7	0.81	0.18	46,47,50,52	0
11	NAG	D	1101	14/15	0.83	0.12	37,41,46,46	0
12	PEG	A	1204	7/7	0.83	0.20	50,52,54,55	0
13	P6G	B	1203	19/19	0.83	0.17	37,39,51,51	0
12	PEG	D	1205	7/7	0.84	0.14	37,40,42,43	0
12	PEG	B	1205	7/7	0.84	0.19	50,51,54,58	0
12	PEG	D	1200	7/7	0.85	0.15	52,53,55,60	0
12	PEG	D	1202	7/7	0.85	0.15	52,55,58,58	0
13	P6G	D	1201	19/19	0.87	0.15	31,36,50,51	0
12	PEG	A	1201	7/7	0.88	0.14	40,43,45,45	0
12	PEG	A	1203	7/7	0.88	0.15	49,50,52,52	0
12	PEG	D	1203	7/7	0.88	0.15	46,49,53,53	0
12	PEG	C	1200	7/7	0.89	0.12	43,44,45,47	0
12	PEG	A	1200	7/7	0.89	0.12	47,48,52,54	0
12	PEG	C	1203	7/7	0.90	0.13	41,43,44,46	0
13	P6G	A	1202	19/19	0.90	0.11	36,39,40,41	0
12	PEG	C	1201	7/7	0.91	0.12	36,38,43,47	0
12	PEG	D	1204	7/7	0.91	0.14	43,45,53,55	0
12	PEG	B	1202	7/7	0.92	0.11	33,33,34,34	0
9	CL	B	1002	1/1	0.99	0.02	16,16,16,16	0
9	CL	D	1002	1/1	0.99	0.02	14,14,14,14	0
9	CL	C	1002	1/1	1.00	0.01	15,15,15,15	0
8	ZN	B	1001	1/1	1.00	0.01	16,16,16,16	0
8	ZN	C	1001	1/1	1.00	0.01	15,15,15,15	0
8	ZN	D	1001	1/1	1.00	0.01	15,15,15,15	0
9	CL	A	1002	1/1	1.00	0.02	18,18,18,18	0
8	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.

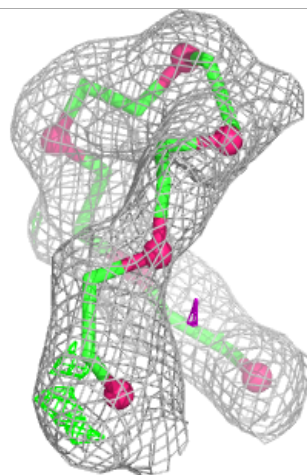
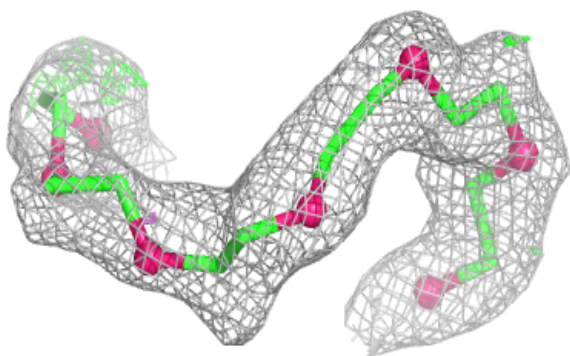
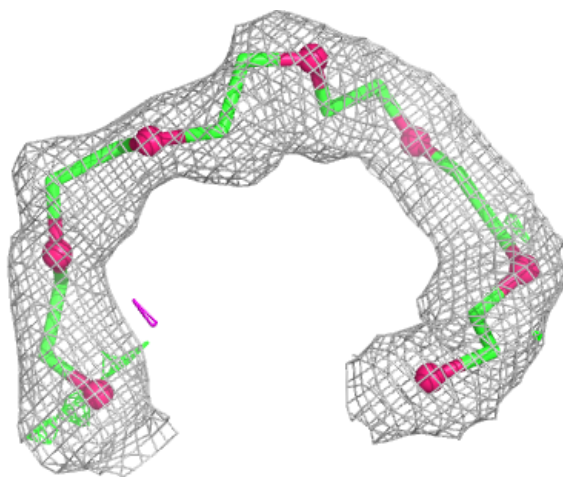
Electron density around P6G B 1203:

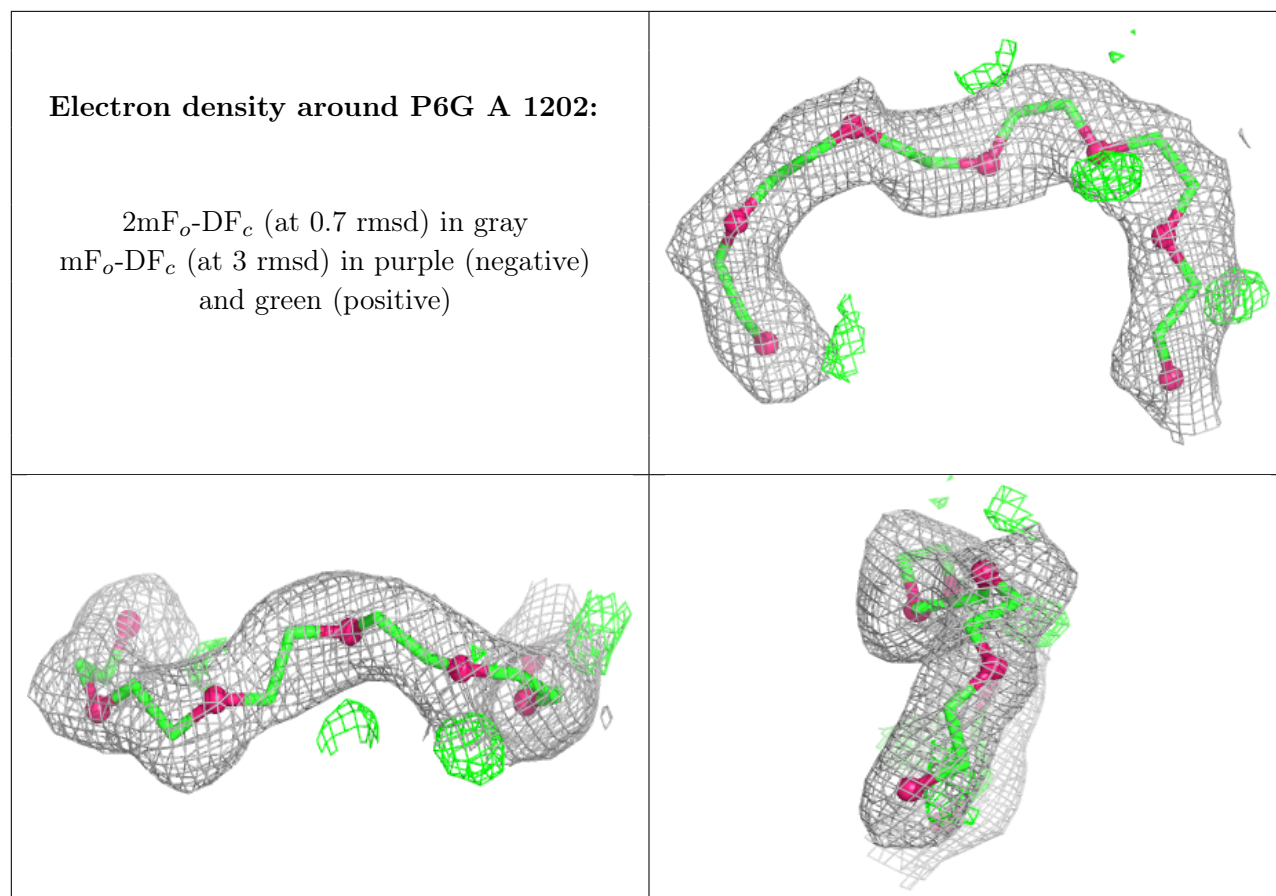
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G D 1201:

$2mF_o-DF_c$ (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.