



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:41 PM UTC

PDB ID : 7OGZ / pdb_00007ogz
Title : Plant peptide hormone receptor complex H1L3S1
Authors : Roman, A.O.; Jimenez-Sandoval, P.; Santiago, J.
Deposited on : 2021-05-07
Resolution : 2.70 Å(reported)

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

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<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
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

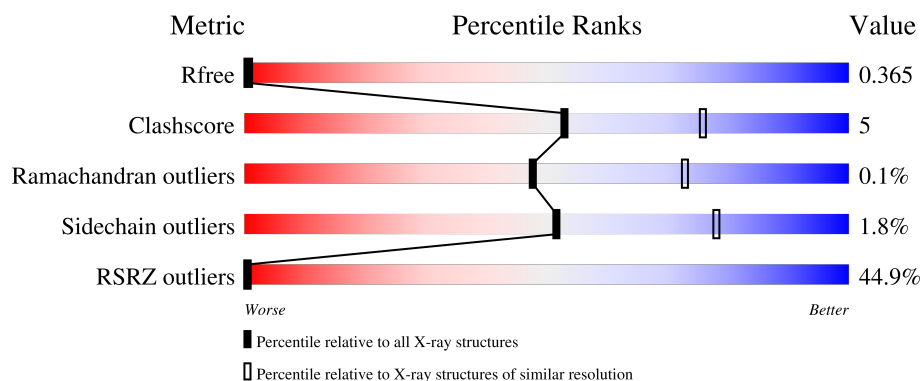
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	AAA	617	42% 81% 14% • •
1	DDD	617	47% 83% 12% • 5%
2	BBB	201	38% 84% 8% 8%
2	EEE	201	37% 82% 10% 8%
3	CCC	12	58% 83% 17%

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Mol	Chain	Length	Quality of chain
3	FFF	12	
4	AaA	2	
4	AgA	2	
4	AiA	2	
4	BaB	2	
4	DbD	2	
4	DcD	2	
4	DeD	2	
4	DhD	2	
4	DkD	2	
4	EaE	2	
5	AeA	3	
5	DaD	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	AaA	2	X	-	-	-
4	NAG	AgA	2	X	-	-	-
4	NAG	AiA	2	X	-	-	-
4	NAG	BaB	1	X	-	-	-
4	NAG	DbD	2	X	-	-	-
4	NAG	DcD	2	X	-	-	-
4	NAG	DeD	2	X	-	-	-
4	NAG	DkD	2	X	-	-	-
4	NAG	EaE	2	X	-	-	-
5	NAG	AeA	2	X	-	-	-
5	BMA	AeA	3	X	-	-	-
5	NAG	DaD	2	X	-	-	-
5	BMA	DaD	3	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12054 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 Receptor-like protein kinase HSL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	591	Total	C	N	O	S	0	1	0
			4348	2750	714	868	16			
1	DDD	589	Total	C	N	O	S	0	1	0
			4350	2756	713	864	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	12	GLY	-	expression tag	UNP Q9SGP2
AAA	13	SER	-	expression tag	UNP Q9SGP2
AAA	14	SER	-	expression tag	UNP Q9SGP2
AAA	15	MET	-	expression tag	UNP Q9SGP2
AAA	16	ASP	-	expression tag	UNP Q9SGP2
AAA	619	LEU	-	expression tag	UNP Q9SGP2
AAA	620	GLU	-	expression tag	UNP Q9SGP2
AAA	621	GLY	-	expression tag	UNP Q9SGP2
AAA	622	SER	-	expression tag	UNP Q9SGP2
AAA	623	GLU	-	expression tag	UNP Q9SGP2
AAA	624	ASN	-	expression tag	UNP Q9SGP2
AAA	625	LEU	-	expression tag	UNP Q9SGP2
AAA	626	TYR	-	expression tag	UNP Q9SGP2
AAA	627	PHE	-	expression tag	UNP Q9SGP2
AAA	628	GLN	-	expression tag	UNP Q9SGP2
DDD	12	GLY	-	expression tag	UNP Q9SGP2
DDD	13	SER	-	expression tag	UNP Q9SGP2
DDD	14	SER	-	expression tag	UNP Q9SGP2
DDD	15	MET	-	expression tag	UNP Q9SGP2
DDD	16	ASP	-	expression tag	UNP Q9SGP2
DDD	619	LEU	-	expression tag	UNP Q9SGP2
DDD	620	GLU	-	expression tag	UNP Q9SGP2
DDD	621	GLY	-	expression tag	UNP Q9SGP2
DDD	622	SER	-	expression tag	UNP Q9SGP2
DDD	623	GLU	-	expression tag	UNP Q9SGP2

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	624	ASN	-	expression tag	UNP Q9SGP2
DDD	625	LEU	-	expression tag	UNP Q9SGP2
DDD	626	TYR	-	expression tag	UNP Q9SGP2
DDD	627	PHE	-	expression tag	UNP Q9SGP2
DDD	628	GLN	-	expression tag	UNP Q9SGP2

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	185	Total	C	N	O	S	0	0	0
			1362	862	232	263	5			
2	EEE	185	Total	C	N	O	S	0	0	0
			1381	871	236	269	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	20	GLY	-	expression tag	UNP Q94AG2
BBB	21	SER	-	expression tag	UNP Q94AG2
BBB	22	SER	-	expression tag	UNP Q94AG2
BBB	23	MET	-	expression tag	UNP Q94AG2
BBB	214	LEU	-	expression tag	UNP Q94AG2
BBB	215	GLU	-	expression tag	UNP Q94AG2
BBB	216	ASN	-	expression tag	UNP Q94AG2
BBB	217	LEU	-	expression tag	UNP Q94AG2
BBB	218	TYR	-	expression tag	UNP Q94AG2
BBB	219	PHE	-	expression tag	UNP Q94AG2
BBB	220	GLN	-	expression tag	UNP Q94AG2
EEE	20	GLY	-	expression tag	UNP Q94AG2
EEE	21	SER	-	expression tag	UNP Q94AG2
EEE	22	SER	-	expression tag	UNP Q94AG2
EEE	23	MET	-	expression tag	UNP Q94AG2
EEE	214	LEU	-	expression tag	UNP Q94AG2
EEE	215	GLU	-	expression tag	UNP Q94AG2
EEE	216	ASN	-	expression tag	UNP Q94AG2
EEE	217	LEU	-	expression tag	UNP Q94AG2
EEE	218	TYR	-	expression tag	UNP Q94AG2
EEE	219	PHE	-	expression tag	UNP Q94AG2
EEE	220	GLN	-	expression tag	UNP Q94AG2

- Molecule 3 is a protein called Peptide hormone IDL3.

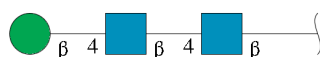
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	12	Total	C	N	O	0	0	0
			81	48	16	17			
3	FFF	12	Total	C	N	O	0	0	0
			81	48	16	17			

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



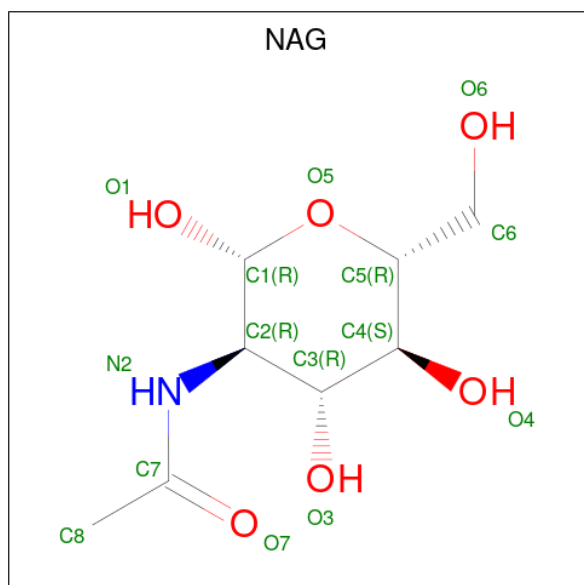
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AaA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AgA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AiA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BaB	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DbD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DcD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DeD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DhD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DkD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	EaE	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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
6	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
6	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
6	DDD	1	Total	C	N	O	0	0
			14	8	1	5		

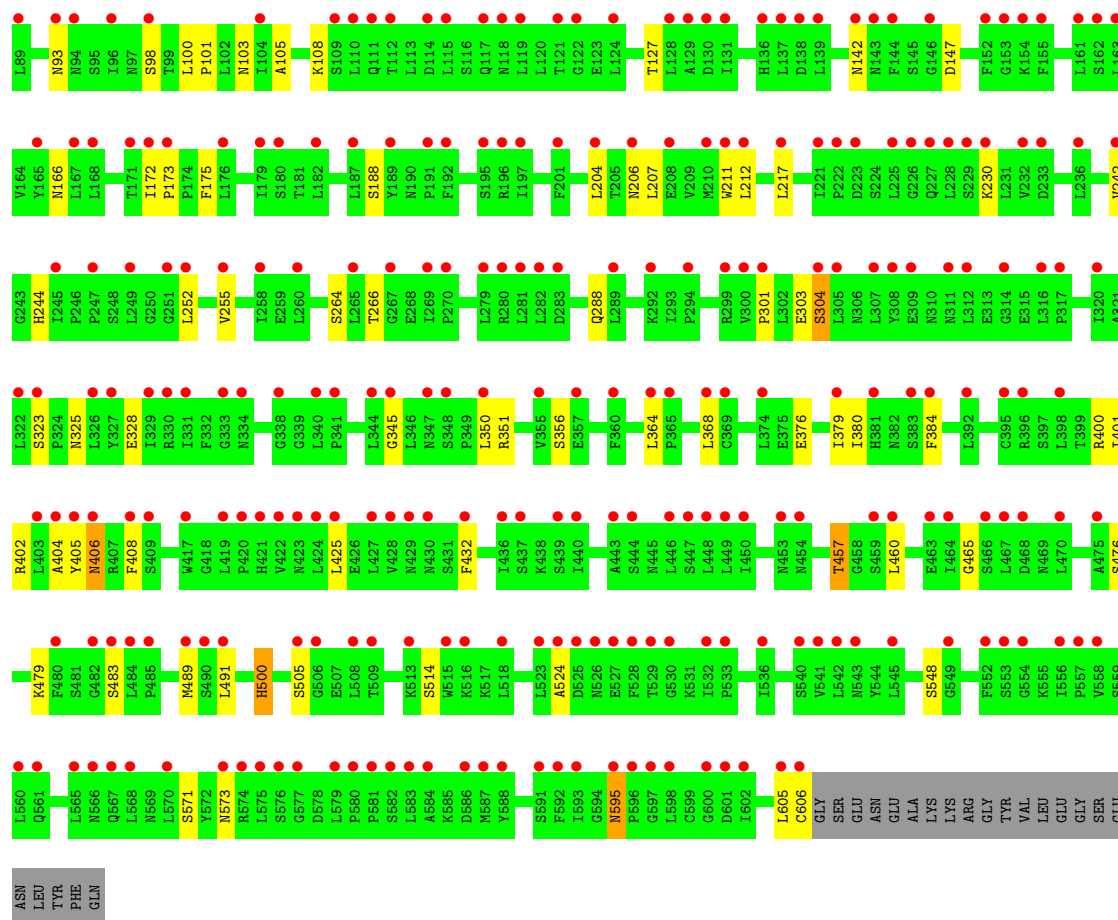
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	10	Total O 10 10	0	0
7	BBB	2	Total O 2 2	0	0

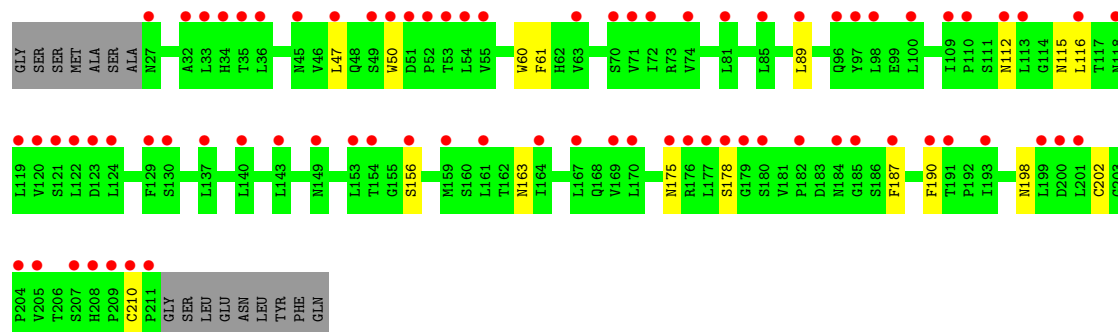
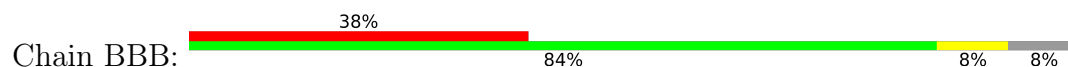
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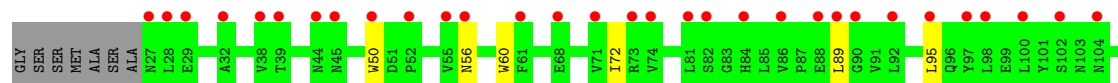
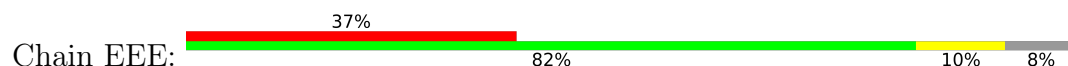
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total	O	0	0
			1	1		
7	DDD	7	Total	O	0	0
			7	7		
7	EEE	3	Total	O	0	0
			3	3		

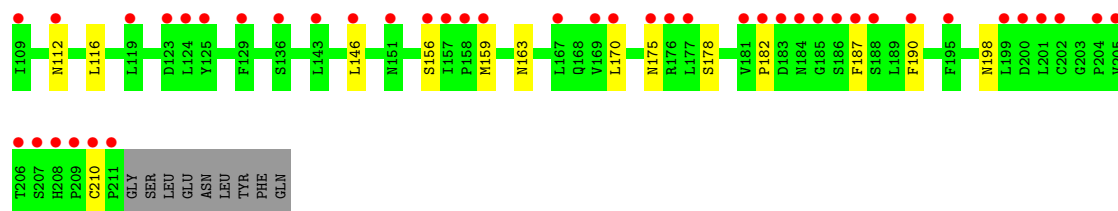


- Molecule 2: Somatic embryogenesis receptor kinase 1

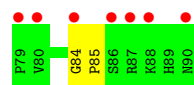
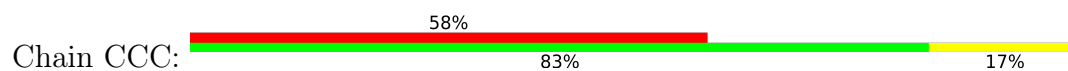


- Molecule 2: Somatic embryogenesis receptor kinase 1

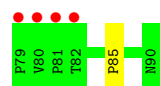




● Molecule 3: Peptide hormone IDL3



● Molecule 3: Peptide hormone IDL3



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



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



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



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



MAG1
MAG2

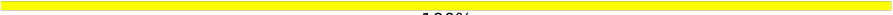
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DbD:  50% 50%MAG1
MAG2

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

Chain DcD:  100%MAG1
MAG2

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

Chain DeD:  100%MAG1
MAG2

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

Chain DhD:  50% 50%MAG1
MAG2

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

Chain DkD:  100%MAG1
MAG2

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

Chain EaE:  100%MAG1
MAG2

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

Chain AeA:  100%

MAG1
MAG2
BMA3

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

Chain DaD:  33%  67%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.84Å 144.50Å 168.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.70 47.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.66-2.70) 99.8 (47.66-2.70)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.353 , 0.371 0.347 , 0.365	Depositor DCC
R_{free} test set	3065 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12054	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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 49.19 % 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 7.7328e-05. 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: NAG, HYP, BMA

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	AAA	0.97	0/4432	1.25	4/6056 (0.1%)
1	DDD	0.96	0/4432	1.23	0/6050
2	BBB	0.97	0/1391	1.27	0/1917
2	EEE	0.95	0/1410	1.28	1/1939 (0.1%)
3	CCC	1.09	0/74	1.00	0/96
3	FFF	1.04	0/74	1.05	0/96
All	All	0.96	0/11813	1.25	5/16154 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	173	PRO	N-CA-C	5.56	117.48	110.70
1	AAA	173	PRO	CB-CA-C	-5.50	104.21	110.92
1	AAA	362	GLY	CA-C-O	-5.37	118.28	122.52
2	EEE	56	ASN	CB-CA-C	5.25	118.30	109.32
1	AAA	256	VAL	N-CA-C	-5.08	107.88	112.96

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	AAA	4348	0	4115	49	0
1	DDD	4350	0	4157	49	0
2	BBB	1362	0	1284	10	0
2	EEE	1381	0	1324	9	0
3	CCC	81	0	66	1	0
3	FFF	81	0	66	0	0
4	AaA	28	0	25	0	0
4	AgA	28	0	25	0	0
4	AiA	28	0	25	0	0
4	BaB	28	0	25	0	0
4	DbD	28	0	25	0	0
4	DcD	28	0	25	0	0
4	DeD	28	0	25	0	0
4	DhD	28	0	25	0	0
4	DkD	28	0	25	0	0
4	EaE	28	0	25	0	0
5	AeA	39	0	34	0	0
5	DaD	39	0	34	0	0
6	AAA	42	0	39	0	0
6	DDD	28	0	26	0	0
7	AAA	10	0	0	0	0
7	BBB	2	0	0	0	0
7	CCC	1	0	0	0	0
7	DDD	7	0	0	0	0
7	EEE	3	0	0	0	0
All	All	12054	0	11395	116	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 5.

The worst 5 of 116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EEE:89:LEU:O	2:EEE:116:LEU:HD21	2.00	0.61
2:EEE:187:PHE:HA	2:EEE:190:PHE:HD2	1.64	0.60
1:DDD:206:ASN:HA	1:DDD:230:LYS:HD2	1.82	0.60
1:AAA:188:SER:HG	1:AAA:211:TRP:CD1	2.20	0.60
1:DDD:188:SER:HG	1:DDD:211:TRP:CD1	2.19	0.60

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	AAA	588/617 (95%)	577 (98%)	10 (2%)	1 (0%)	43	68
1	DDD	586/617 (95%)	576 (98%)	9 (2%)	1 (0%)	43	68
2	BBB	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
2	EEE	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
3	CCC	9/12 (75%)	9 (100%)	0	0	100	100
3	FFF	9/12 (75%)	9 (100%)	0	0	100	100
All	All	1558/1660 (94%)	1531 (98%)	25 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	98	SER
1	DDD	98	SER

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	AAA	469/540 (87%)	457 (97%)	12 (3%)	40	70
1	DDD	473/540 (88%)	466 (98%)	7 (2%)	57	81
2	BBB	150/182 (82%)	149 (99%)	1 (1%)	76	90
2	EEE	157/182 (86%)	154 (98%)	3 (2%)	50	77
3	CCC	7/10 (70%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FFF	7/10 (70%)	7 (100%)	0	100	100
All	All	1263/1464 (86%)	1240 (98%)	23 (2%)	51	78

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	304	SER
1	DDD	457	THR
1	DDD	406	ASN
1	DDD	500	HIS
1	AAA	394	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	HYP	CCC	85	3	7,8,9	0.68	0	5,10,12	1.04	1 (20%)
3	HYP	FFF	85	3	7,8,9	0.64	0	5,10,12	1.12	1 (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	HYP	CCC	85	3	-	0/0/11/13	0/1/1/1
3	HYP	FFF	85	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FFF	85	HYP	O-C-CA	-2.17	119.18	124.77
3	CCC	85	HYP	O-C-CA	-2.11	119.34	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

26 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	$\# Z > 2$
4	NAG	AaA	1	1,4	14,14,15	0.35	0	17,19,21	1.30	3 (17%)
4	NAG	AaA	2	4	14,14,15	0.34	0	17,19,21	0.72	0
5	NAG	AeA	1	1,5	14,14,15	0.36	0	17,19,21	1.10	2 (11%)
5	NAG	AeA	2	5	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
5	BMA	AeA	3	5	11,11,12	0.33	0	15,15,17	0.72	1 (6%)
4	NAG	AgA	1	1,4	14,14,15	0.29	0	17,19,21	1.00	1 (5%)
4	NAG	AgA	2	4	14,14,15	0.40	0	17,19,21	0.65	0
4	NAG	AiA	1	1,4	14,14,15	0.47	0	17,19,21	1.41	2 (11%)
4	NAG	AiA	2	4	14,14,15	0.37	0	17,19,21	0.79	0
4	NAG	BaB	1	2,4	14,14,15	0.39	0	17,19,21	0.56	0
4	NAG	BaB	2	4	14,14,15	0.49	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	DaD	1	1,5	14,14,15	0.33	0	17,19,21	0.96	1 (5%)
5	NAG	DaD	2	5	14,14,15	0.53	0	17,19,21	1.08	0
5	BMA	DaD	3	5	11,11,12	0.36	0	15,15,17	0.76	1 (6%)
4	NAG	DbD	1	1,4	14,14,15	0.35	0	17,19,21	1.08	3 (17%)
4	NAG	DbD	2	4	14,14,15	0.38	0	17,19,21	0.62	0
4	NAG	DcD	1	1,4	14,14,15	0.49	0	17,19,21	1.20	1 (5%)
4	NAG	DcD	2	4	14,14,15	0.30	0	17,19,21	0.75	1 (5%)
4	NAG	DeD	1	1,4	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
4	NAG	DeD	2	4	14,14,15	0.33	0	17,19,21	10.45	5 (29%)
4	NAG	DhD	1	1,4	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
4	NAG	DhD	2	4	14,14,15	0.36	0	17,19,21	0.69	0
4	NAG	DkD	1	1,4	14,14,15	0.35	0	17,19,21	0.83	0
4	NAG	DkD	2	4	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	EaE	1	2,4	14,14,15	0.42	0	17,19,21	1.03	1 (5%)
4	NAG	EaE	2	4	14,14,15	0.41	0	17,19,21	0.80	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	AaA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AaA	2	4	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	AeA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	AeA	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	BMA	AeA	3	5	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	AgA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AgA	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	AiA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	AiA	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	BaB	1	2,4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	BaB	2	4	-	0/6/23/26	0/1/1/1
5	NAG	DaD	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	DaD	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	BMA	DaD	3	5	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	DbD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	DbD	2	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	DcD	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	DcD	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	DeD	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	DeD	2	4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	DhD	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	DhD	2	4	-	0/6/23/26	0/1/1/1
4	NAG	DkD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	DkD	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	EaE	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	EaE	2	4	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DeD	2	NAG	C8-C7-N2	27.83	162.27	116.12
4	DeD	2	NAG	O7-C7-C8	-23.31	80.54	122.05
4	DeD	2	NAG	O7-C7-N2	-22.77	81.74	121.98
4	AiA	1	NAG	C1-O5-C5	3.88	117.39	112.19
4	AaA	1	NAG	C1-O5-C5	3.24	116.53	112.19

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AaA	2	NAG	C1
4	AgA	2	NAG	C1
4	AiA	2	NAG	C1
4	BaB	1	NAG	C1
4	DbD	2	NAG	C1

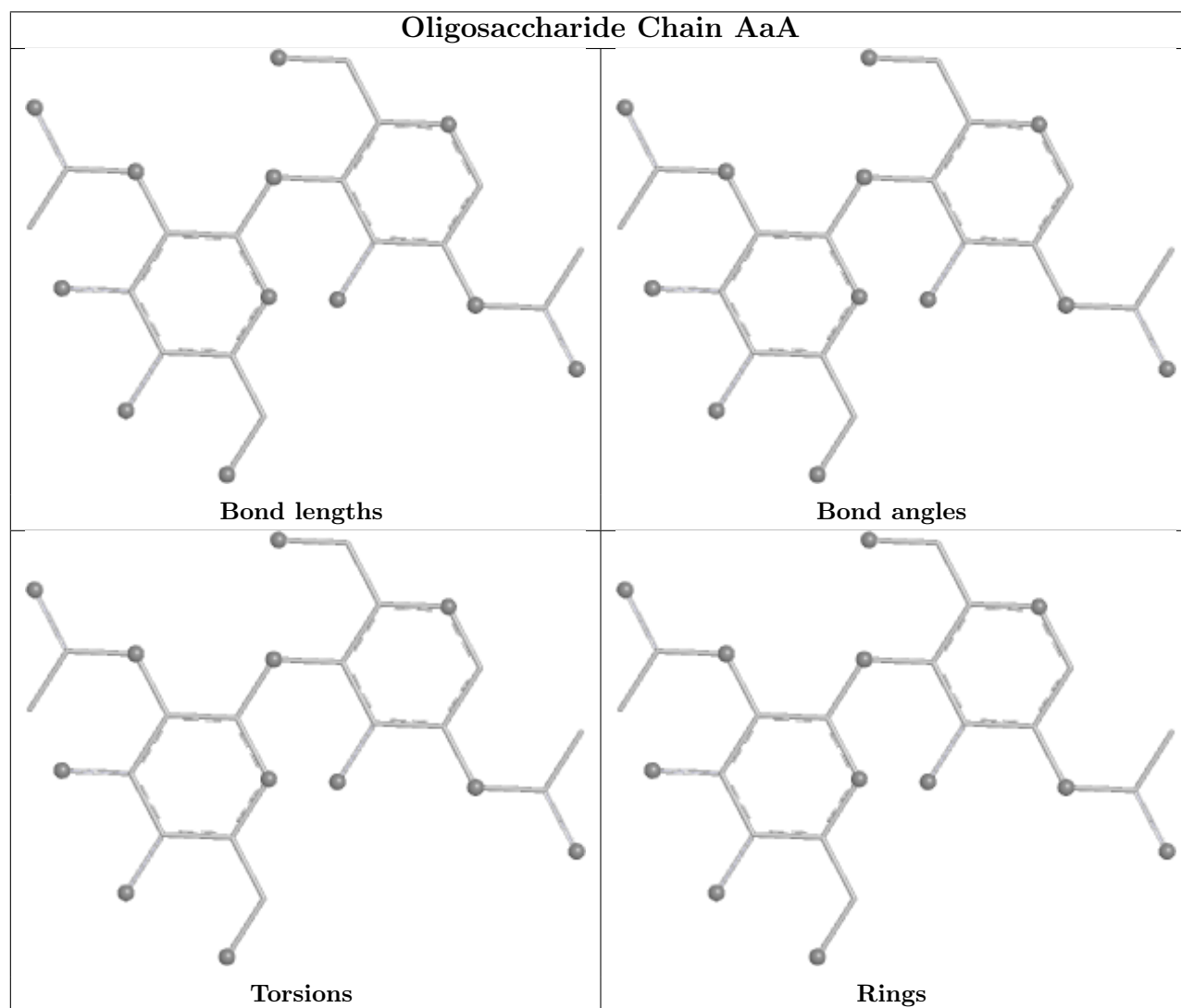
5 of 22 torsion outliers are listed below:

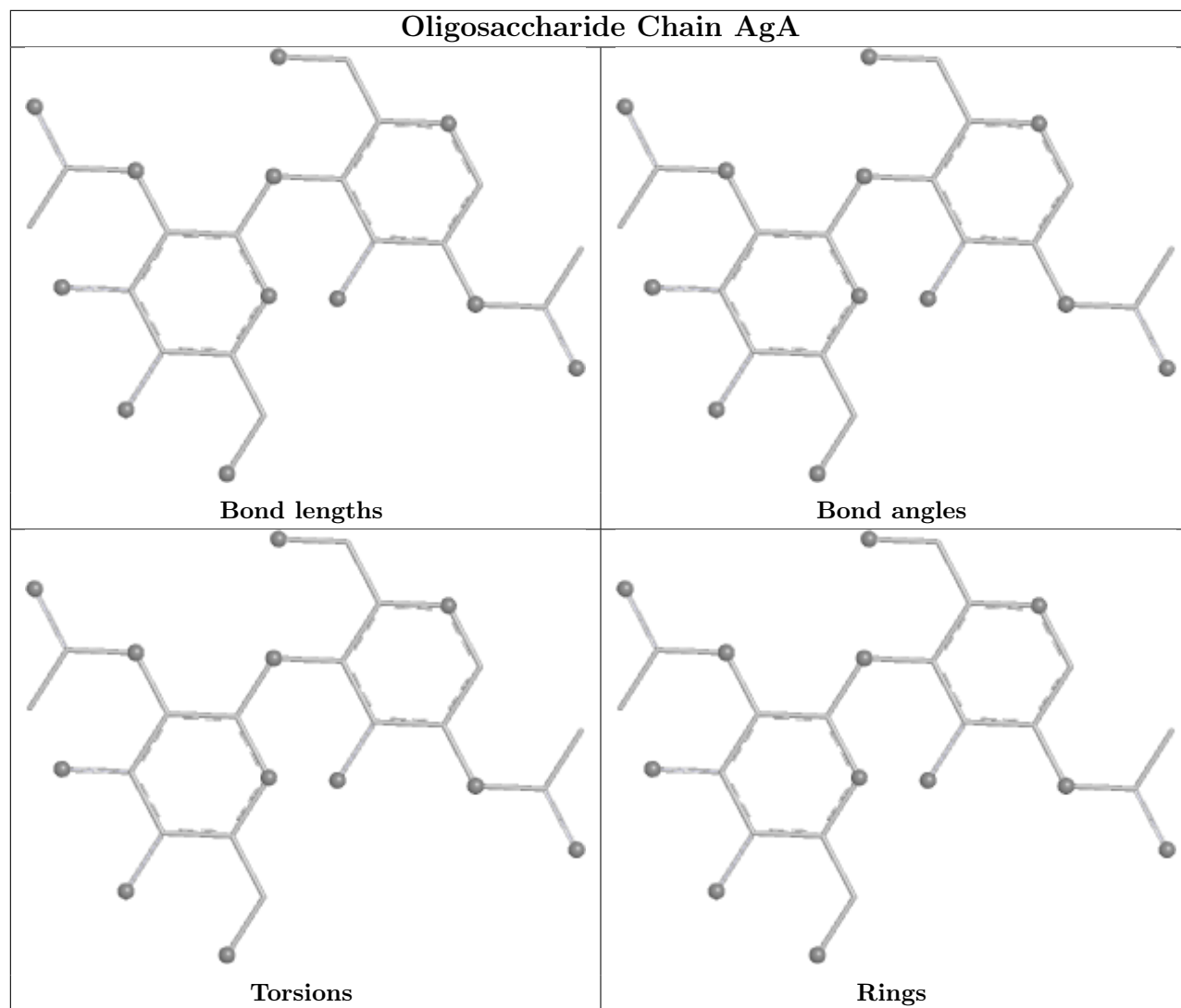
Mol	Chain	Res	Type	Atoms
4	DcD	1	NAG	O5-C5-C6-O6
4	AgA	2	NAG	O5-C5-C6-O6
4	AiA	1	NAG	O5-C5-C6-O6
4	DcD	1	NAG	C4-C5-C6-O6
4	DkD	2	NAG	O5-C5-C6-O6

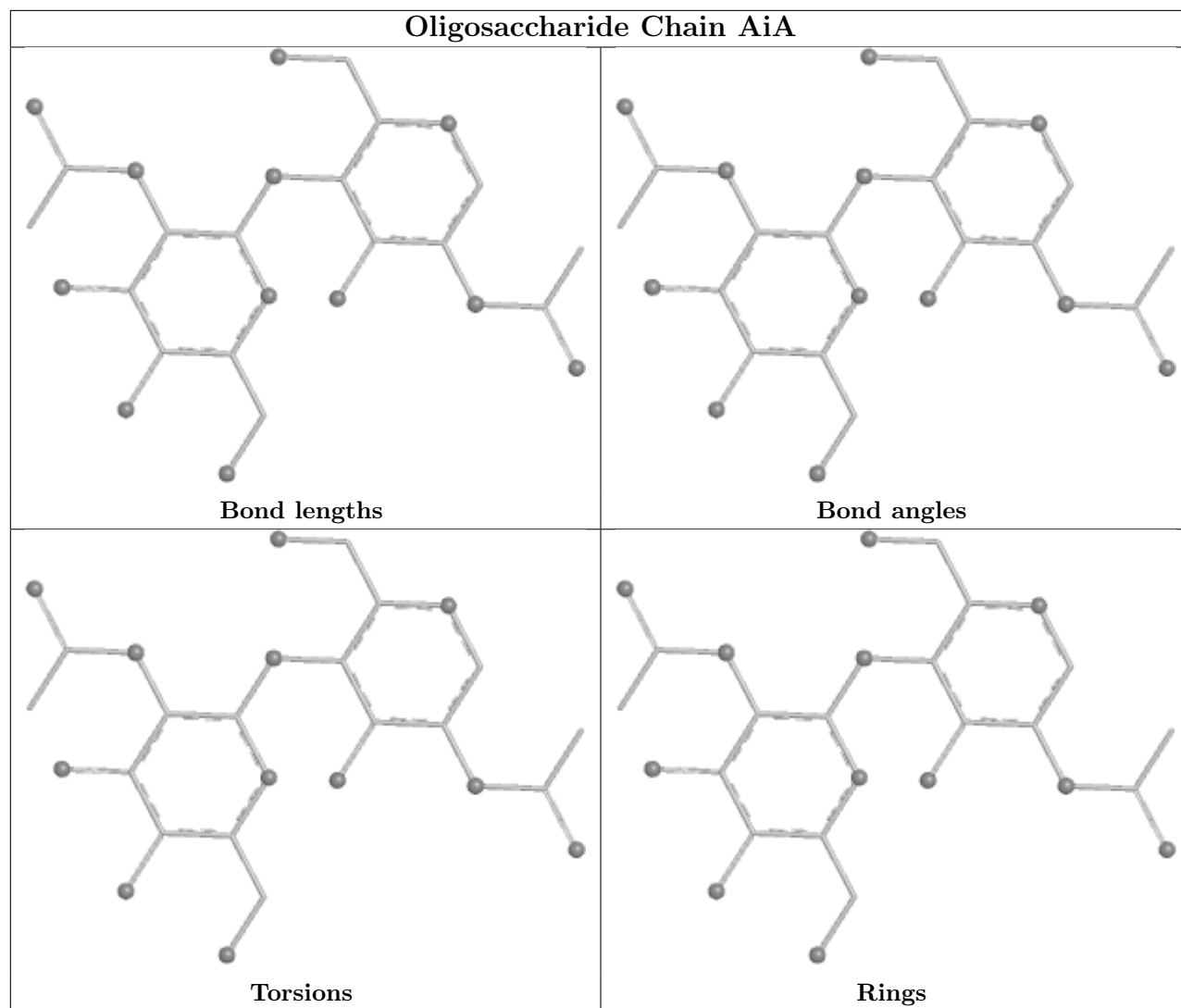
There are no ring outliers.

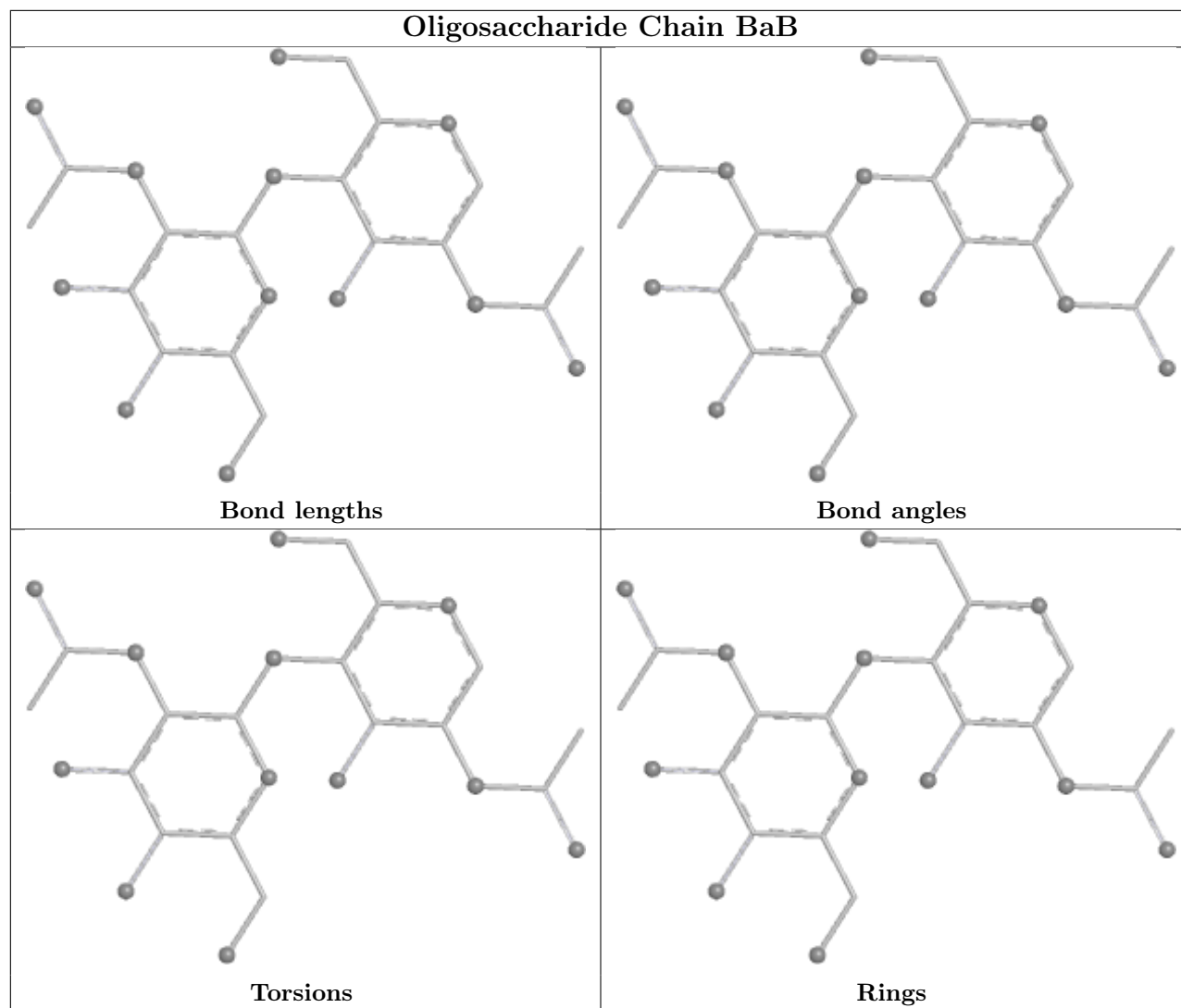
No monomer is involved in short contacts.

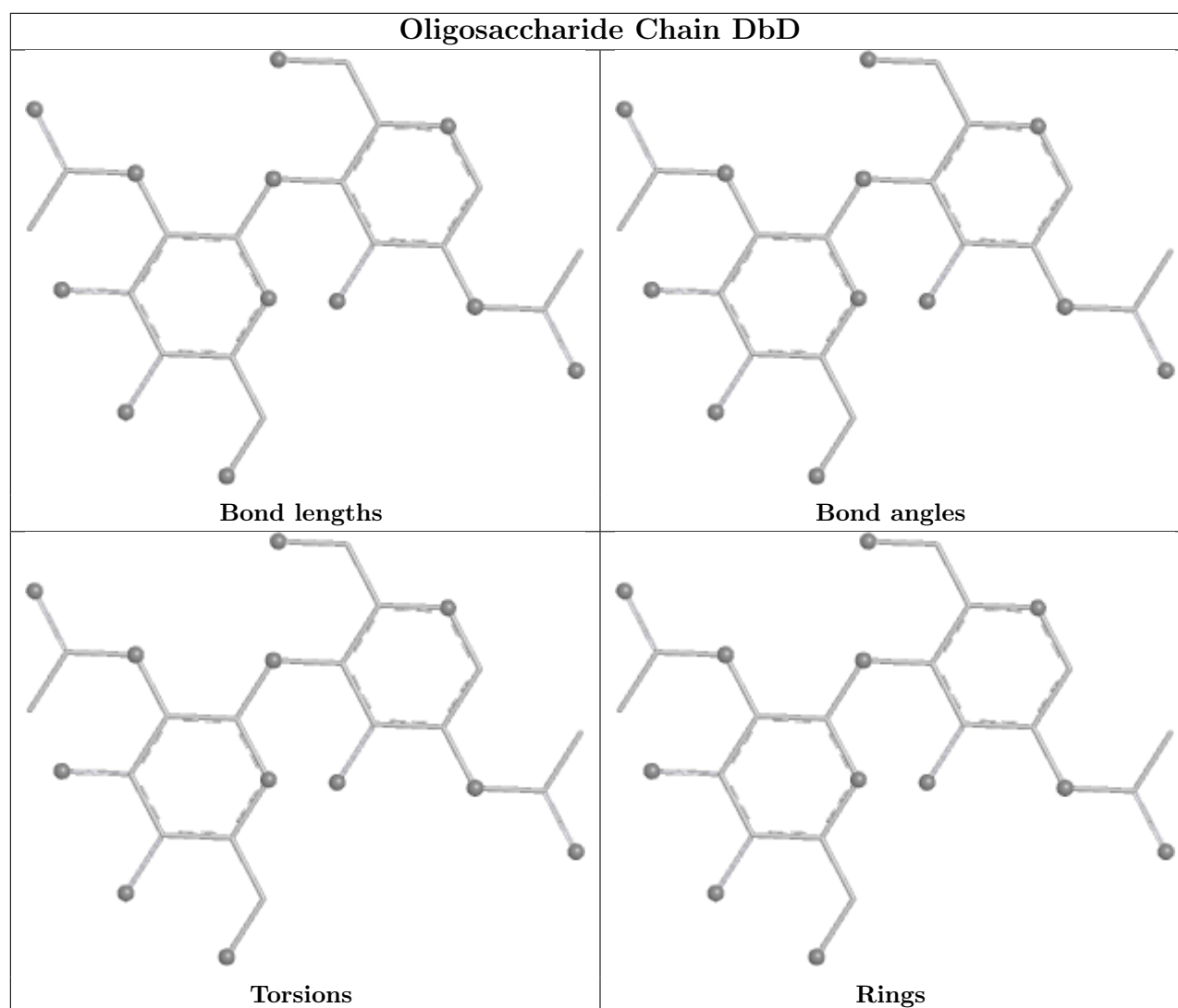
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

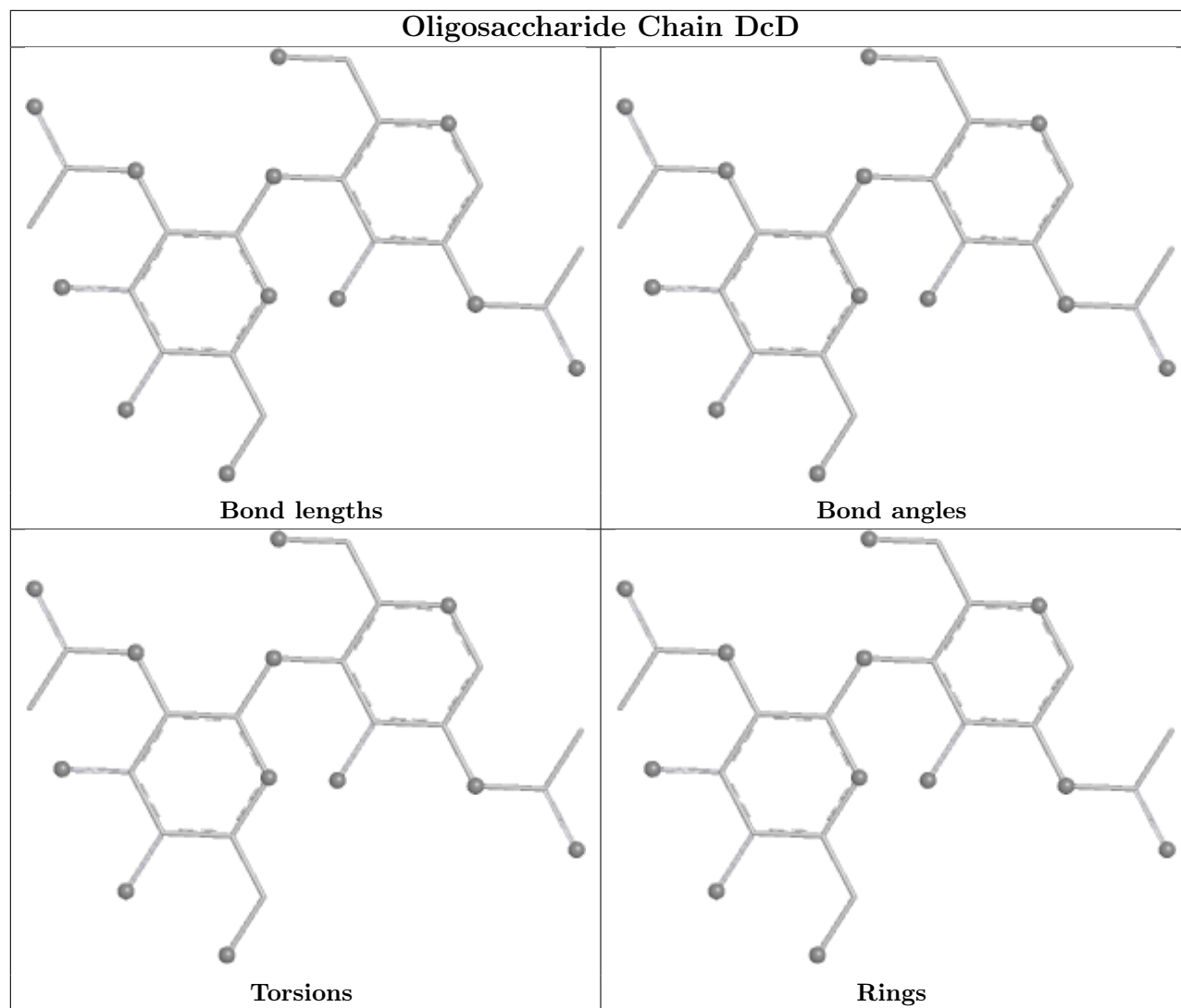


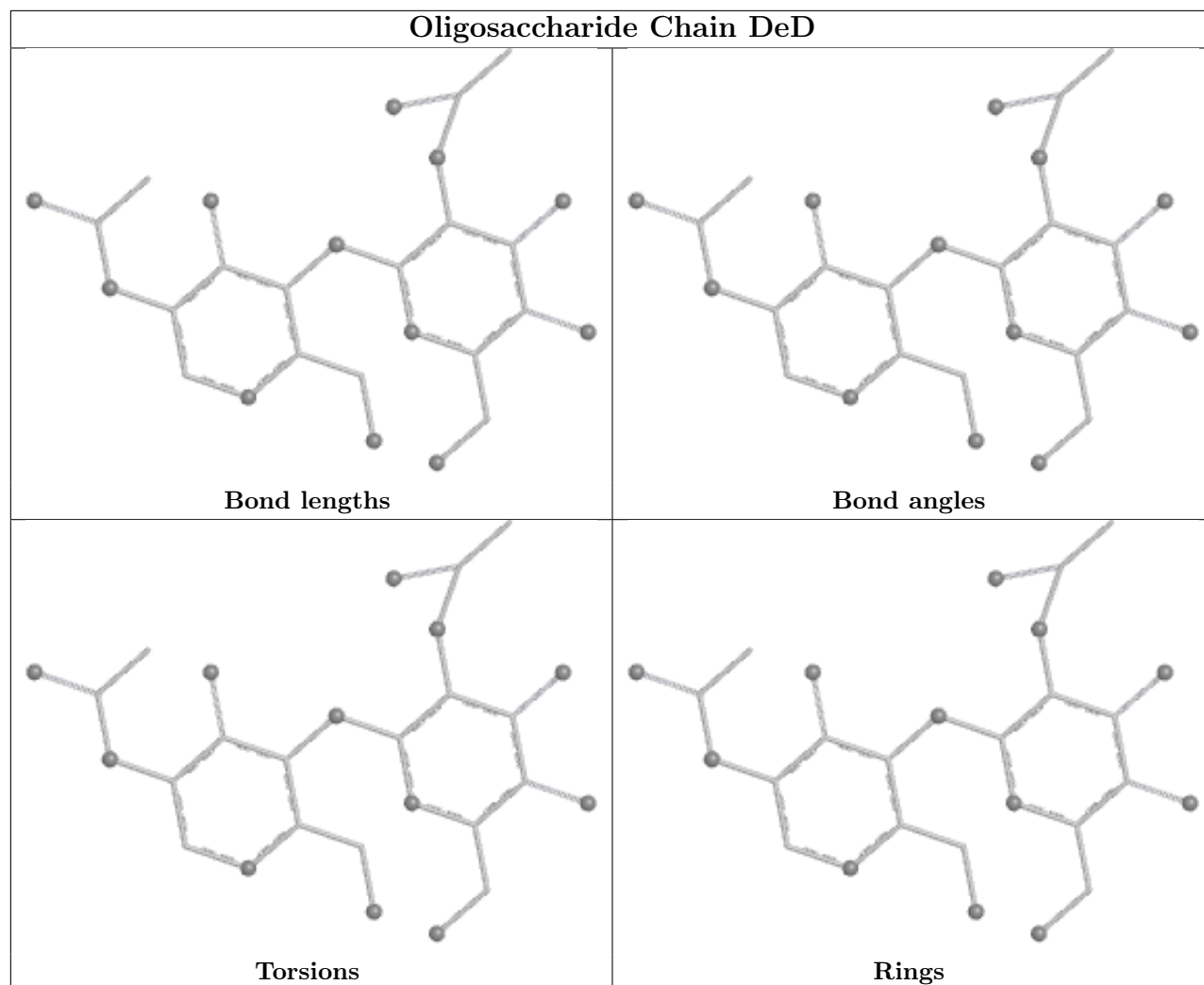


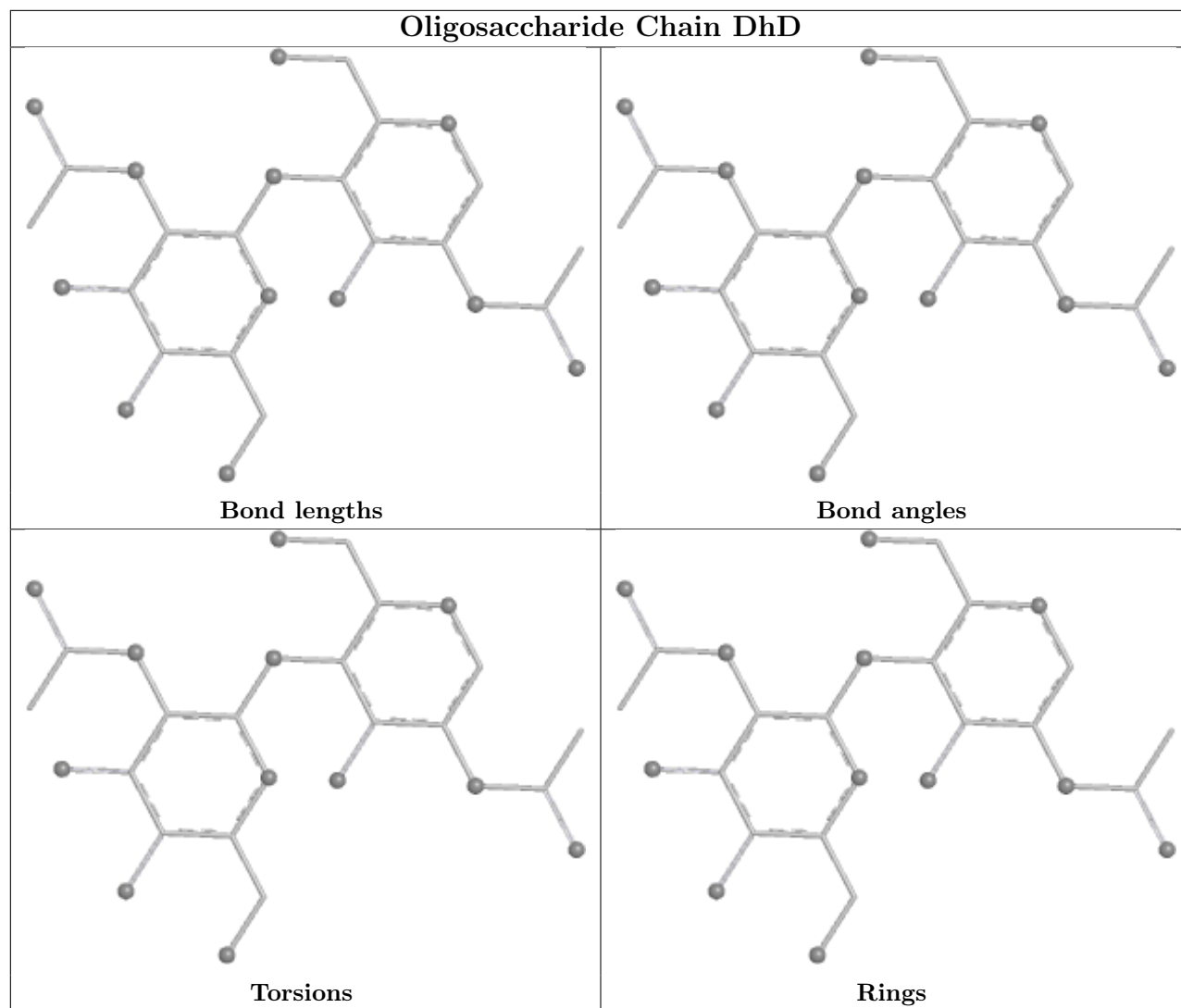


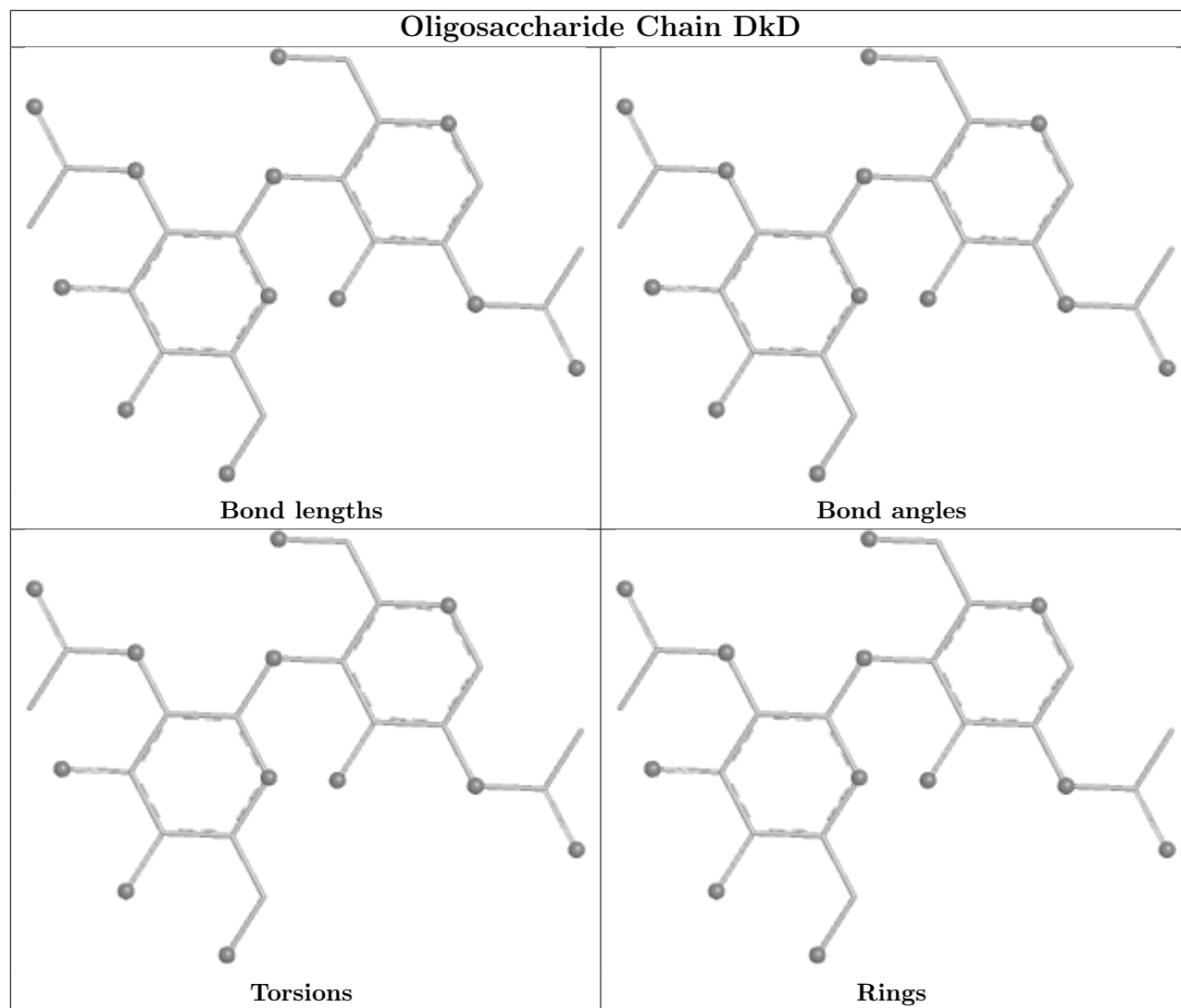


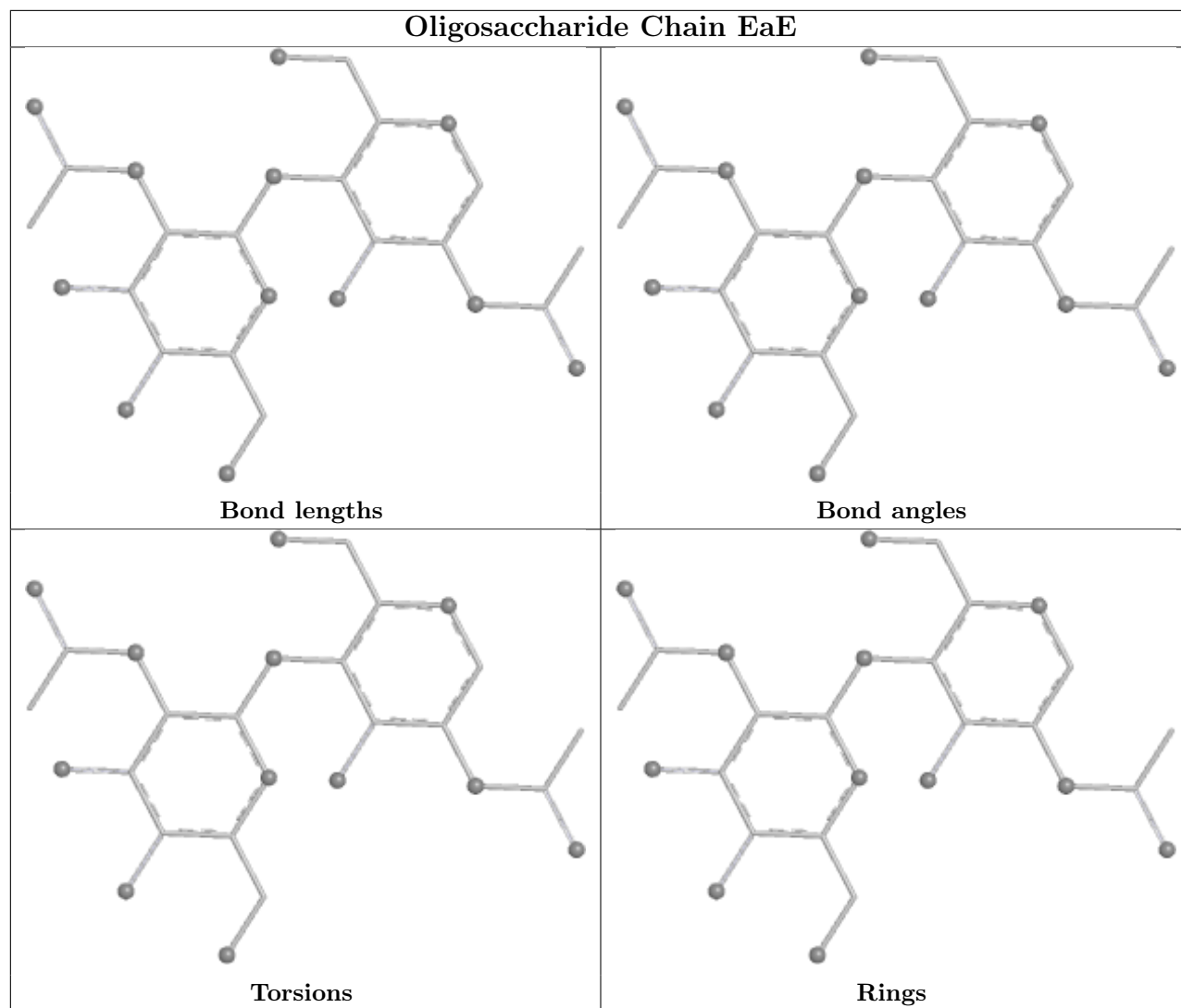




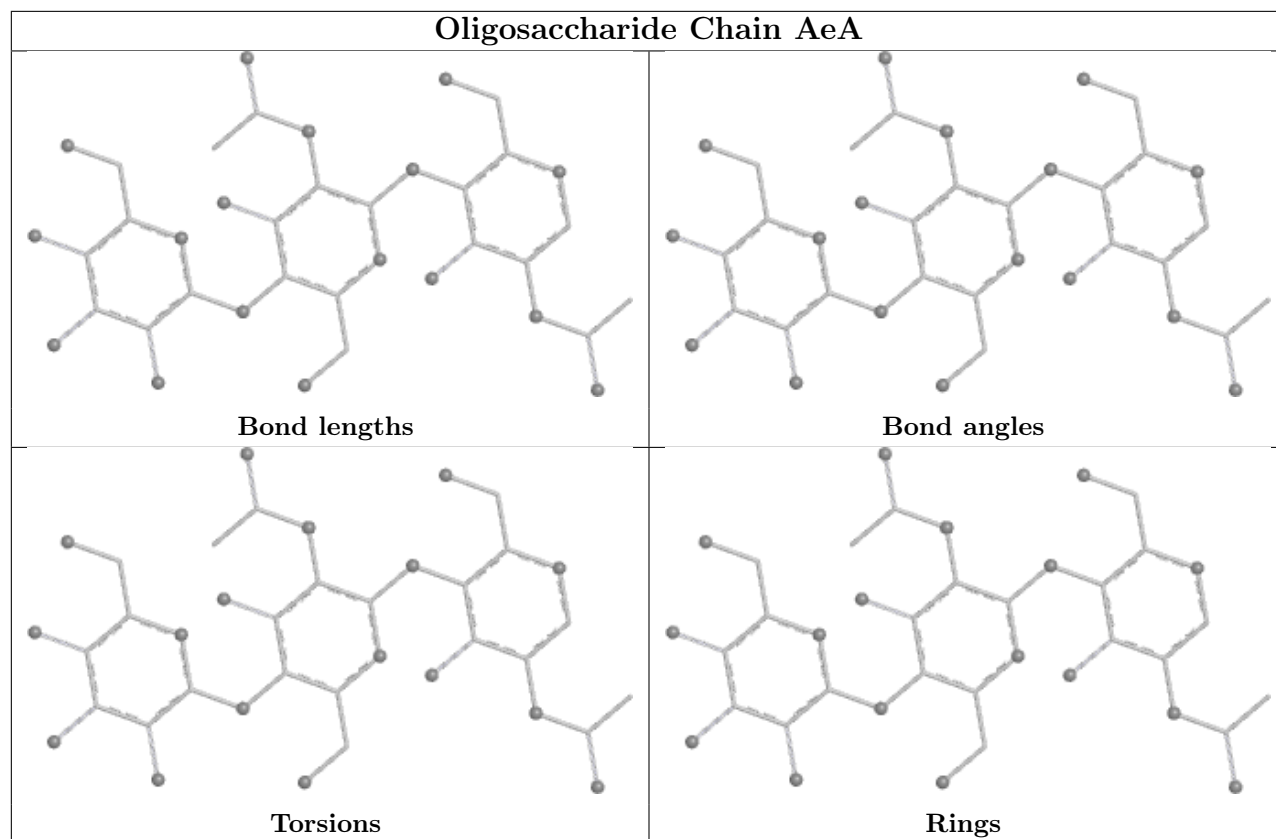




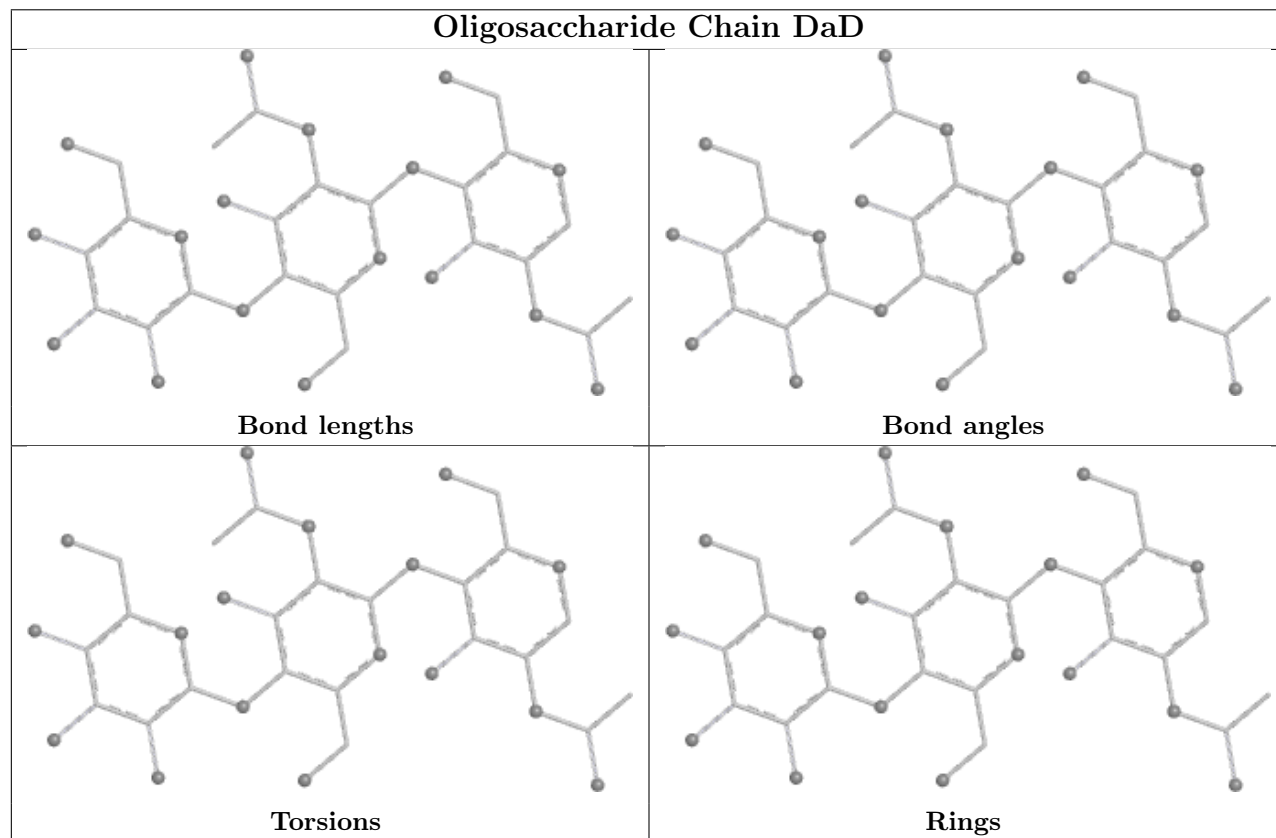




Oligosaccharide Chain AeA



Oligosaccharide Chain DaD



5.6 Ligand geometry

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	AAA	702	1	14,14,15	0.44	0	17,19,21	0.76	0
6	NAG	DDD	701	1	14,14,15	0.35	0	17,19,21	0.87	0
6	NAG	AAA	701	1	14,14,15	0.45	0	17,19,21	1.20	3 (17%)
6	NAG	AAA	703	1	14,14,15	0.38	0	17,19,21	0.76	0
6	NAG	DDD	702	1	14,14,15	0.44	0	17,19,21	1.07	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	AAA	702	1	-	2/6/23/26	0/1/1/1
6	NAG	DDD	701	1	-	0/6/23/26	0/1/1/1
6	NAG	AAA	701	1	-	0/6/23/26	0/1/1/1
6	NAG	AAA	703	1	-	3/6/23/26	0/1/1/1
6	NAG	DDD	702	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	AAA	701	NAG	C1-O5-C5	2.50	115.53	112.19
6	DDD	702	NAG	O5-C5-C6	2.40	112.33	107.66
6	AAA	701	NAG	O5-C1-C2	-2.21	107.86	111.29
6	DDD	702	NAG	C2-N2-C7	2.20	125.85	122.90
6	AAA	701	NAG	C4-C3-C2	-2.16	107.85	111.02

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	DDD	702	NAG	O5-C5-C6-O6
6	DDD	702	NAG	C4-C5-C6-O6
6	AAA	703	NAG	C4-C5-C6-O6
6	AAA	703	NAG	O5-C5-C6-O6
6	AAA	702	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	591/617 (95%)	1.93	257 (43%) 0 0	18, 53, 72, 99	1 (0%)
1	DDD	589/617 (95%)	2.03	287 (48%) 0 0	16, 55, 79, 106	1 (0%)
2	BBB	185/201 (92%)	1.77	77 (41%) 0 0	30, 45, 76, 94	0
2	EEE	185/201 (92%)	1.85	74 (40%) 1 0	27, 45, 83, 96	0
3	CCC	11/12 (91%)	2.19	7 (63%) 0 0	32, 48, 63, 72	0
3	FFF	11/12 (91%)	2.03	4 (36%) 1 0	35, 46, 75, 83	0
All	All	1572/1660 (94%)	1.94	706 (44%) 0 0	16, 53, 78, 106	2 (0%)

The worst 5 of 706 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	EEE	187	PHE	6.4
1	DDD	270	PRO	6.0
2	EEE	182	PRO	5.9
1	DDD	427	LEU	5.7
1	AAA	364	LEU	5.7

6.2 Non-standard residues in protein, DNA, RNA chains [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	HYP	CCC	85	8/9	0.76	0.20	47,48,49,53	0
3	HYP	FFF	85	8/9	0.79	0.15	45,46,46,47	0

6.3 Carbohydrates ⓘ

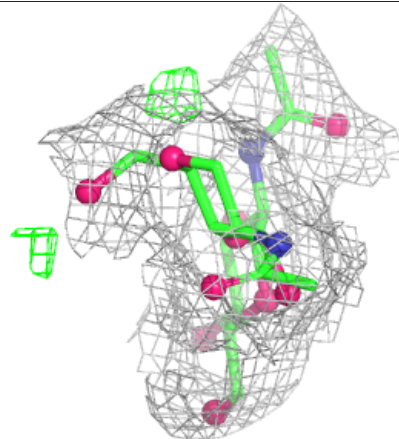
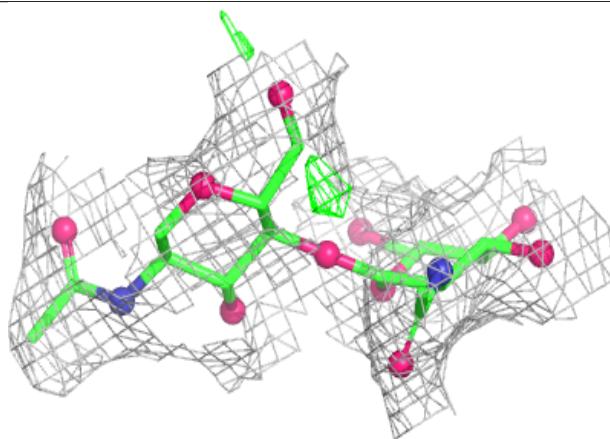
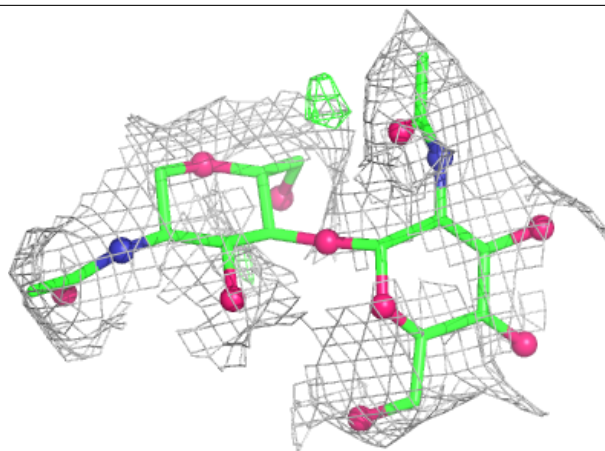
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	AaA	1	14/15	-	-	62,64,66,67	0
4	NAG	AaA	2	14/15	-	-	74,77,78,80	0
4	NAG	AgA	1	14/15	-	-	82,89,92,95	0
4	NAG	AgA	2	14/15	-	-	90,94,98,100	0
4	NAG	AiA	1	14/15	-	-	53,55,62,65	0
4	NAG	AiA	2	14/15	-	-	60,67,69,70	0
4	NAG	BaB	1	14/15	-	-	110,118,126,133	0
4	NAG	BaB	2	14/15	-	-	83,105,109,109	0
4	NAG	DbD	1	14/15	-	-	59,63,67,70	0
4	NAG	DbD	2	14/15	-	-	83,87,88,88	0
4	NAG	DcD	1	14/15	-	-	46,50,56,61	0
4	NAG	DcD	2	14/15	-	-	65,67,68,68	0
4	NAG	DeD	1	14/15	-	-	74,78,86,92	0
4	NAG	DeD	2	14/15	-	-	110,115,120,122	0
4	NAG	DhD	1	14/15	-	-	83,95,101,105	0
4	NAG	DhD	2	14/15	-	-	103,116,120,121	0
4	NAG	DkD	1	14/15	-	-	90,94,101,107	0
4	NAG	DkD	2	14/15	-	-	106,108,111,113	0
4	NAG	EaE	1	14/15	-	-	99,104,118,119	0
4	NAG	EaE	2	14/15	-	-	99,106,108,109	0
5	NAG	AeA	1	14/15	-	-	53,58,62,67	0
5	NAG	AeA	2	14/15	-	-	89,97,100,104	0
5	BMA	AeA	3	11/12	-	-	99,106,107,108	0
5	NAG	DaD	1	14/15	-	-	48,49,55,61	0
5	NAG	DaD	2	14/15	-	-	78,86,89,91	0
5	BMA	DaD	3	11/12	-	-	93,97,99,100	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.

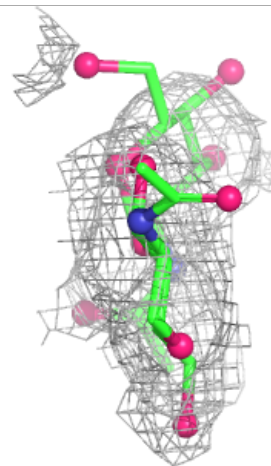
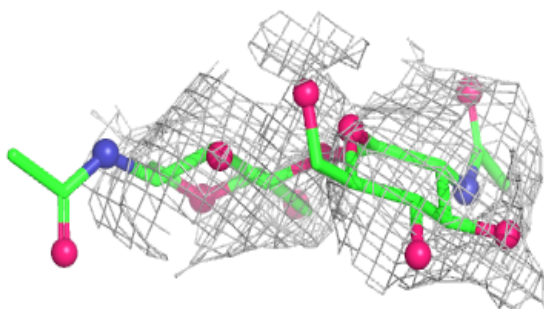
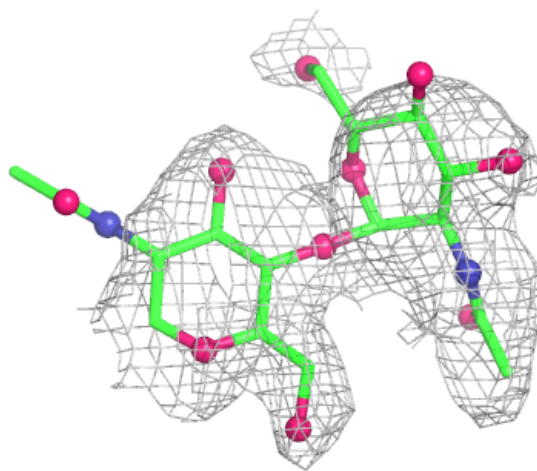
Electron density around Chain AaA:

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



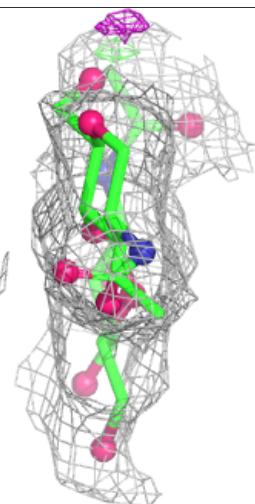
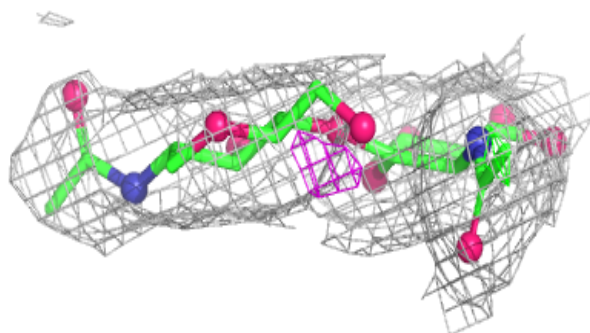
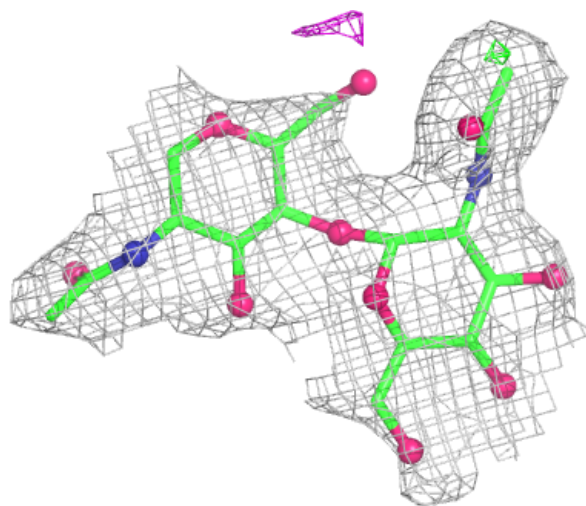
Electron density around Chain AgA:

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



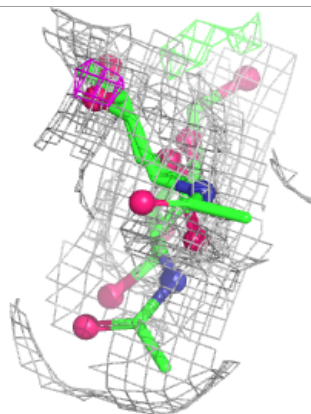
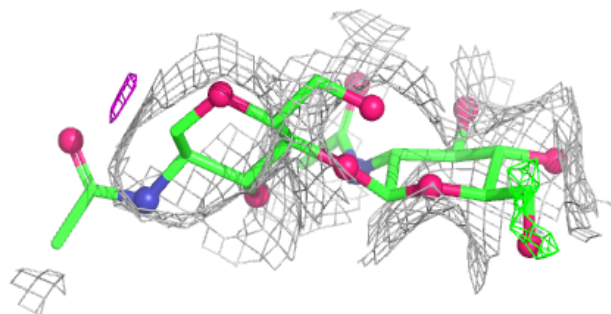
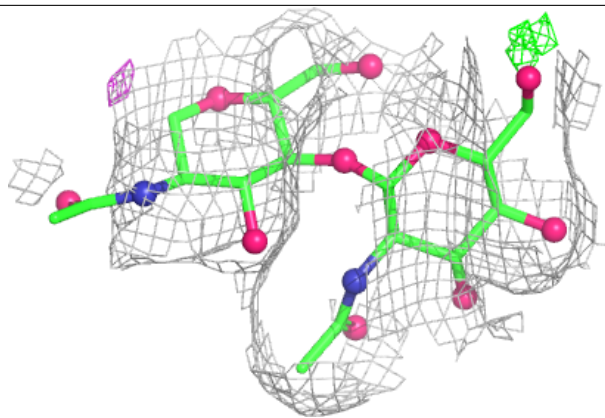
Electron density around Chain AiA:

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



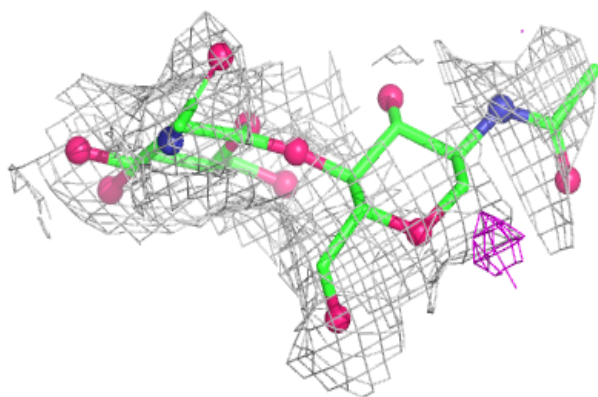
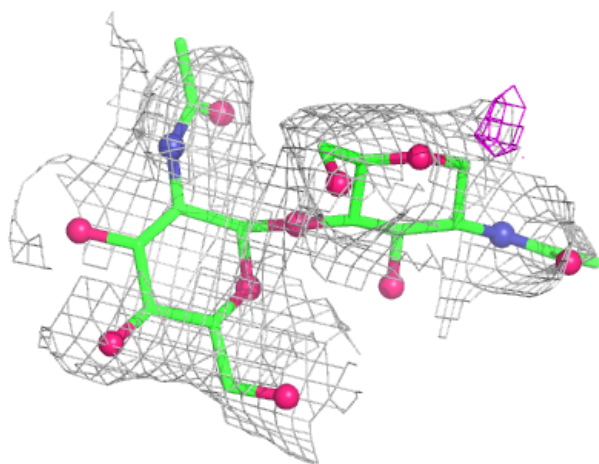
Electron density around Chain BaB:

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



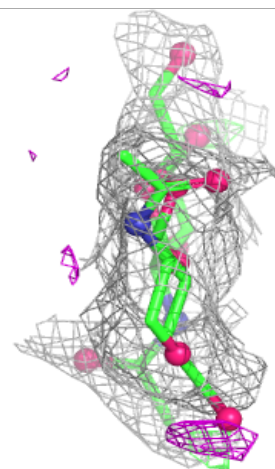
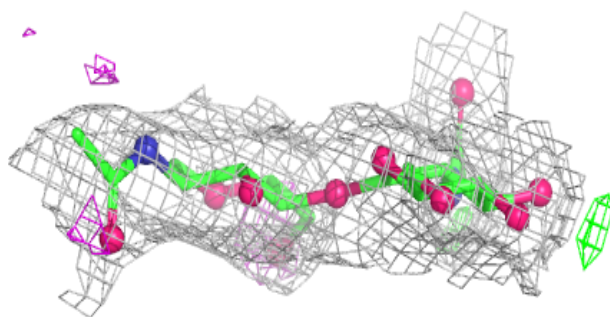
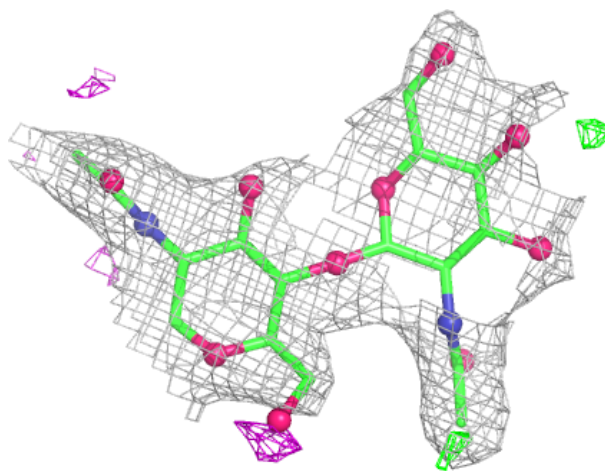
Electron density around Chain DbD:

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



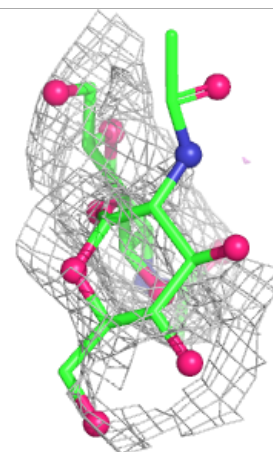
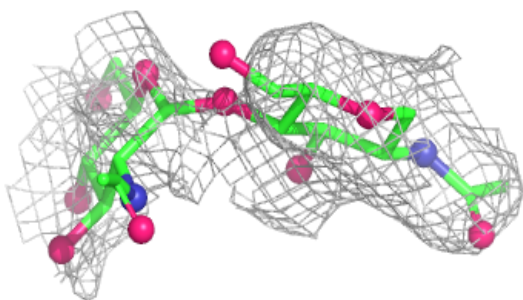
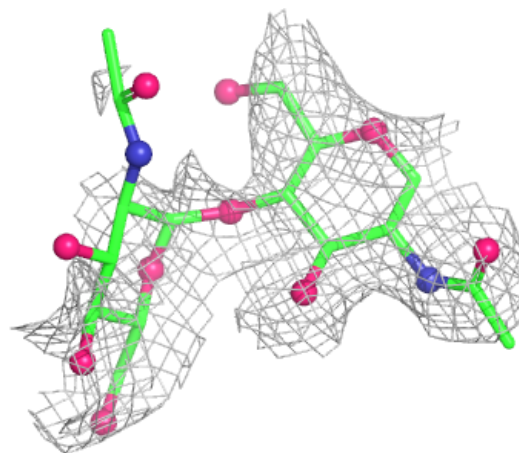
Electron density around Chain DcD:

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



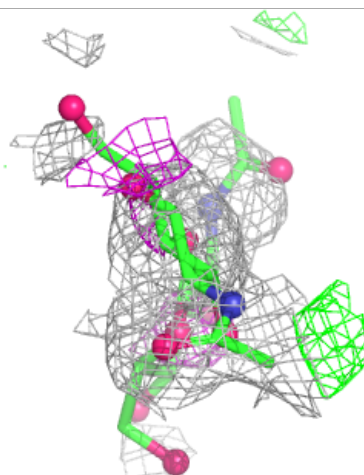
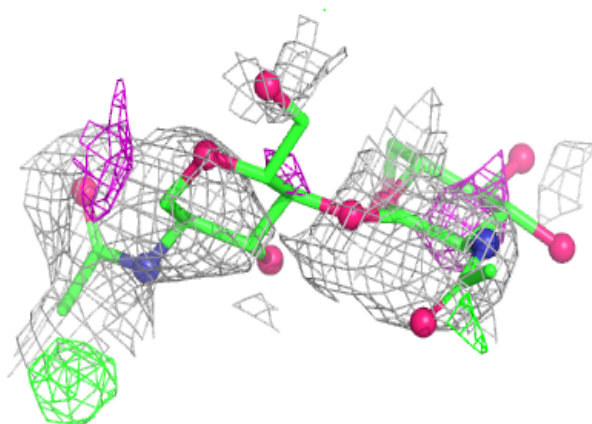
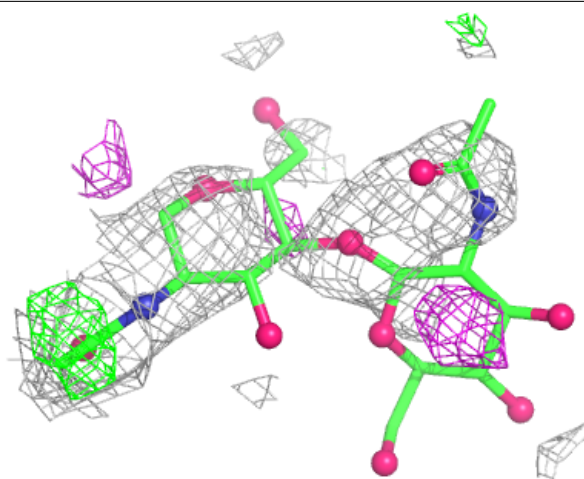
Electron density around Chain DeD:

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



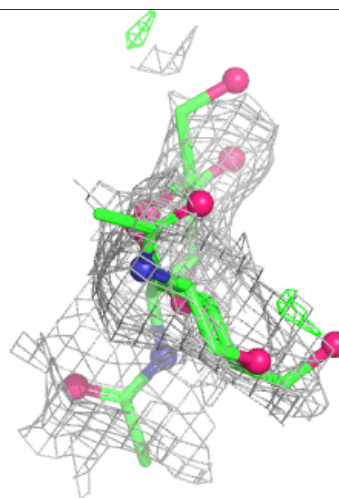
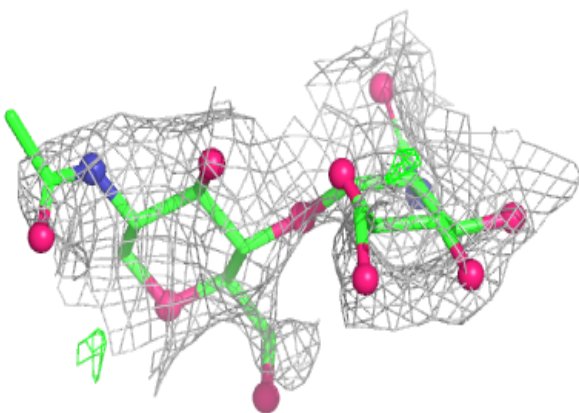
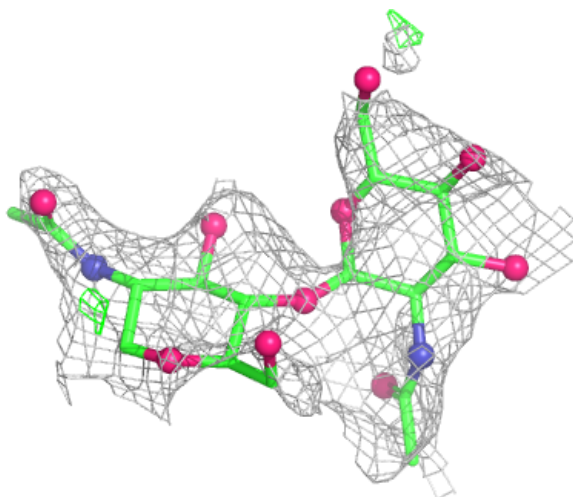
Electron density around Chain DhD:

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



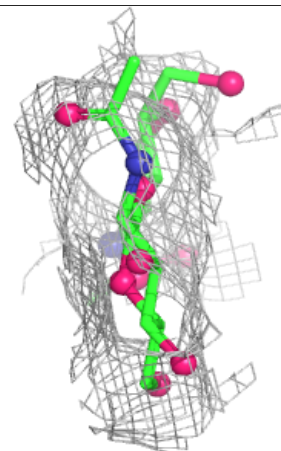
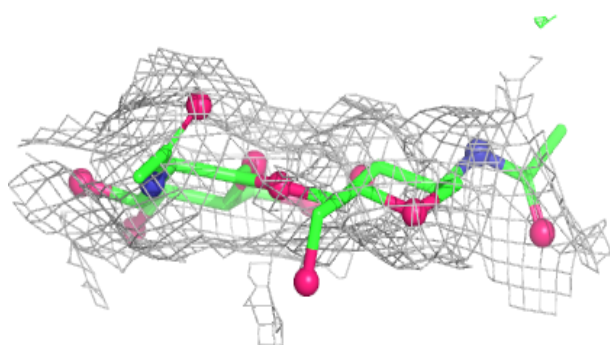
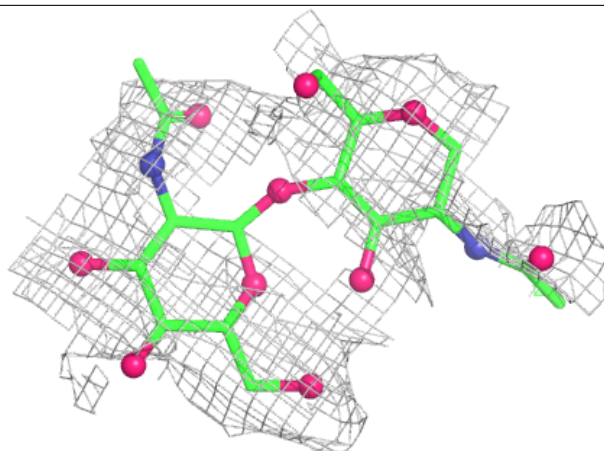
Electron density around Chain DkD:

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

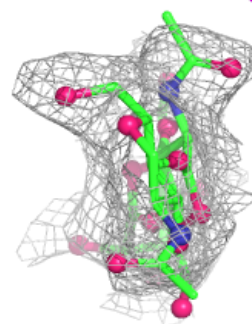
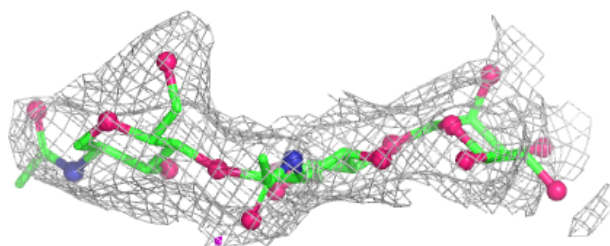
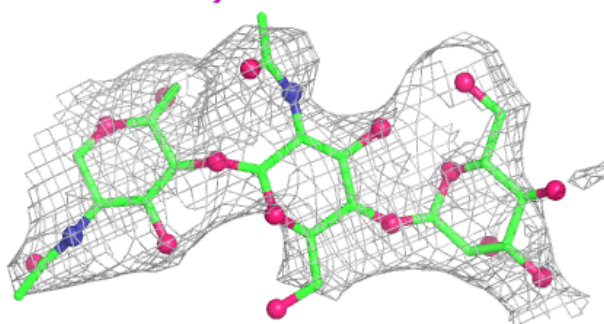


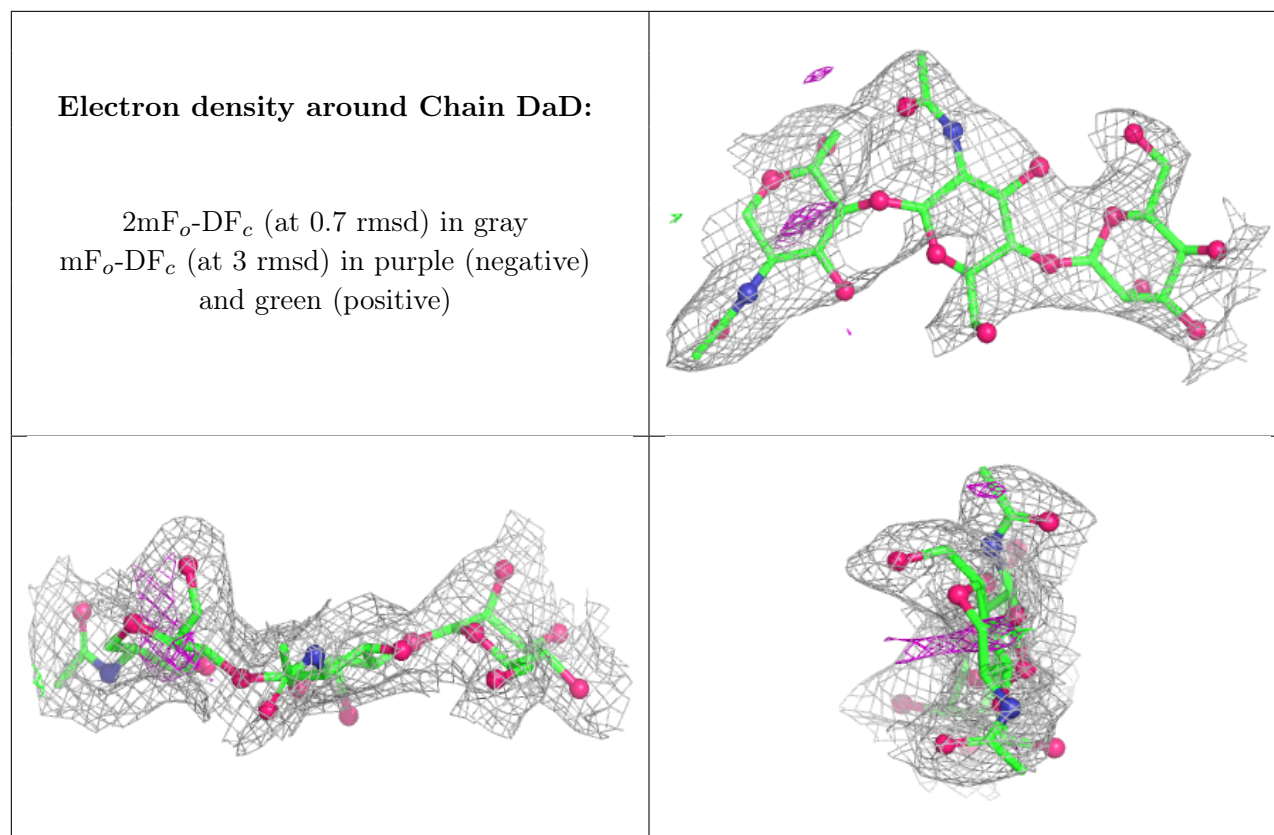
Electron density around Chain EaE:

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

**Electron density around Chain AeA:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
6	NAG	DDD	702	14/15	0.33	0.24	61,67,74,80	0
6	NAG	AAA	702	14/15	0.48	0.20	74,82,85,88	0
6	NAG	AAA	703	14/15	0.68	0.17	85,89,92,92	0
6	NAG	AAA	701	14/15	0.72	0.17	61,64,65,66	0
6	NAG	DDD	701	14/15	0.74	0.18	82,85,87,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.