



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:19 PM EST

PDB ID : 5VEM  
Title : Human ectonucleotide pyrophosphatase / phosphodiesterase 5 (ENPP5, NPP5)  
Authors : Gorelik, A.; Randriamihaja, A.; Illes, K.; Nagar, B.  
Deposited on : 2017-04-05  
Resolution : 2.60 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](mailto: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>.

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

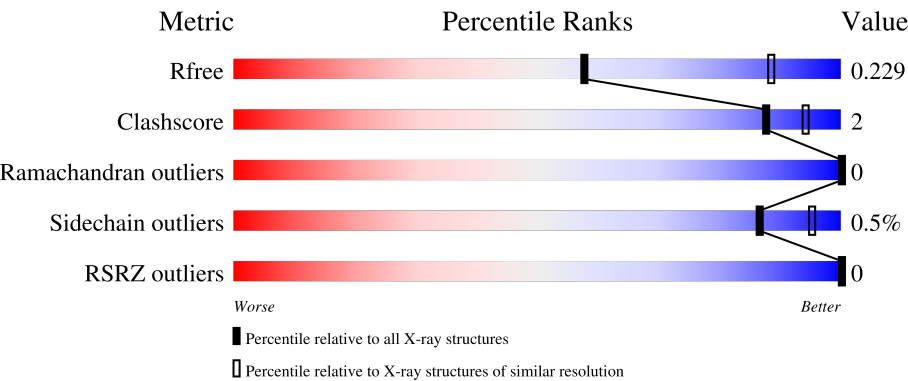
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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 <sub>free</sub>	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	416	<div><div>88%</div><div>• 8%</div></div>
1	B	416	<div><div>88%</div><div>• 8%</div></div>
1	C	416	<div><div>83%</div><div>7% 10%</div></div>
2	D	2	<div><div>100%</div></div>
2	F	2	<div><div>50%</div><div>50%</div></div>
2	G	2	<div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	2	<div><div></div><div>100%</div></div>
3	E	2	<div><div></div><div>50%</div><div>50%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19013 atoms, of which 9242 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	H	N	O	S	0	0	0
			6169	2032	3024	531	568	14			
1	B	383	Total	C	H	N	O	S	0	0	0
			6167	2032	3022	531	568	14			
1	C	374	Total	C	H	N	O	S	0	0	0
			6016	1982	2952	512	556	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASP	-	expression tag	UNP Q9UJA9
A	16	ARG	-	expression tag	UNP Q9UJA9
A	17	HIS	-	expression tag	UNP Q9UJA9
A	18	HIS	-	expression tag	UNP Q9UJA9
A	19	HIS	-	expression tag	UNP Q9UJA9
A	20	HIS	-	expression tag	UNP Q9UJA9
A	21	HIS	-	expression tag	UNP Q9UJA9
A	22	HIS	-	expression tag	UNP Q9UJA9
A	23	LYS	-	expression tag	UNP Q9UJA9
A	24	LEU	-	expression tag	UNP Q9UJA9
B	15	ASP	-	expression tag	UNP Q9UJA9
B	16	ARG	-	expression tag	UNP Q9UJA9
B	17	HIS	-	expression tag	UNP Q9UJA9
B	18	HIS	-	expression tag	UNP Q9UJA9
B	19	HIS	-	expression tag	UNP Q9UJA9
B	20	HIS	-	expression tag	UNP Q9UJA9
B	21	HIS	-	expression tag	UNP Q9UJA9
B	22	HIS	-	expression tag	UNP Q9UJA9
B	23	LYS	-	expression tag	UNP Q9UJA9
B	24	LEU	-	expression tag	UNP Q9UJA9
C	15	ASP	-	expression tag	UNP Q9UJA9
C	16	ARG	-	expression tag	UNP Q9UJA9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	HIS	-	expression tag	UNP Q9UJA9
C	18	HIS	-	expression tag	UNP Q9UJA9
C	19	HIS	-	expression tag	UNP Q9UJA9
C	20	HIS	-	expression tag	UNP Q9UJA9
C	21	HIS	-	expression tag	UNP Q9UJA9
C	22	HIS	-	expression tag	UNP Q9UJA9
C	23	LYS	-	expression tag	UNP Q9UJA9
C	24	LEU	-	expression tag	UNP Q9UJA9

- Molecule 2 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
2	D	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	F	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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

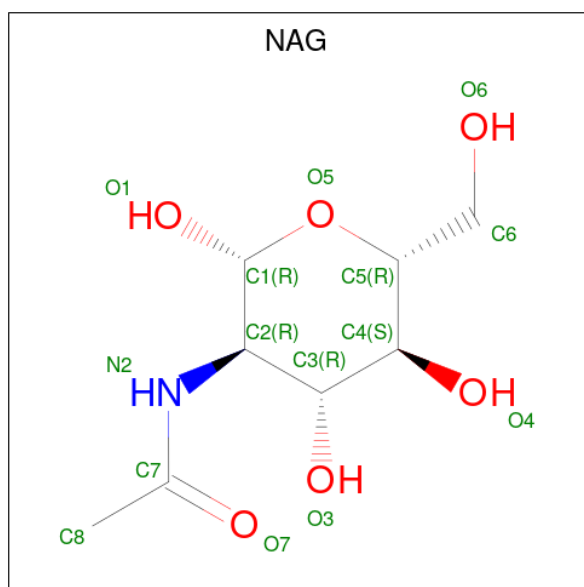


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	0	0	0
			48	14	24	1	9			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Zn 3	0	0
4	B	3	Total 3	Zn 3	0	0
4	C	3	Total 3	Zn 3	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	A	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	B	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	C	1	Total 28	C 8	H 14	N 1	O 5	0	0
5	C	1	Total 28	C 8	H 14	N 1	O 5	0	0


- Molecule 6 is water.

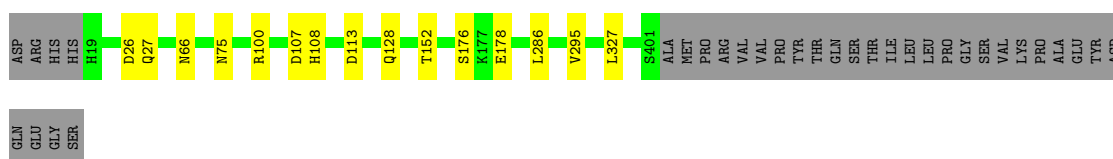
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total 77	O 77	0	0
6	B	72	Total 72	O 72	0	0
6	C	11	Total 11	O 11	0	0

### 3 Residue-property plots [i](#)

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. 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. 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.

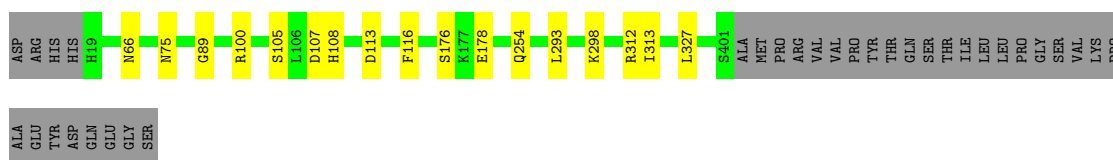
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 5

Chain A: 




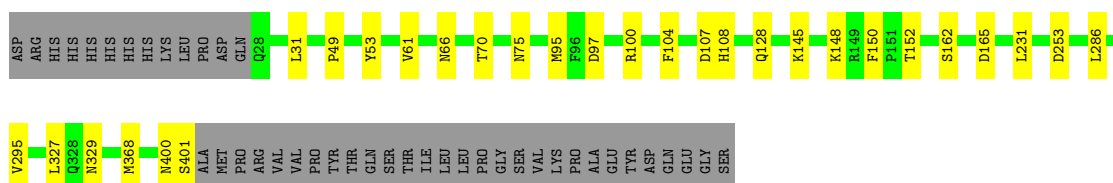
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 5

Chain B: 



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 5

Chain C: 



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

Chain D: 



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



Chain F:  50% 50%

MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain H:  100%

MAG1  
MAG2

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

Chain E:  50% 50%

MAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.41 Å   109.41 Å   134.82 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	44.94 – 2.60 44.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	80.8 (44.94-2.60) 0.1 (44.94-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.196 , 0.227 0.201 , 0.229	Depositor DCC
$R_{free}$ test set	1836 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 64.4	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical 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: FUC, ZN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/3249	0.44	0/4423
1	B	0.24	0/3249	0.45	0/4423
1	C	0.25	0/3163	0.44	0/4306
All	All	0.25	0/9661	0.44	0/13152

There are no bond length outliers.

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	3145	3024	3023	7	0
1	B	3145	3022	3021	12	0
1	C	3064	2952	2953	17	1
2	D	28	27	25	0	0
2	F	28	27	25	0	1
2	G	28	27	25	0	0
2	H	28	27	25	0	0
3	E	24	24	22	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	3	0	0	0	0
5	A	42	42	39	0	0
5	B	42	42	39	0	0
5	C	28	28	26	0	0
6	A	77	0	0	0	0
6	B	72	0	0	3	0
6	C	11	0	0	0	0
All	All	9771	9242	9223	36	1

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 (36) 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:254:GLN:OE1	6:B:601:HOH:O	2.04	0.75
1:C:97:ASP:OD1	1:C:100:ARG:NH1	2.21	0.74
1:C:253:ASP:OD2	1:C:329:ASN:ND2	2.22	0.72
1:C:128:GLN:OE1	1:C:152:THR:N	2.30	0.64
1:A:100:ARG:NH2	1:A:113:ASP:OD2	2.30	0.63
1:A:176:SER:OG	1:A:178:GLU:O	2.16	0.62
1:B:100:ARG:NH2	1:B:113:ASP:OD2	2.33	0.62
1:A:107:ASP:OD1	1:A:108:HIS:N	2.39	0.54
1:B:116:PHE:O	6:B:602:HOH:O	2.18	0.54
1:C:107:ASP:OD1	1:C:108:HIS:N	2.40	0.54
1:A:66:ASN:HB2	1:A:75:ASN:OD1	2.10	0.51
1:B:89:GLY:O	1:B:312:ARG:NH1	2.43	0.51
1:C:400:ASN:O	1:C:401:SER:CB	2.59	0.50
1:B:107:ASP:OD1	1:B:108:HIS:N	2.45	0.50
1:C:286:LEU:HB3	1:C:295:VAL:HG21	1.94	0.49
1:B:66:ASN:HB2	1:B:75:ASN:OD1	2.12	0.49
1:C:162:SER:OG	1:C:165:ASP:OD1	2.30	0.49
1:C:66:ASN:HB2	1:C:75:ASN:OD1	2.15	0.47
1:A:286:LEU:HB3	1:A:295:VAL:HG21	1.96	0.46
1:B:176:SER:OG	1:B:178:GLU:O	2.34	0.46
1:B:178:GLU:O	1:B:178:GLU:HG2	2.15	0.45
1:B:298:LYS:HE2	1:B:313:ILE:HB	1.98	0.45
1:B:293:LEU:O	6:B:603:HOH:O	2.21	0.44
1:C:400:ASN:O	1:C:401:SER:OG	2.29	0.44
1:A:128:GLN:OE1	1:A:152:THR:N	2.50	0.43
1:C:145:LYS:HB2	1:C:150:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:CB	1:C:231:LEU:HD21	2.50	0.42
1:C:31:LEU:HB3	1:C:231:LEU:HD21	2.02	0.41
1:B:178:GLU:O	1:B:178:GLU:CG	2.68	0.41
1:C:70:THR:HA	1:C:75:ASN:HD21	1.85	0.41
1:C:95:MET:HG3	1:C:104:PHE:HB3	2.03	0.41
1:C:49:PRO:O	1:C:53:TYR:N	2.51	0.41
1:C:145:LYS:HB2	1:C:150:PHE:CZ	2.56	0.41
1:B:105:SER:OG	1:B:107:ASP:OD1	2.36	0.40
1:C:61:VAL:HG11	1:C:368:MET:HB3	2.04	0.40
1:A:178:GLU:O	1:A:178:GLU:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LYS:HZ2	2:F:2:NAG:O3[3_565]	1.55	0.05

## 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	381/416 (92%)	366 (96%)	15 (4%)	0	100	100
1	B	381/416 (92%)	366 (96%)	15 (4%)	0	100	100
1	C	372/416 (89%)	357 (96%)	15 (4%)	0	100	100
All	All	1134/1248 (91%)	1089 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/373 (92%)	341 (99%)	3 (1%)	75	90
1	B	344/373 (92%)	343 (100%)	1 (0%)	91	97
1	C	335/373 (90%)	334 (100%)	1 (0%)	91	97
All	All	1023/1119 (91%)	1018 (100%)	5 (0%)	86	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	27	GLN
1	A	327	LEU
1	B	327	LEU
1	C	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

10 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	$\# Z  > 2$
2	NAG	D	1	2,1	14,14,15	0.38	0	17,19,21	0.60	0
2	NAG	D	2	2	14,14,15	0.17	0	17,19,21	0.50	0
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.50	0
3	FUC	E	2	3	10,10,11	0.95	1 (10%)	14,14,16	0.97	1 (7%)
2	NAG	F	1	2,1	14,14,15	0.36	0	17,19,21	0.54	0
2	NAG	F	2	2	14,14,15	1.40	1 (7%)	17,19,21	2.01	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.19	0	17,19,21	0.68	0
2	NAG	G	2	2	14,14,15	0.16	0	17,19,21	0.49	0
2	NAG	H	1	2,1	14,14,15	0.54	0	17,19,21	0.63	0
2	NAG	H	2	2	14,14,15	0.27	0	17,19,21	0.52	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C1	5.04	1.52	1.43
3	E	2	FUC	C1-C2	2.32	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	8.04	122.97	112.19
3	E	2	FUC	C1-C2-C3	2.60	113.43	109.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7

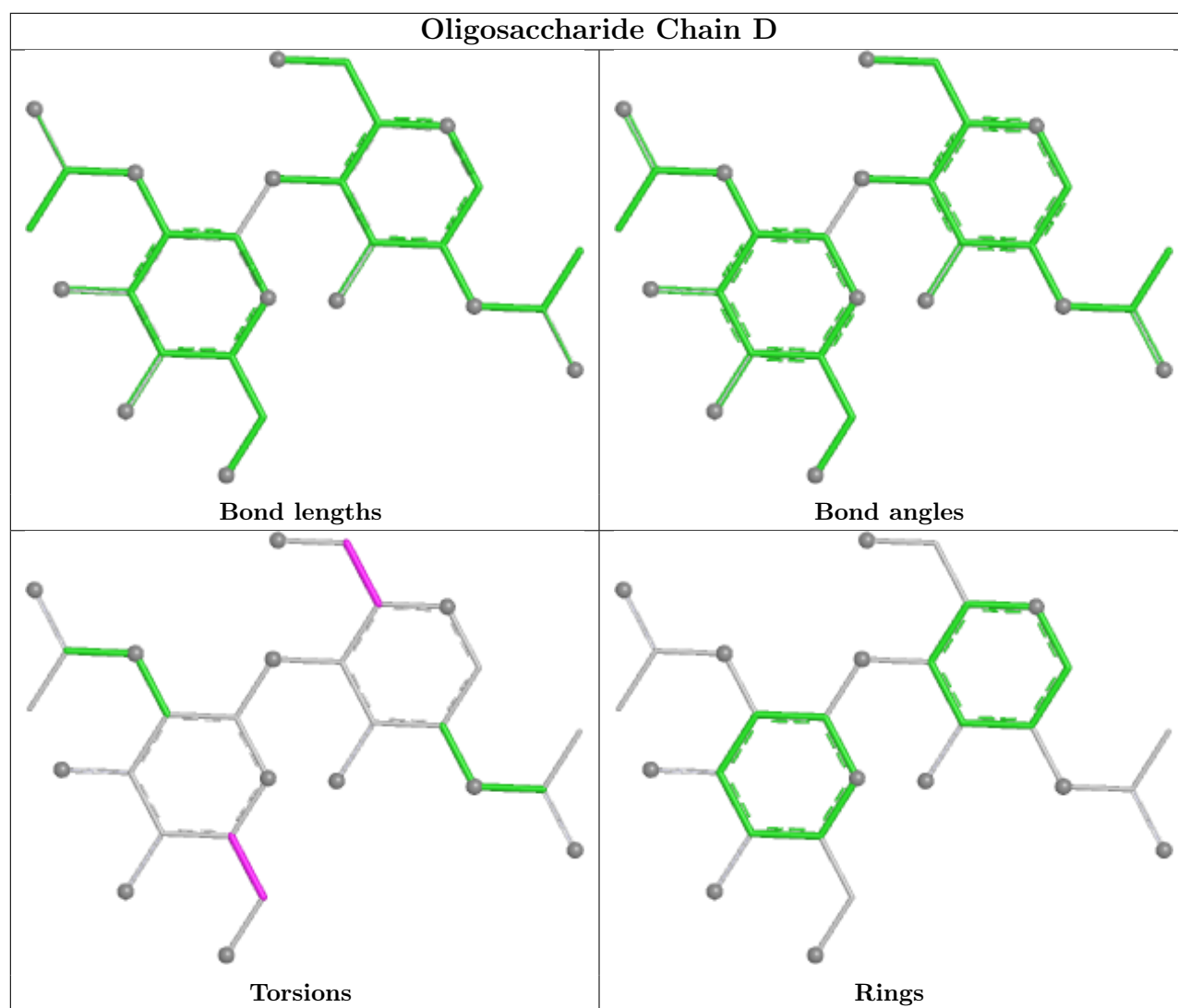
There are no ring outliers.

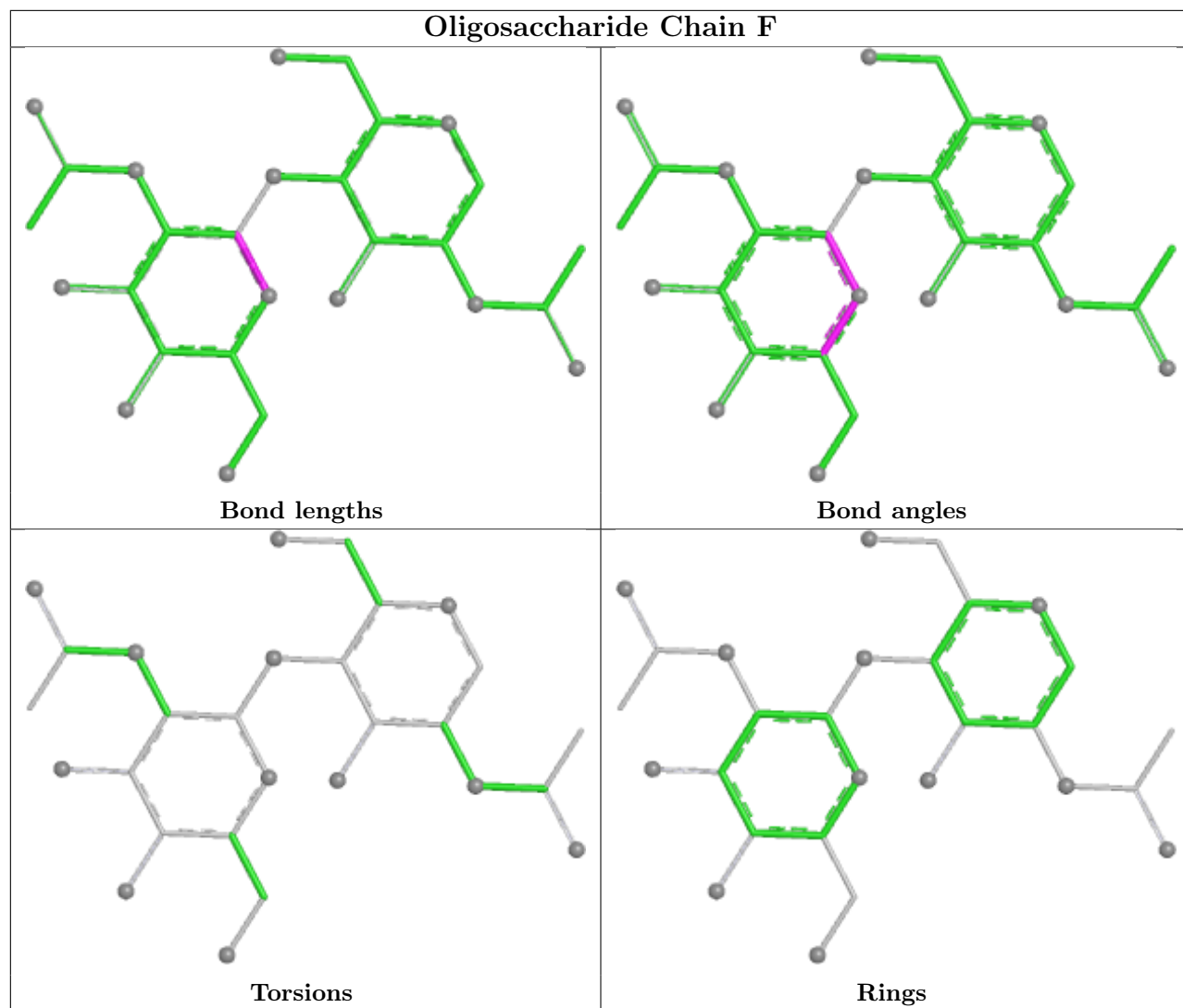
1 monomer is involved in 1 short contact:

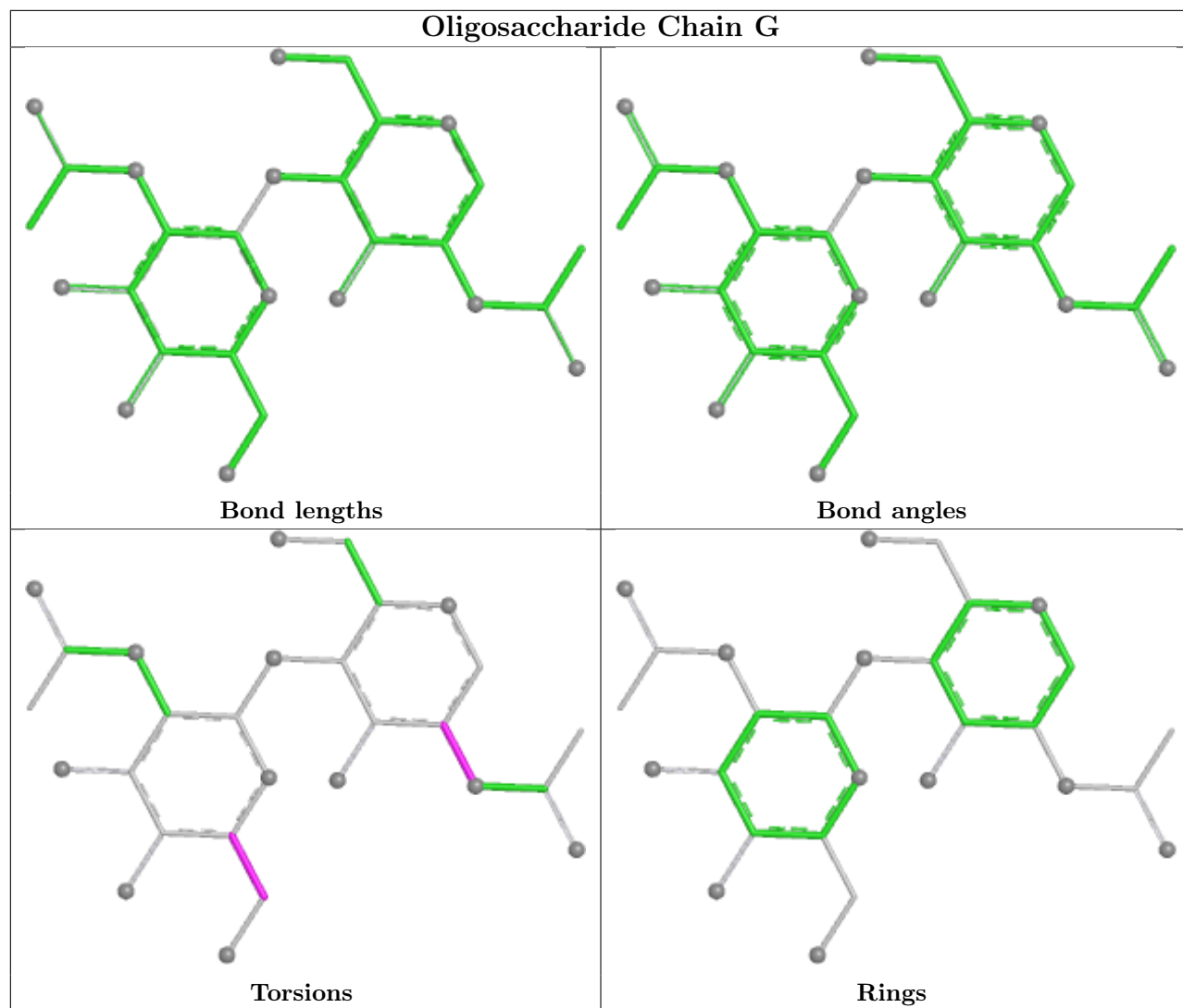
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	0	1

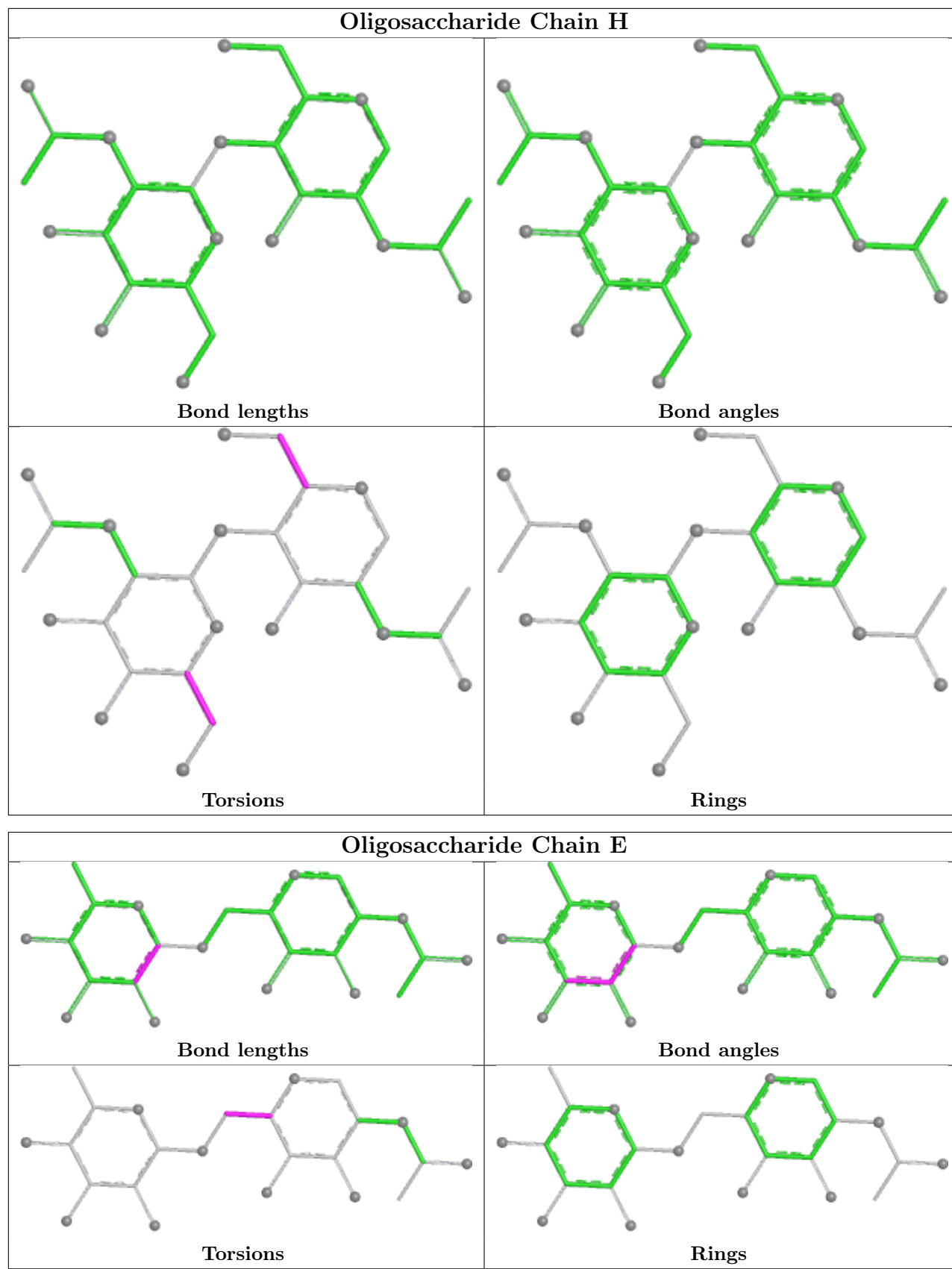
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	506	1	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
5	NAG	B	506	1	14,14,15	0.44	0	17,19,21	0.62	0
5	NAG	B	509	1	14,14,15	0.46	0	17,19,21	0.56	0
5	NAG	B	510	1	14,14,15	0.51	0	17,19,21	0.52	0
5	NAG	A	504	1	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
5	NAG	A	506	1	14,14,15	0.44	0	17,19,21	0.56	0
5	NAG	A	505	1	14,14,15	0.40	0	17,19,21	0.50	0
5	NAG	C	507	1	14,14,15	0.21	0	17,19,21	0.70	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
5	NAG	C	506	1	-	2/6/23/26	0/1/1/1
5	NAG	B	506	1	-	3/6/23/26	0/1/1/1
5	NAG	B	509	1	-	0/6/23/26	0/1/1/1
5	NAG	B	510	1	-	0/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	A	506	1	-	2/6/23/26	0/1/1/1
5	NAG	A	505	1	-	0/6/23/26	0/1/1/1
5	NAG	C	507	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	NAG	C1-O5-C5	3.72	117.17	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	506	NAG	C1-O5-C5	2.15	115.06	112.19
5	C	507	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	NAG	O5-C5-C6-O6
5	A	506	NAG	C4-C5-C6-O6
5	C	506	NAG	O5-C5-C6-O6
5	B	506	NAG	O5-C5-C6-O6
5	B	506	NAG	C4-C5-C6-O6
5	C	506	NAG	C4-C5-C6-O6
5	C	507	NAG	C4-C5-C6-O6
5	C	507	NAG	O5-C5-C6-O6
5	B	506	NAG	C1-C2-N2-C7

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](#)

**Warning:** The R factor obtained from EDS is 0.3199, which does not match the depositor's R factor of 0.196. Please interpret the results in this section carefully.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	383/416 (92%)	-2.42	0 100 100	23, 34, 60, 84	0
1	B	383/416 (92%)	-2.43	0 100 100	21, 34, 65, 83	0
1	C	374/416 (89%)	-2.39	0 100 100	43, 65, 94, 108	0
All	All	1140/1248 (91%)	-2.41	0 100 100	21, 41, 84, 108	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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.

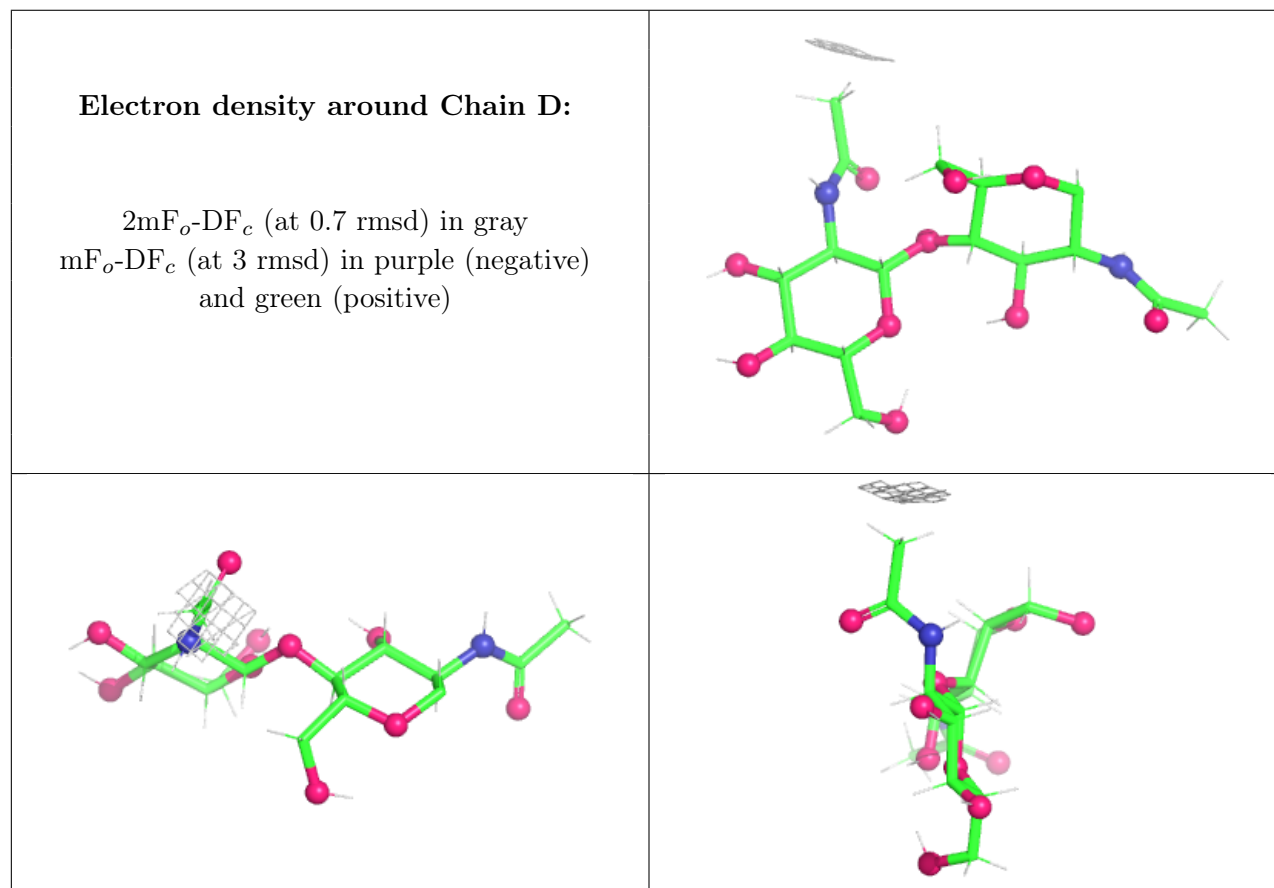
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	H	1	14/15	0.59	0.00	45,61,81,83	0
3	NAG	E	1	14/15	0.72	0.00	60,73,82,93	0
2	NAG	D	2	14/15	0.88	0.01	59,78,90,103	0
2	NAG	F	2	14/15	0.88	0.00	62,75,88,95	0
2	NAG	D	1	14/15	0.91	0.00	38,52,62,73	0
2	NAG	G	1	14/15	0.91	0.01	42,53,62,69	0
2	NAG	H	2	14/15	0.92	0.00	61,83,100,104	0
2	NAG	G	2	14/15	0.93	0.00	60,83,105,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FUC	E	2	10/11	0.96	0.00	56,72,87,90	0
2	NAG	F	1	14/15	0.97	0.00	34,47,67,69	0

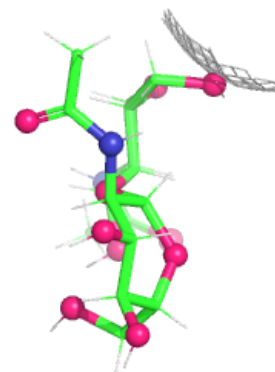
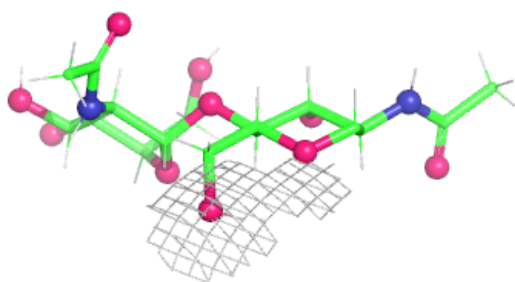
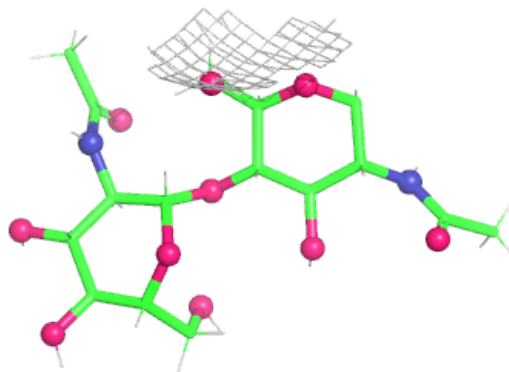
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



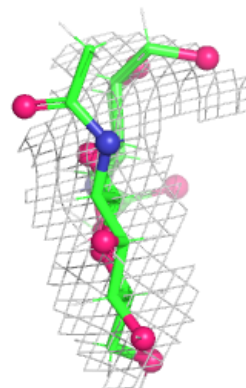
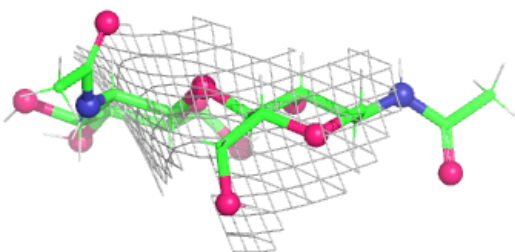
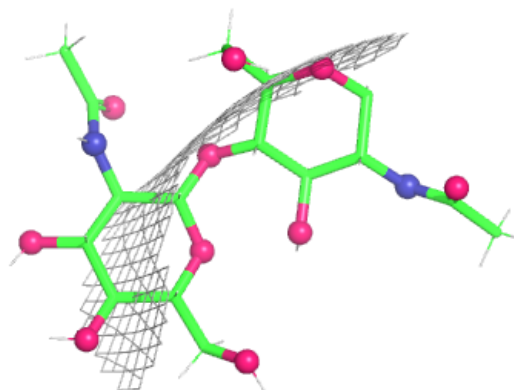


**Electron density around Chain F:**

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

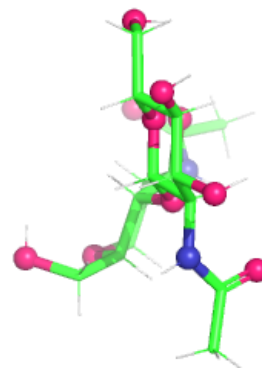
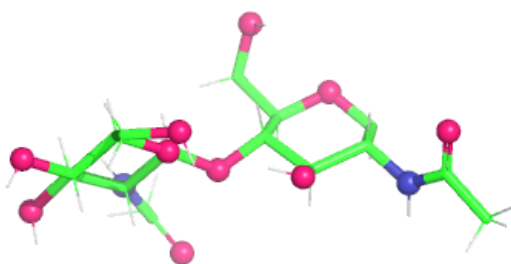
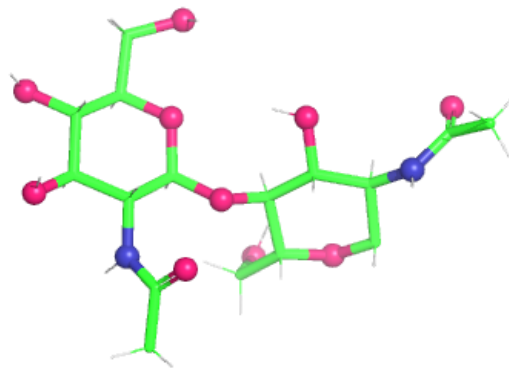
**Electron density around Chain G:**

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

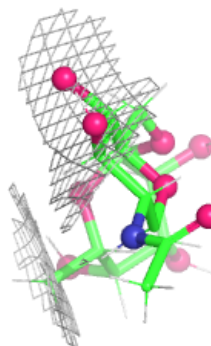
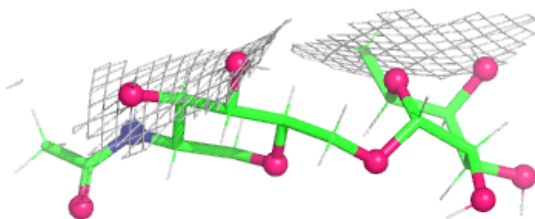
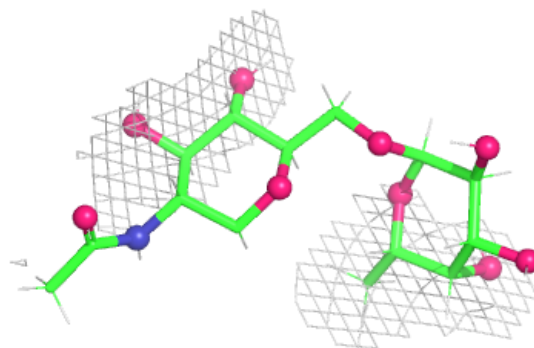


**Electron density around Chain H:**

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

**Electron density around Chain E:**

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



## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ZN	B	503	1/1	-0.19	0.02	102,102,102,102	0
4	ZN	B	501	1/1	-0.08	0.01	24,24,24,24	0
4	ZN	C	501	1/1	0.22	0.01	46,46,46,46	0
4	ZN	B	502	1/1	0.39	0.01	27,27,27,27	0
4	ZN	C	502	1/1	0.43	0.01	51,51,51,51	0
5	NAG	A	506	14/15	0.47	0.00	39,57,79,85	0
5	NAG	A	505	14/15	0.58	0.00	30,38,51,61	0
4	ZN	A	503	1/1	0.68	0.01	90,90,90,90	0
5	NAG	A	504	14/15	0.68	0.00	66,90,108,110	0
4	ZN	C	503	1/1	0.74	0.00	111,111,111,111	0
5	NAG	B	510	14/15	0.81	0.00	65,81,97,104	0
5	NAG	C	506	14/15	0.84	0.00	46,71,89,91	0
5	NAG	C	507	14/15	0.84	0.00	58,72,86,95	0
4	ZN	A	501	1/1	0.89	0.00	26,26,26,26	0
5	NAG	B	506	14/15	0.91	0.00	55,69,88,96	0
5	NAG	B	509	14/15	0.96	0.00	38,53,65,68	0
4	ZN	A	502	1/1	0.96	0.01	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.