



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2023 – 06:08 am GMT

PDB ID : 1V0Z
Title : Structure of Neuraminidase from English duck subtype N6
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on : 2004-03-12
Resolution : 1.84 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

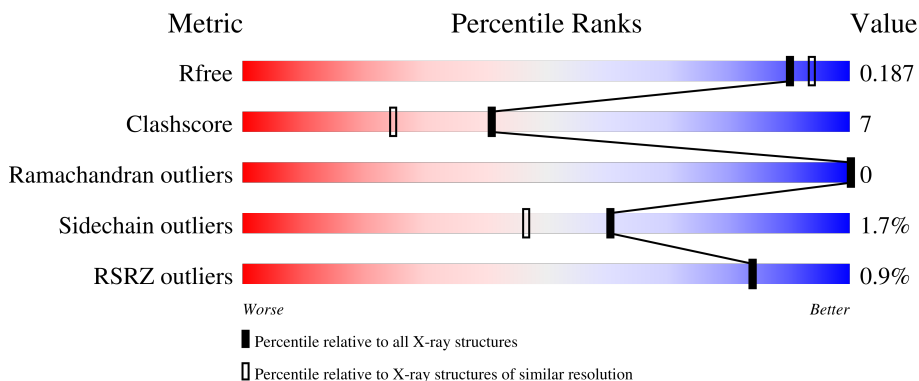
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	389	
1	B	389	
1	C	389	
1	D	389	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	I	2	
3	F	4	
4	G	6	
5	H	3	
6	J	2	

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
11	PEG	C	503	-	X	X	-
2	NAG	E	2	-	-	-	X
3	MAN	F	3	-	-	-	X
6	MAN	J	2	-	-	-	X
9	NAG	A	506	-	-	X	-
9	NAG	A	513	-	-	-	X
9	NAG	B	503	-	-	-	X
9	NAG	C	501	-	-	-	X
9	NAG	D	506	-	-	-	X
9	NAG	D	508	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 14347 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 NEURAMINIDASE.

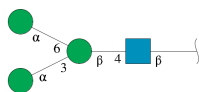
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	Total 3009	C 1875	N 535	O 572	S 27	0	0	0
1	B	389	Total 3009	C 1875	N 535	O 572	S 27	0	0	0
1	C	389	Total 3009	C 1875	N 535	O 572	S 27	0	0	0
1	D	389	Total 3009	C 1875	N 535	O 572	S 27	0	0	0

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



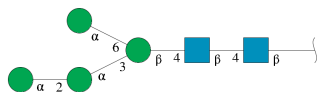
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	Total 28	C 16	N 2	O 10	0	0	0
2	I	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



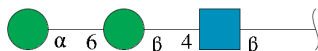
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	4	Total 47	C 26	N 1	O 20	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O			
4	G	6	72	40	2	30	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	3	36	20	1	15	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
6	J	2	22	12	10	0	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

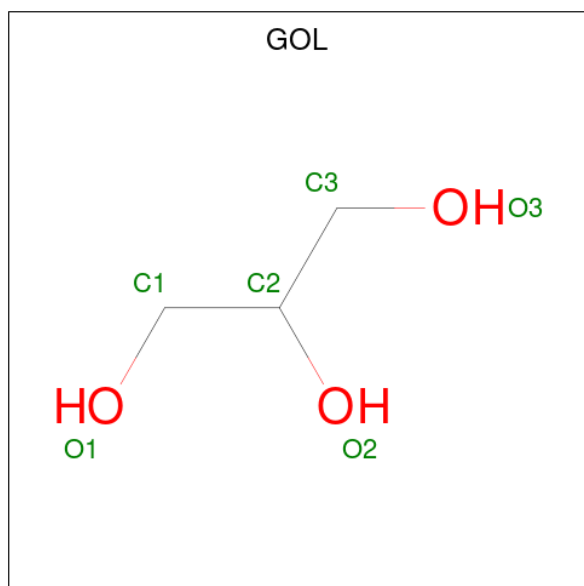
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



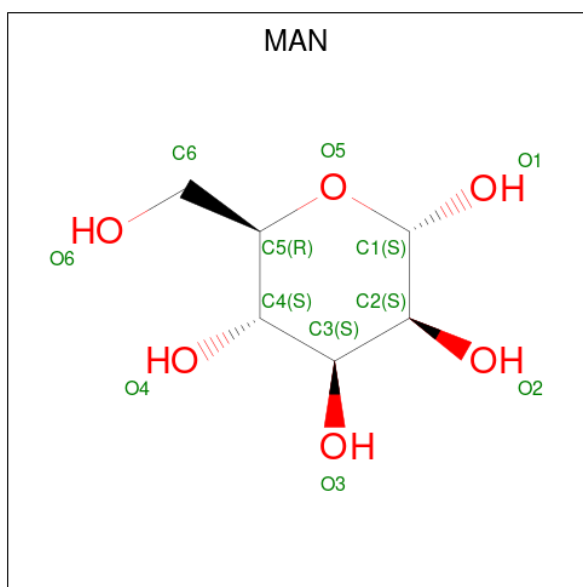
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 11 6 5	0	0
10	A	1	Total C O 11 6 5	0	0
10	A	1	Total C O 11 6 5	0	0
10	A	1	Total C O 11 6 5	0	0
10	B	1	Total C O 11 6 5	0	0
10	B	1	Total C O 11 6 5	0	0
10	D	1	Total C O 11 6 5	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

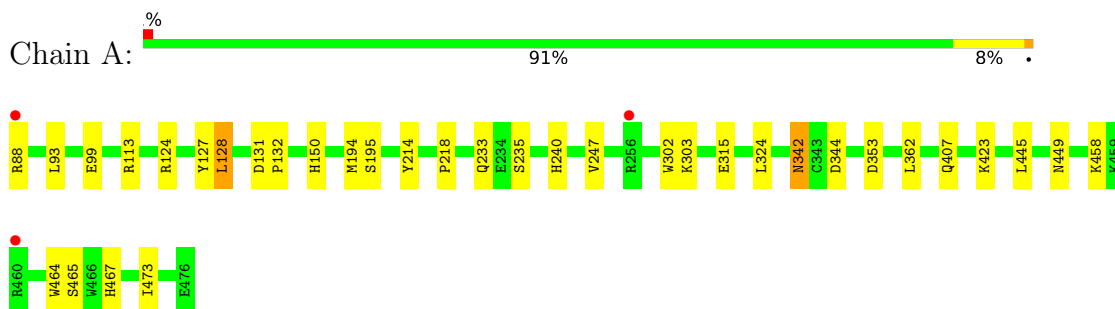
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	460	Total O 460 460	0	0
12	B	442	Total O 442 442	0	0
12	C	454	Total O 454 454	0	0
12	D	442	Total O 442 442	0	0

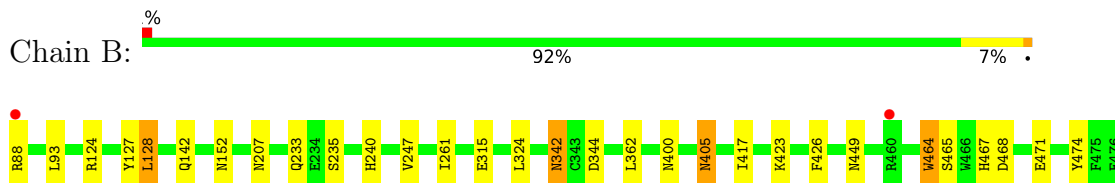
3 Residue-property plots [i](#)

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 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.

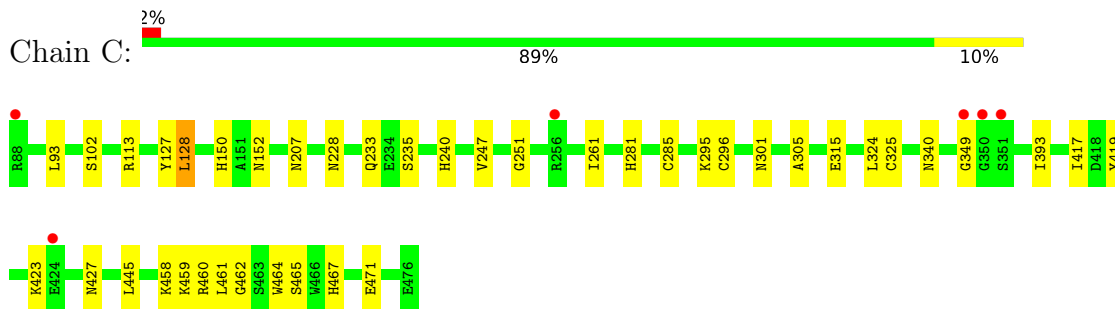
- Molecule 1: NEURAMINIDASE



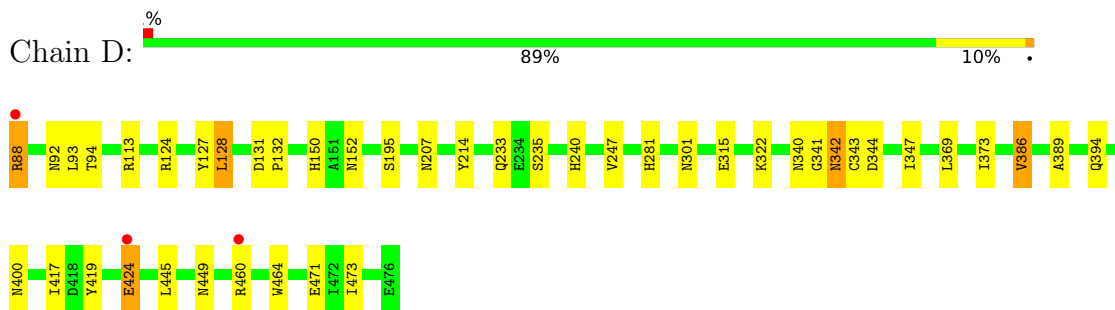
- Molecule 1: NEURAMINIDASE



- Molecule 1: NEURAMINIDASE



- Molecule 1: NEURAMINIDASE




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

Chain E:  50% 50%

 MAG1
MAG2

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

Chain I:  50% 50%

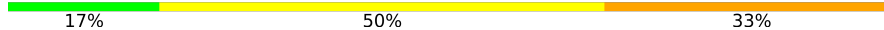
 MAG1
MAG2

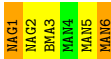
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  25% 50% 25%

 MAG1
MAG2
MAN3
MAN4

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  17% 50% 33%

 MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

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

Chain H:  33% 67%

 MAG1
MAN2
MAN3

- Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain J:  100%

 MAN1
MAN2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.48Å 73.75Å 106.81Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	19.96 – 1.84 19.98 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.84) 93.2 (19.98-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.84Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.149 , 0.190 0.150 , 0.187	Depositor DCC
R_{free} test set	6696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtrriage
Anisotropy	1.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for l,k,-h 0.016 for h,-k,-l 0.012 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14347	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, GOL, NAG, PEG, MAN

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	0/3084	0.67	1/4185 (0.0%)
1	B	0.65	1/3084 (0.0%)	0.67	1/4185 (0.0%)
1	C	0.66	0/3084	0.66	1/4185 (0.0%)
1	D	0.65	0/3084	0.69	1/4185 (0.0%)
All	All	0.65	1/12336 (0.0%)	0.67	4/16740 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	464	TRP	CB-CG	-5.11	1.41	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LEU	CA-CB-CG	7.07	131.57	115.30
1	D	128	LEU	CA-CB-CG	6.70	130.71	115.30
1	B	128	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	128	LEU	CA-CB-CG	6.12	129.38	115.30

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	3009	0	2885	26	0
1	B	3009	0	2888	31	0
1	C	3009	0	2888	53	0
1	D	3009	0	2888	50	0
2	E	28	0	25	0	0
2	I	28	0	25	7	0
3	F	47	0	40	7	0
4	G	72	0	61	8	0
5	H	36	0	31	6	0
6	J	22	0	19	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	6	0	8	2	0
8	B	6	0	8	1	0
8	C	6	0	8	1	0
8	D	6	0	8	0	0
9	A	42	0	39	9	0
9	B	28	0	26	4	0
9	C	42	0	39	5	0
9	D	56	0	52	16	0
10	A	44	0	40	9	0
10	B	22	0	20	1	0
10	D	11	0	10	2	0
11	C	7	0	10	16	0
12	A	460	0	0	5	0
12	B	442	0	0	1	0
12	C	454	0	0	6	0
12	D	442	0	0	1	0
All	All	14347	0	12018	174	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 7.

The worst 5 of 174 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:D:207:ASN:HD21	9:D:508:NAG:C1	1.03	1.63
1:D:152:ASN:HD21	9:D:507:NAG:C1	1.01	1.55
1:B:152:ASN:HD21	9:B:504:NAG:C1	0.97	1.54
1:C:152:ASN:HD21	9:C:506:NAG:C1	0.92	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ASN:HD21	2:I:1:NAG:C1	0.94	1.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	B	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	C	387/389 (100%)	374 (97%)	13 (3%)	0	100	100
1	D	387/389 (100%)	373 (96%)	14 (4%)	0	100	100
All	All	1548/1556 (100%)	1497 (97%)	51 (3%)	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	331/331 (100%)	327 (99%)	4 (1%)	71	61
1	B	331/331 (100%)	325 (98%)	6 (2%)	59	44
1	C	331/331 (100%)	327 (99%)	4 (1%)	71	61
1	D	331/331 (100%)	323 (98%)	8 (2%)	49	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1324/1324 (100%)	1302 (98%)	22 (2%)	60 47

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	88	ARG
1	D	386	VAL
1	D	342	ASN
1	D	424	GLU
1	B	142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	ASN
1	C	406	ASN
1	D	422	ASN
1	C	207	ASN
1	C	281	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](#)

19 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	E	1	2,1	14,14,15	0.64	0	17,19,21	0.93	0
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	0.77	1 (5%)
3	NAG	F	1	3	14,14,15	0.59	0	17,19,21	0.65	0
3	BMA	F	2	3	11,11,12	0.26	0	15,15,17	1.20	2 (13%)
3	MAN	F	3	3	11,11,12	0.41	0	15,15,17	0.86	0
3	MAN	F	4	3	11,11,12	0.54	0	15,15,17	1.45	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.77	0	17,19,21	2.50	6 (35%)
4	NAG	G	2	4	14,14,15	0.61	0	17,19,21	1.41	2 (11%)
4	BMA	G	3	4	11,11,12	0.56	0	15,15,17	0.99	1 (6%)
4	MAN	G	4	4	11,11,12	0.51	0	15,15,17	0.86	0
4	MAN	G	5	4	11,11,12	0.43	0	15,15,17	0.94	1 (6%)
4	MAN	G	6	4	11,11,12	0.38	0	15,15,17	1.34	2 (13%)
5	NAG	H	1	5	14,14,15	0.68	0	17,19,21	2.54	6 (35%)
5	BMA	H	2	5	11,11,12	0.42	0	15,15,17	1.16	1 (6%)
5	MAN	H	3	5	11,11,12	0.41	0	15,15,17	1.07	1 (6%)
2	NAG	I	1	2	14,14,15	0.63	0	17,19,21	1.56	3 (17%)
2	NAG	I	2	2	14,14,15	0.61	0	17,19,21	0.63	0
6	BMA	J	1	6	11,11,12	0.45	0	15,15,17	1.13	2 (13%)
6	MAN	J	2	6	11,11,12	0.50	0	15,15,17	1.61	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	H	2	5	-	0/2/19/22	0/1/1/1
5	MAN	H	3	5	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
6	BMA	J	1	6	-	0/2/19/22	0/1/1/1
6	MAN	J	2	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C3-C4-C5	-6.03	99.49	110.24
5	H	1	NAG	C4-C3-C2	-5.51	102.94	111.02
4	G	1	NAG	O5-C5-C6	5.18	115.32	107.20
5	H	1	NAG	C2-N2-C7	4.49	129.29	122.90
5	H	1	NAG	O5-C1-C2	-4.32	104.47	111.29

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

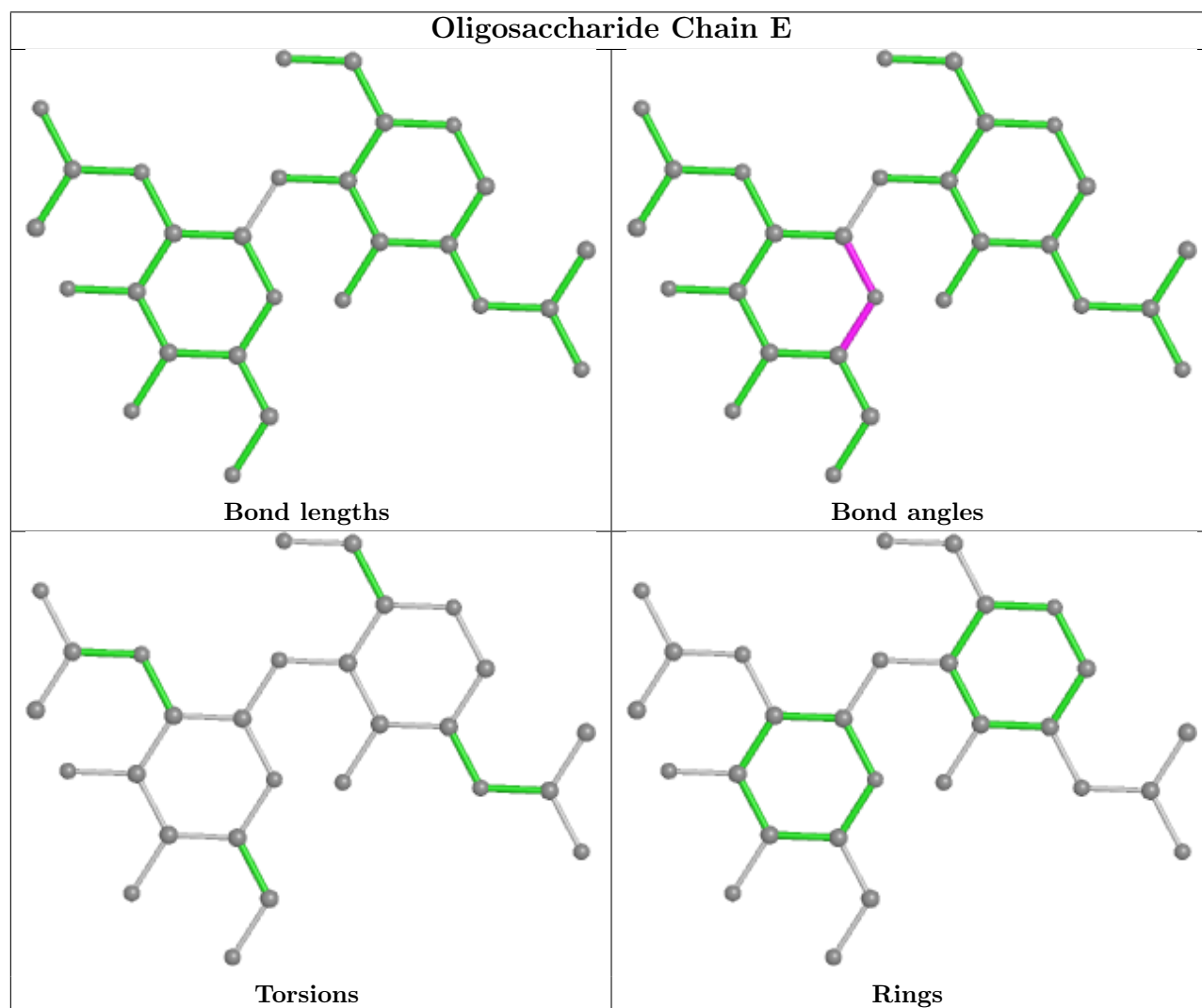
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	1	NAG	O5-C5-C6-O6
3	F	3	MAN	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6

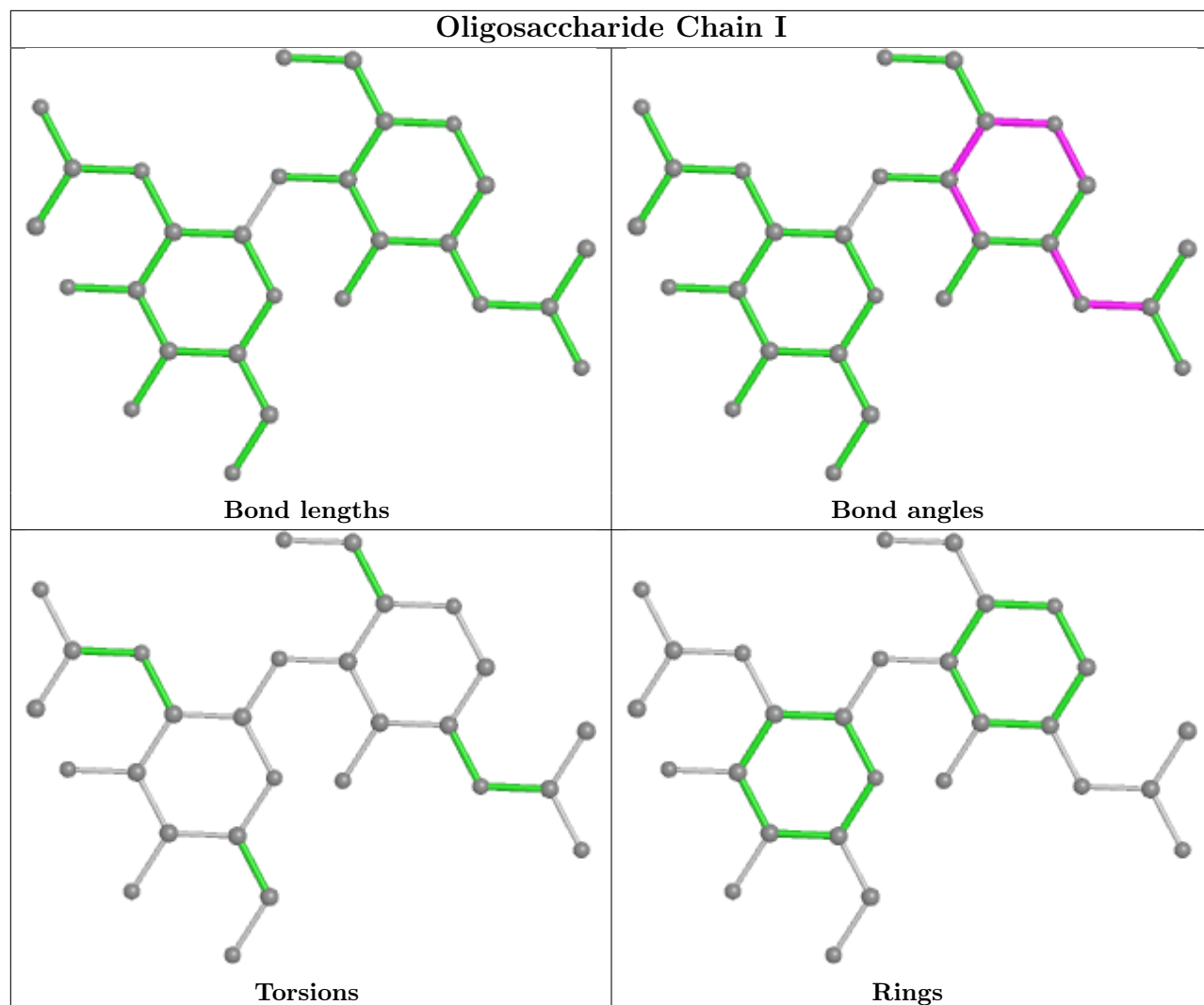
There are no ring outliers.

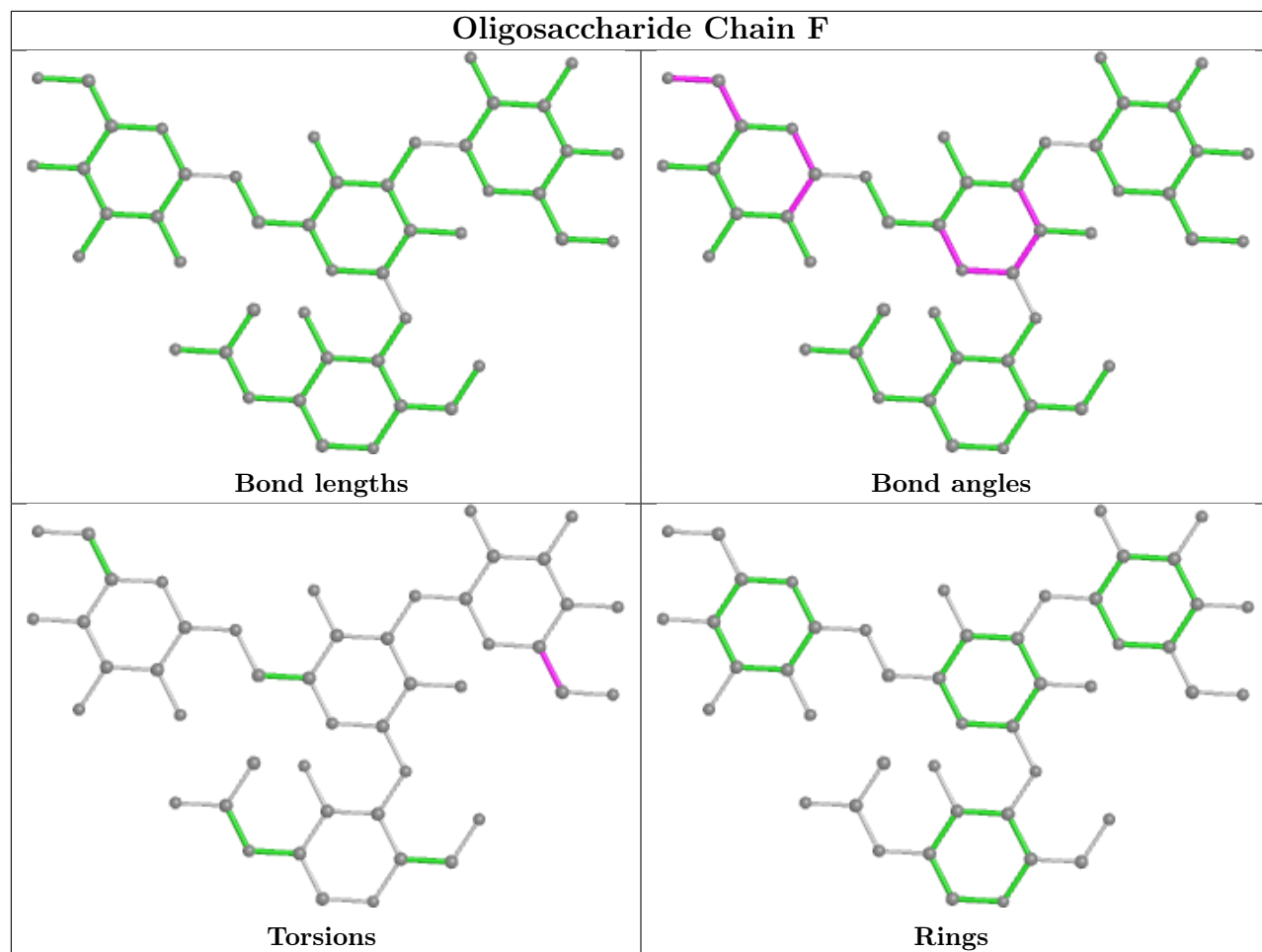
10 monomers are involved in 30 short contacts:

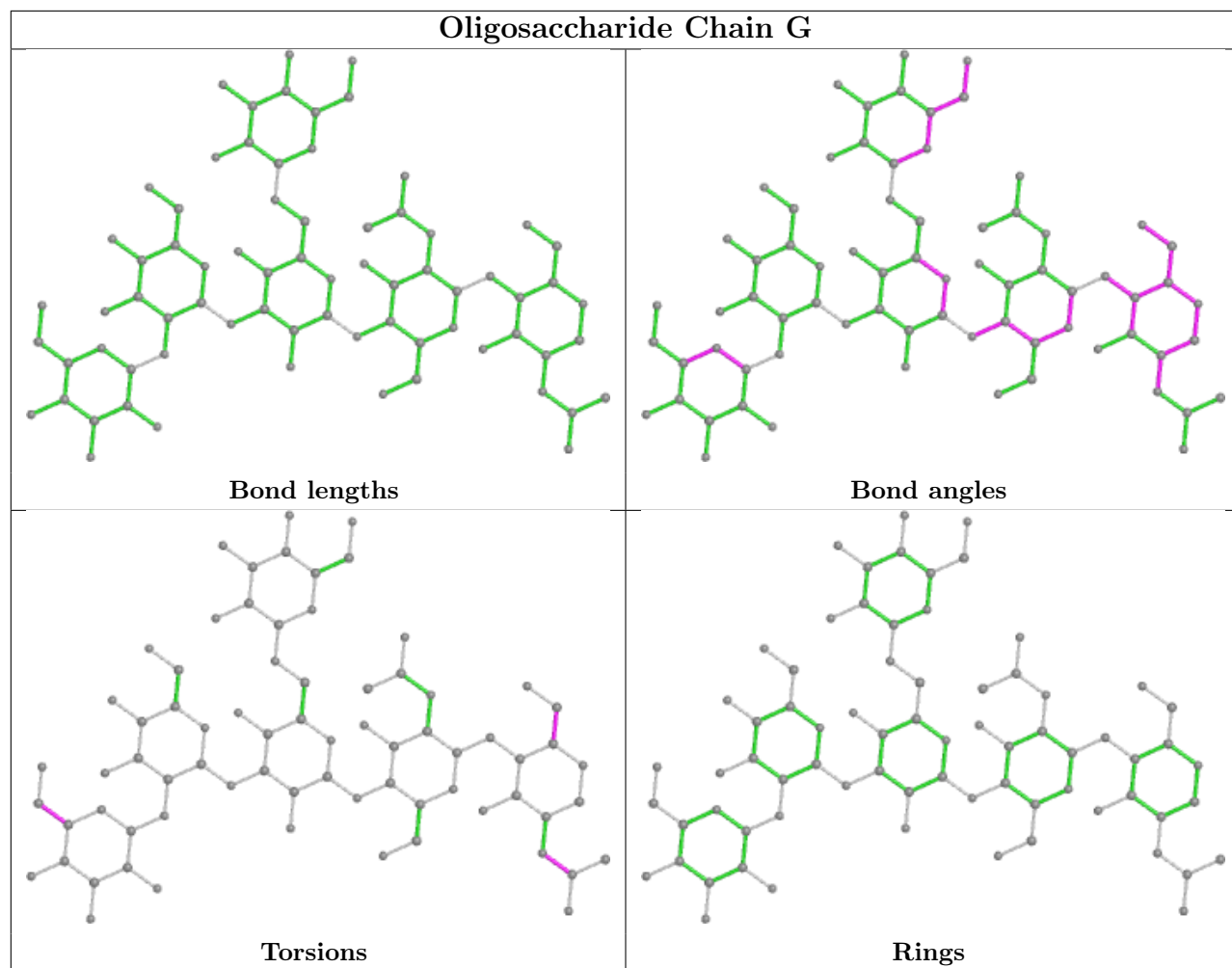
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	3	0
5	H	3	MAN	1	0
6	J	2	MAN	2	0
5	H	1	NAG	5	0
3	F	1	NAG	3	0
3	F	4	MAN	4	0
6	J	1	BMA	3	0
2	I	1	NAG	4	0
4	G	1	NAG	3	0
4	G	6	MAN	5	0

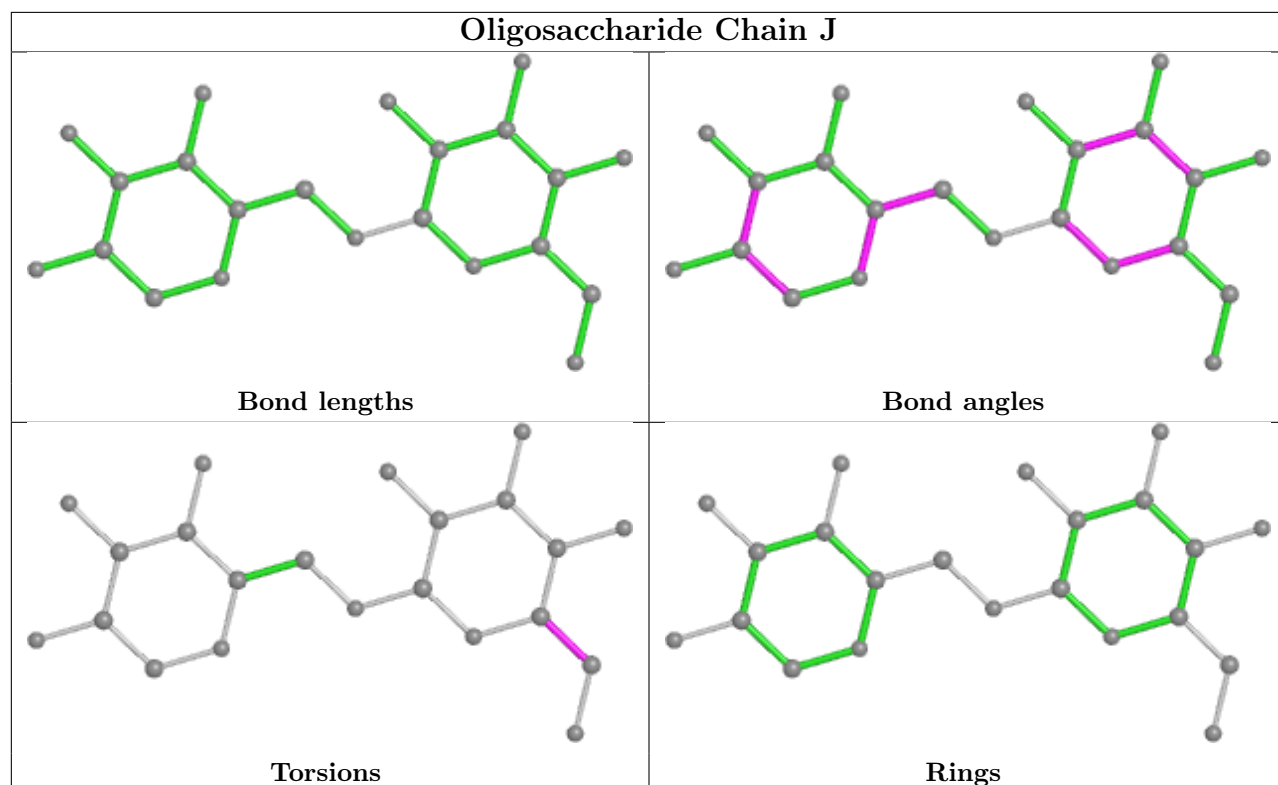
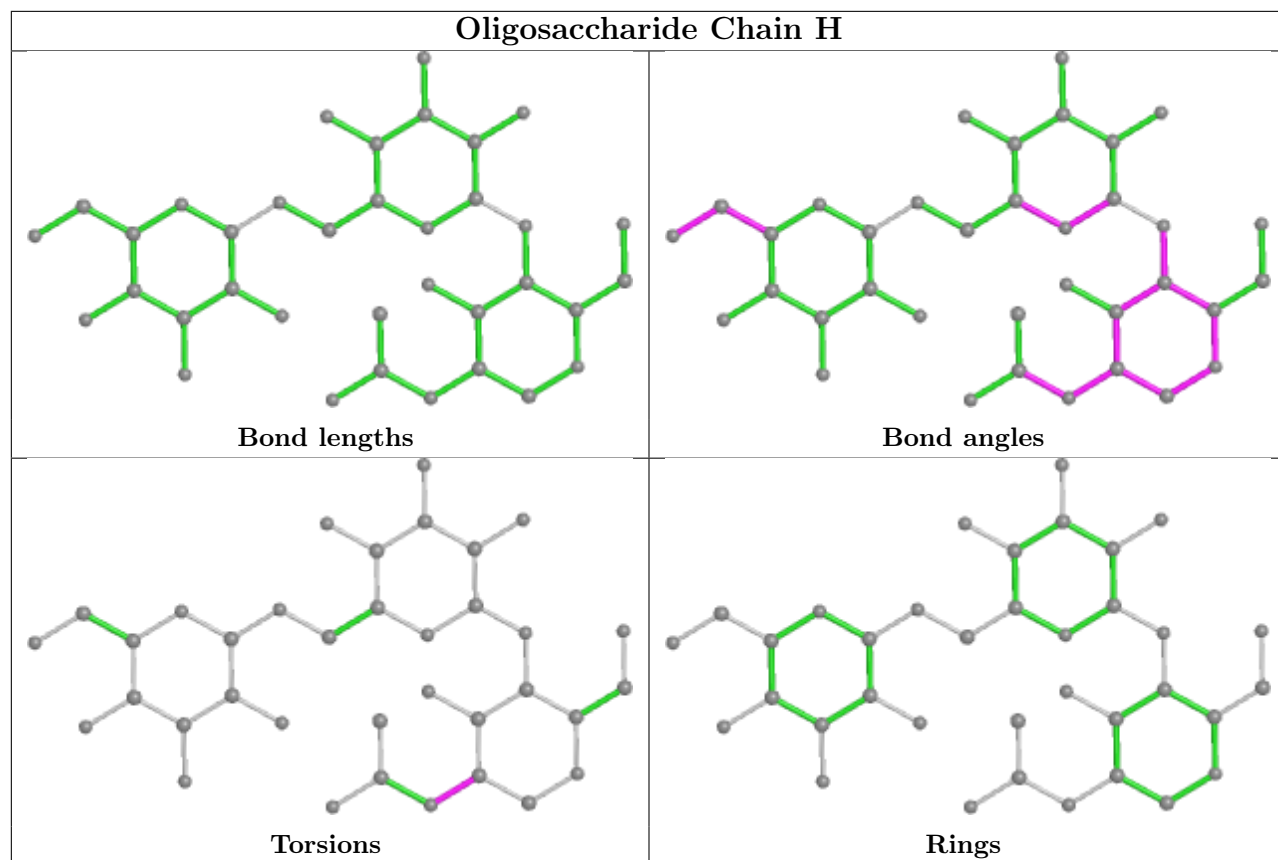
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	A	521	-	11,11,12	0.59	0	15,15,17	1.78	4 (26%)
9	NAG	D	508	-	14,14,15	0.64	0	17,19,21	1.69	3 (17%)
10	MAN	A	514	-	11,11,12	0.43	0	15,15,17	1.55	2 (13%)
10	MAN	B	506	-	11,11,12	0.37	0	15,15,17	1.14	1 (6%)
9	NAG	A	506	-	14,14,15	0.58	0	17,19,21	1.66	3 (17%)
11	PEG	C	503	-	6,6,6	0.27	0	5,5,5	6.29	5 (100%)
10	MAN	A	509	-	11,11,12	0.52	0	15,15,17	1.39	2 (13%)
9	NAG	C	505	-	14,14,15	0.56	0	17,19,21	1.49	5 (29%)
9	NAG	D	507	-	14,14,15	0.60	0	17,19,21	1.20	2 (11%)
9	NAG	C	506	-	14,14,15	0.67	0	17,19,21	1.11	1 (5%)
9	NAG	A	505	1	14,14,15	0.63	0	17,19,21	0.91	0
10	MAN	D	509	-	11,11,12	0.59	0	15,15,17	1.22	2 (13%)
10	MAN	A	508	-	11,11,12	0.37	0	15,15,17	1.44	2 (13%)
9	NAG	A	513	-	14,14,15	0.52	0	17,19,21	1.12	2 (11%)
9	NAG	D	506	-	14,14,15	0.46	0	17,19,21	1.07	1 (5%)
9	NAG	D	501	-	14,14,15	0.50	0	17,19,21	0.93	1 (5%)
8	GOL	B	502	-	5,5,5	1.72	1 (20%)	5,5,5	2.12	2 (40%)
8	GOL	C	504	-	5,5,5	1.62	1 (20%)	5,5,5	2.10	2 (40%)
8	GOL	A	502	-	5,5,5	1.20	0	5,5,5	1.83	1 (20%)
10	MAN	B	509	-	11,11,12	0.50	0	15,15,17	1.87	3 (20%)
8	GOL	D	505	-	5,5,5	1.38	0	5,5,5	1.88	1 (20%)
9	NAG	C	501	-	14,14,15	0.54	0	17,19,21	1.21	2 (11%)
9	NAG	B	504	-	14,14,15	0.71	0	17,19,21	1.06	2 (11%)
9	NAG	B	503	-	14,14,15	0.45	0	17,19,21	1.33	3 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	A	521	-	-	0/2/19/22	0/1/1/1
9	NAG	D	508	-	-	0/6/23/26	0/1/1/1
10	MAN	A	514	-	-	2/2/19/22	0/1/1/1
10	MAN	B	506	-	-	0/2/19/22	0/1/1/1
9	NAG	A	506	-	-	4/6/23/26	0/1/1/1
11	PEG	C	503	-	-	2/4/4/4	-
10	MAN	A	509	-	-	0/2/19/22	0/1/1/1
9	NAG	C	505	-	-	2/6/23/26	0/1/1/1
9	NAG	D	507	-	-	0/6/23/26	0/1/1/1
9	NAG	C	506	-	-	0/6/23/26	0/1/1/1
9	NAG	A	505	1	-	0/6/23/26	0/1/1/1
10	MAN	D	509	-	-	2/2/19/22	0/1/1/1
10	MAN	A	508	-	-	1/2/19/22	0/1/1/1
9	NAG	A	513	-	-	4/6/23/26	0/1/1/1
9	NAG	D	506	-	-	2/6/23/26	0/1/1/1
9	NAG	D	501	-	-	4/6/23/26	0/1/1/1
8	GOL	B	502	-	-	0/4/4/4	-
8	GOL	C	504	-	-	1/4/4/4	-
8	GOL	A	502	-	-	1/4/4/4	-
10	MAN	B	509	-	-	0/2/19/22	0/1/1/1
8	GOL	D	505	-	-	1/4/4/4	-
9	NAG	C	501	-	-	1/6/23/26	0/1/1/1
9	NAG	B	504	-	-	0/6/23/26	0/1/1/1
9	NAG	B	503	-	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	GOL	O3-C3	2.69	1.53	1.42
8	C	504	GOL	O3-C3	2.33	1.52	1.42

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	503	PEG	O1-C1-C2	9.11	164.65	111.81
11	C	503	PEG	O2-C2-C1	7.83	144.49	110.07
11	C	503	PEG	C3-O2-C2	-6.14	86.66	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	509	MAN	C1-O5-C5	4.93	118.86	112.19
10	A	514	MAN	C1-O5-C5	4.73	118.59	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	506	NAG	C8-C7-N2-C2
9	A	506	NAG	O7-C7-N2-C2
9	B	503	NAG	C8-C7-N2-C2
9	B	503	NAG	O7-C7-N2-C2
9	D	501	NAG	C8-C7-N2-C2

There are no ring outliers.

17 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	521	MAN	3	0
9	D	508	NAG	8	0
10	A	514	MAN	2	0
10	B	506	MAN	1	0
9	A	506	NAG	9	0
11	C	503	PEG	16	0
10	A	509	MAN	2	0
9	D	507	NAG	4	0
9	C	506	NAG	5	0
10	D	509	MAN	2	0
10	A	508	MAN	2	0
9	D	506	NAG	3	0
9	D	501	NAG	1	0
8	B	502	GOL	1	0
8	C	504	GOL	1	0
8	A	502	GOL	2	0
9	B	504	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	389/389 (100%)	-0.48	3 (0%) 86 86	7, 12, 20, 31	0
1	B	389/389 (100%)	-0.49	2 (0%) 91 91	7, 12, 18, 37	0
1	C	389/389 (100%)	-0.52	6 (1%) 73 73	7, 11, 19, 33	0
1	D	389/389 (100%)	-0.47	3 (0%) 86 86	7, 12, 18, 33	0
All	All	1556/1556 (100%)	-0.49	14 (0%) 84 84	7, 12, 19, 37	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ARG	4.3
1	C	350	GLY	3.5
1	C	349	GLY	3.2
1	A	88	ARG	3.2
1	C	88	ARG	2.9

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
6	MAN	J	2	11/12	0.60	0.42	45,49,51,51	0
2	NAG	E	2	14/15	0.68	0.45	39,43,45,45	0

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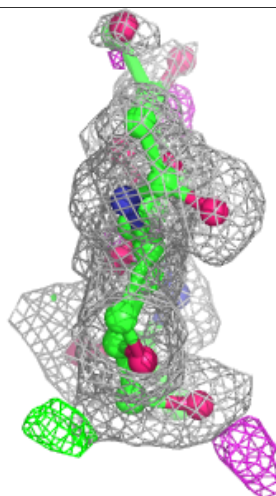
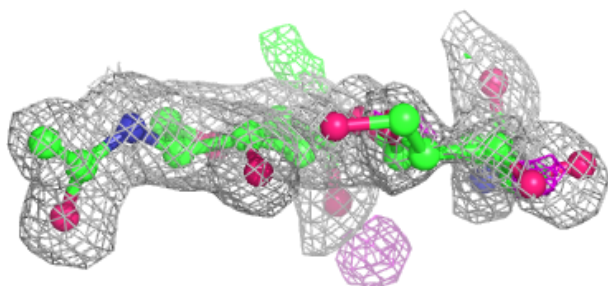
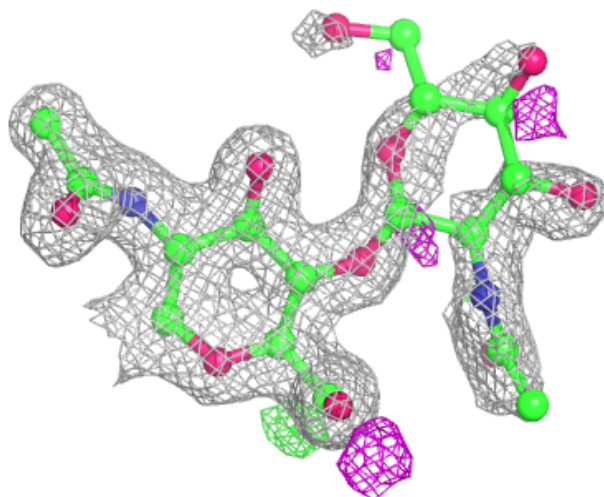
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	H	1	14/15	0.69	0.26	26,35,39,43	0
3	MAN	F	3	11/12	0.75	0.44	45,48,49,50	0
3	NAG	F	1	14/15	0.80	0.28	20,24,27,30	0
2	NAG	I	2	14/15	0.81	0.21	18,24,29,33	0
4	NAG	G	1	14/15	0.81	0.32	26,31,35,38	0
5	MAN	H	3	11/12	0.82	0.26	35,37,37,37	0
4	MAN	G	5	11/12	0.84	0.41	38,42,44,44	0
6	BMA	J	1	11/12	0.85	0.28	32,35,36,40	0
5	BMA	H	2	11/12	0.85	0.24	35,36,37,38	0
2	NAG	I	1	14/15	0.86	0.24	25,29,32,34	0
3	MAN	F	4	11/12	0.90	0.20	22,24,24,27	0
2	NAG	E	1	14/15	0.90	0.16	20,22,26,32	0
4	NAG	G	2	14/15	0.92	0.15	14,20,24,25	0
4	MAN	G	4	11/12	0.94	0.13	24,25,27,27	0
3	BMA	F	2	11/12	0.94	0.21	21,25,26,31	0
4	MAN	G	6	11/12	0.94	0.14	14,15,16,19	0
4	BMA	G	3	11/12	0.94	0.13	16,19,19,21	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.

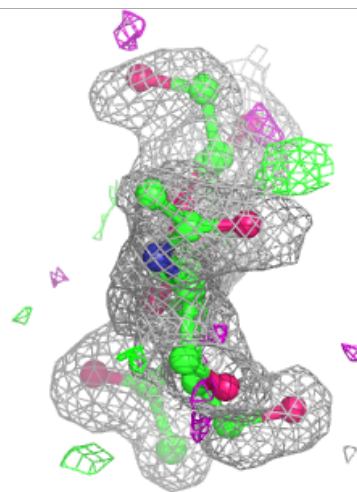
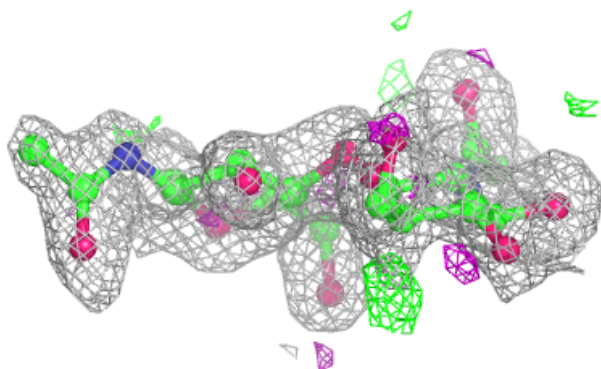
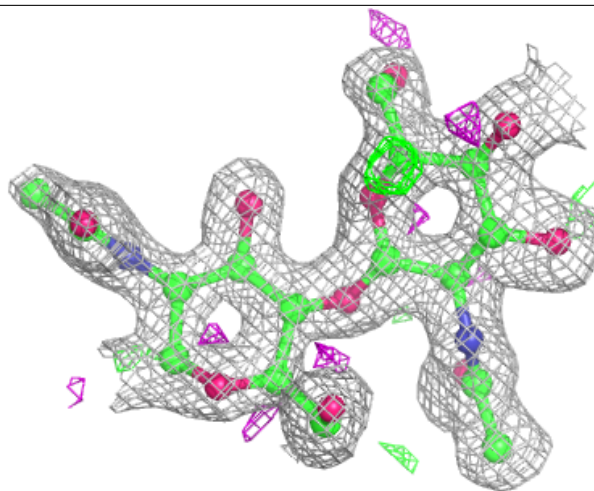
Electron density around Chain E:

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



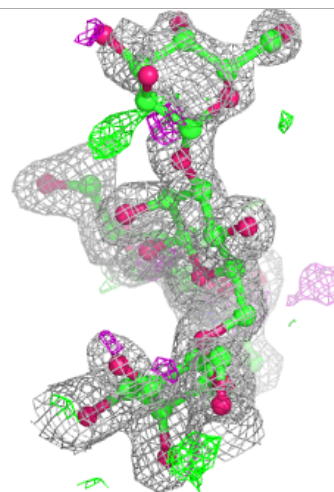
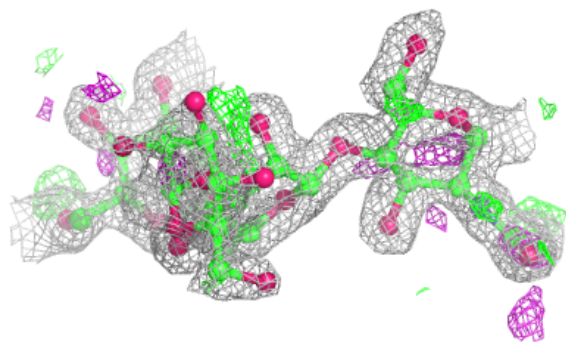
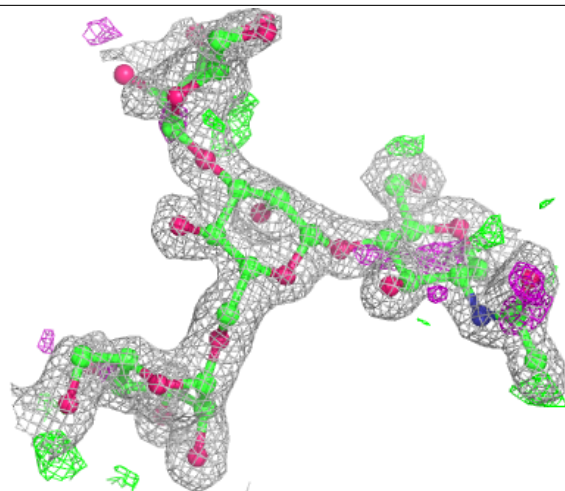
Electron density around Chain I:

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



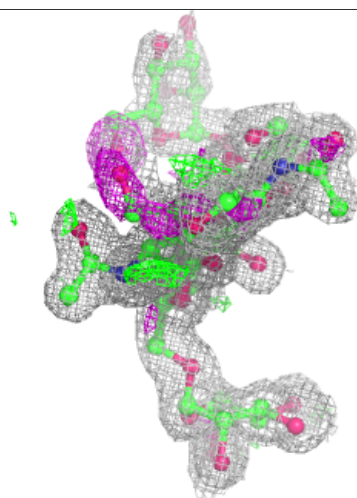
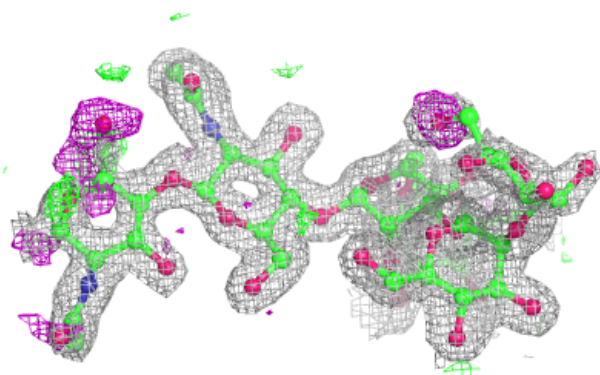
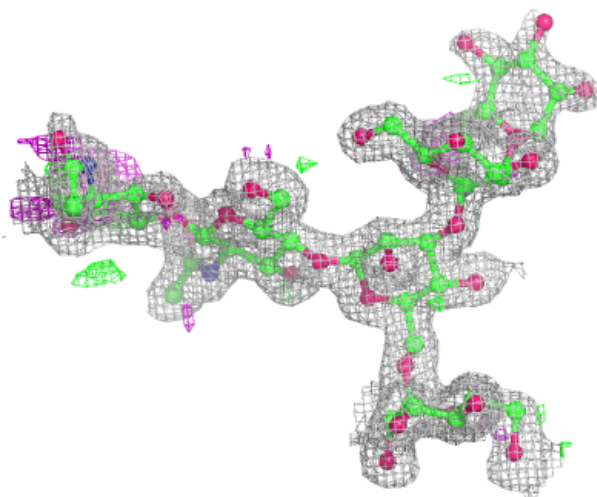
Electron density around Chain F:

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



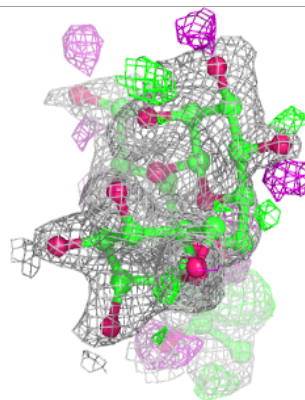
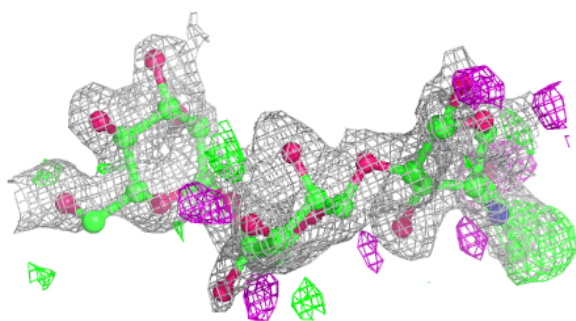
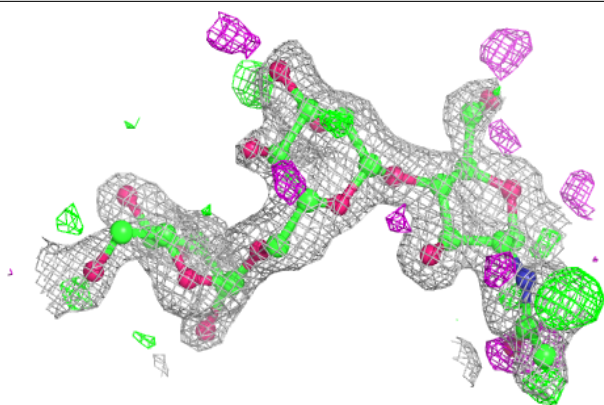
Electron density around Chain G:

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

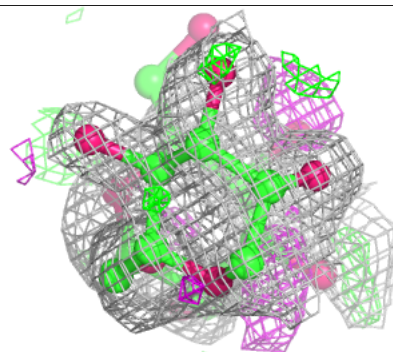
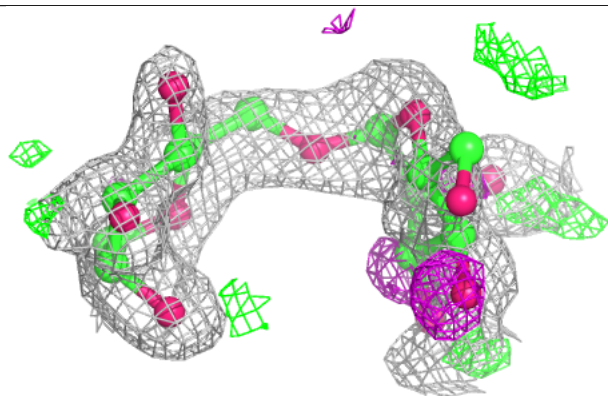
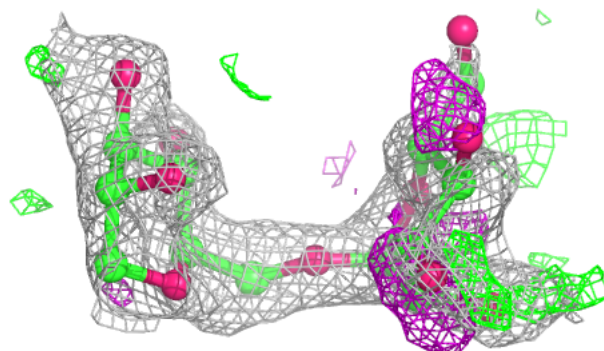


Electron density around Chain H:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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
9	NAG	A	513	14/15	0.15	0.47	95,96,97,97	0
9	NAG	B	503	14/15	0.31	0.43	98,99,99,99	0
9	NAG	D	501	14/15	0.42	0.37	74,77,77,77	0
9	NAG	C	505	14/15	0.46	0.37	62,63,64,64	0
9	NAG	C	501	14/15	0.47	0.49	64,67,68,68	0
9	NAG	D	506	14/15	0.50	0.43	105,105,106,106	0
10	MAN	D	509	11/12	0.53	0.39	67,68,68,68	0
8	GOL	B	502	6/6	0.67	0.29	12,25,26,28	0
11	PEG	C	503	7/7	0.67	0.25	20,24,28,29	0
8	GOL	A	502	6/6	0.69	0.25	19,29,30,31	0
8	GOL	D	505	6/6	0.73	0.29	17,29,30,30	0
9	NAG	A	506	14/15	0.73	0.30	42,44,45,45	0
10	MAN	B	509	11/12	0.74	0.33	44,47,48,49	0
8	GOL	C	504	6/6	0.76	0.26	13,26,28,29	0
10	MAN	B	506	11/12	0.79	0.29	32,33,36,38	0
10	MAN	A	508	11/12	0.81	0.20	26,30,35,38	0
9	NAG	D	508	14/15	0.82	0.21	23,26,27,27	0
10	MAN	A	509	11/12	0.85	0.18	24,27,28,29	0
10	MAN	A	514	11/12	0.85	0.19	30,33,36,38	0
9	NAG	A	505	14/15	0.89	0.16	19,22,27,28	0
9	NAG	B	504	14/15	0.90	0.15	16,22,26,29	0
10	MAN	A	521	11/12	0.91	0.14	19,20,21,21	0
9	NAG	D	507	14/15	0.92	0.15	17,22,26,26	0
9	NAG	C	506	14/15	0.93	0.13	15,18,25,26	0
7	CA	C	502	1/1	0.98	0.17	19,19,19,19	0
7	CA	B	501	1/1	0.99	0.09	19,19,19,19	0
7	CA	A	501	1/1	0.99	0.14	20,20,20,20	0
7	CA	D	504	1/1	0.99	0.14	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.