



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:06 PM UTC

PDB ID : 9NRR / pdb_00009nrr
Title : Crystal structure of the H5 influenza virus hemagglutinin from A/duck/France/161108h/2016 (H5N8) clade 2.3.4.4b
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2025-03-14
Resolution : 1.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

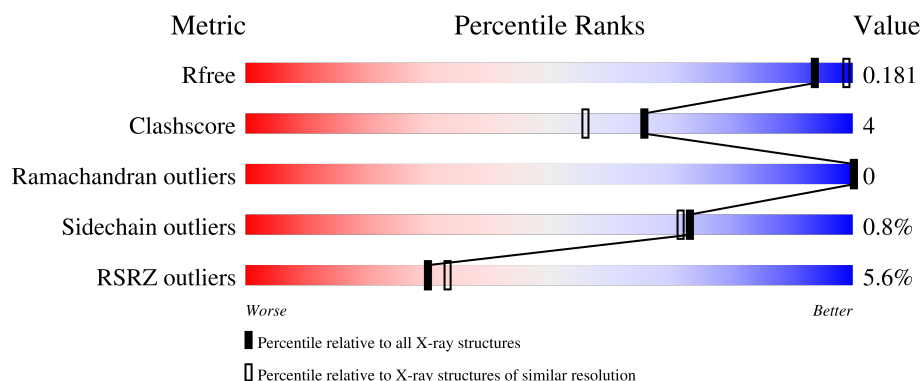
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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.



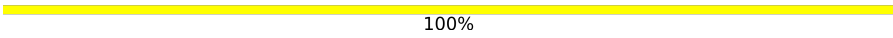
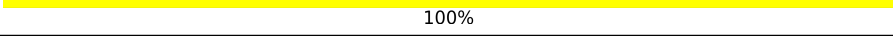
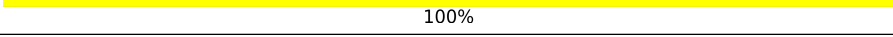
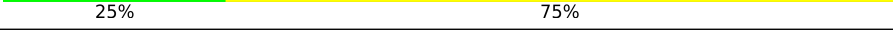
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	329	6% 89% 7% ..
1	C	329	4% 91% 6% ..
1	E	329	5% 90% 8% ..
2	B	181	7% 84% 9% 7%
2	D	181	7% 85% 8% 7%

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Mol	Chain	Length	Quality of chain
2	F	181	
3	G	5	
4	H	3	
5	I	3	
5	L	3	
6	J	4	
7	K	2	
8	M	3	
9	N	4	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 14217 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2537	1605	442	476	14			
1	C	323	Total	C	N	O	S	0	0	0
			2555	1619	444	478	14			
1	E	322	Total	C	N	O	S	0	0	0
			2545	1609	443	479	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	-	expression tag	UNP A0A6M2RJB8
A	9	PRO	-	expression tag	UNP A0A6M2RJB8
A	10	GLY	-	expression tag	UNP A0A6M2RJB8
C	8	ASP	-	expression tag	UNP A0A6M2RJB8
C	9	PRO	-	expression tag	UNP A0A6M2RJB8
C	10	GLY	-	expression tag	UNP A0A6M2RJB8
E	8	ASP	-	expression tag	UNP A0A6M2RJB8
E	9	PRO	-	expression tag	UNP A0A6M2RJB8
E	10	GLY	-	expression tag	UNP A0A6M2RJB8

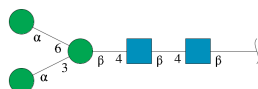
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	D	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	F	172	Total	C	N	O	S	0	0	0
			1399	866	246	279	8			

There are 21 discrepancies between the modelled and reference sequences:

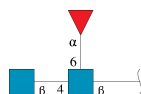
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6M2RJB8
B	176	GLY	-	expression tag	UNP A0A6M2RJB8
B	177	ARG	-	expression tag	UNP A0A6M2RJB8
B	178	LEU	-	expression tag	UNP A0A6M2RJB8
B	179	VAL	-	expression tag	UNP A0A6M2RJB8
B	180	PRO	-	expression tag	UNP A0A6M2RJB8
B	181	ARG	-	expression tag	UNP A0A6M2RJB8
D	175	SER	-	expression tag	UNP A0A6M2RJB8
D	176	GLY	-	expression tag	UNP A0A6M2RJB8
D	177	ARG	-	expression tag	UNP A0A6M2RJB8
D	178	LEU	-	expression tag	UNP A0A6M2RJB8
D	179	VAL	-	expression tag	UNP A0A6M2RJB8
D	180	PRO	-	expression tag	UNP A0A6M2RJB8
D	181	ARG	-	expression tag	UNP A0A6M2RJB8
F	175	SER	-	expression tag	UNP A0A6M2RJB8
F	176	GLY	-	expression tag	UNP A0A6M2RJB8
F	177	ARG	-	expression tag	UNP A0A6M2RJB8
F	178	LEU	-	expression tag	UNP A0A6M2RJB8
F	179	VAL	-	expression tag	UNP A0A6M2RJB8
F	180	PRO	-	expression tag	UNP A0A6M2RJB8
F	181	ARG	-	expression tag	UNP A0A6M2RJB8

- 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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



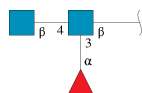
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



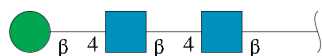
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



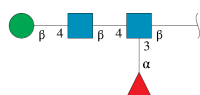
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 8 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.



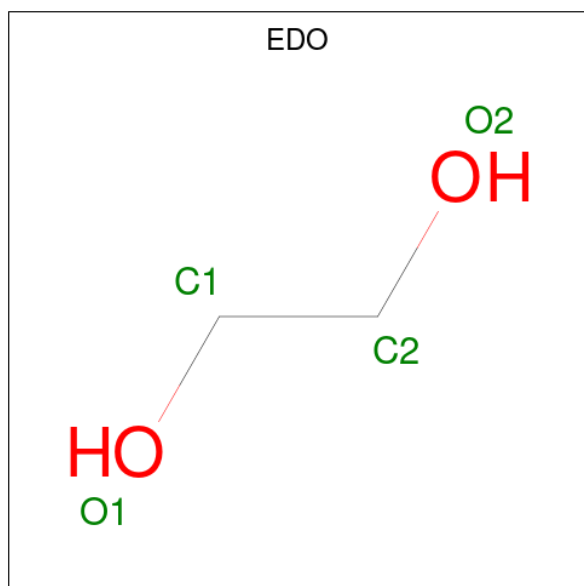
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

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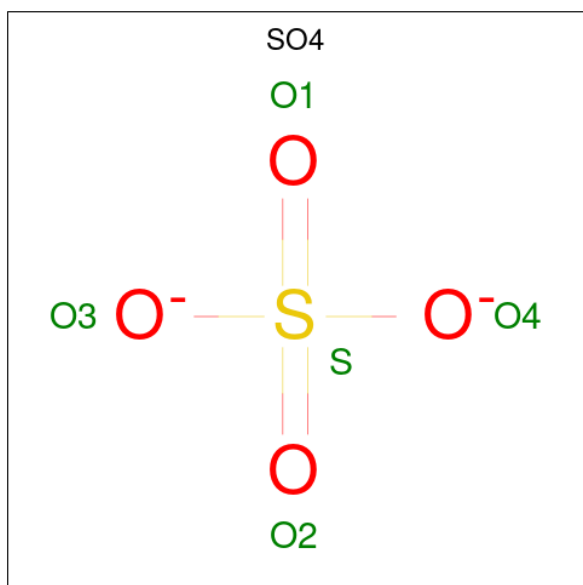
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	B	1	Total 4	C 2	O 2	0	0
10	B	1	Total 4	C 2	O 2	0	0
10	C	1	Total 4	C 2	O 2	0	0
10	C	1	Total 4	C 2	O 2	0	0
10	C	1	Total 4	C 2	O 2	0	0
10	C	1	Total 4	C 2	O 2	0	0
10	C	1	Total 4	C 2	O 2	0	0
10	C	1	Total 4	C 2	O 2	0	0
10	D	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	E	1	Total 4	C 2	O 2	0	0
10	F	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



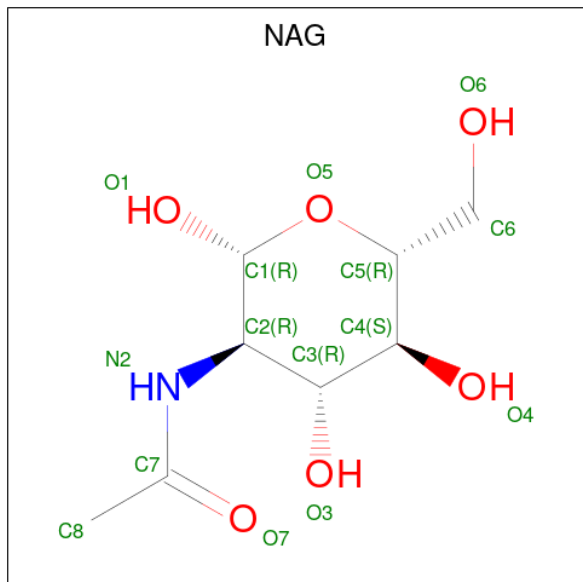
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		

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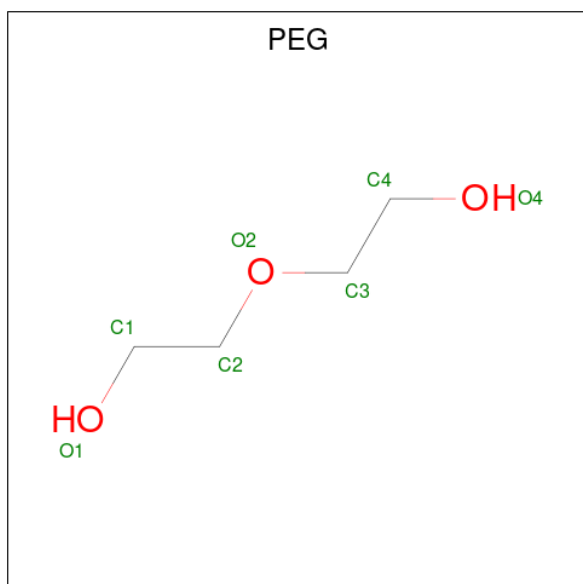
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	C	1	Total	O	S	0	0
			5	4	1		
11	C	1	Total	O	S	0	0
			5	4	1		
11	C	1	Total	O	S	0	0
			5	4	1		
11	C	1	Total	O	S	0	0
			5	4	1		
11	C	1	Total	O	S	0	0
			5	4	1		
11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

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

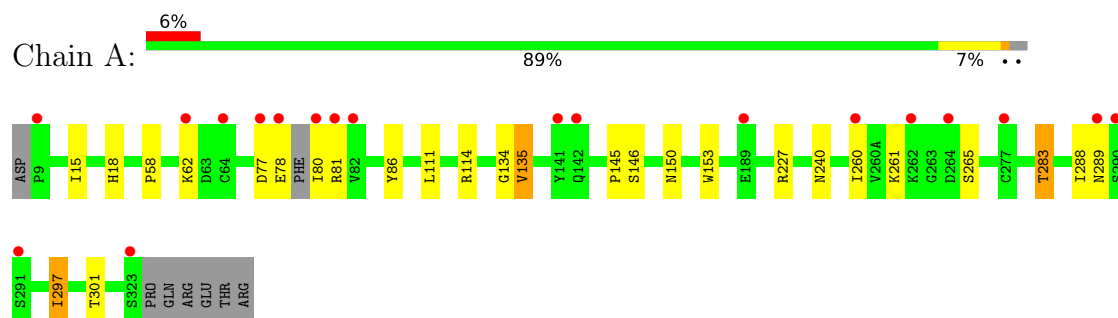
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	390	Total	O	0	0
			390	390		
14	B	187	Total	O	0	0
			187	187		
14	C	416	Total	O	0	0
			416	416		
14	D	146	Total	O	0	0
			146	146		
14	E	433	Total	O	0	0
			433	433		
14	F	238	Total	O	0	0
			238	238		

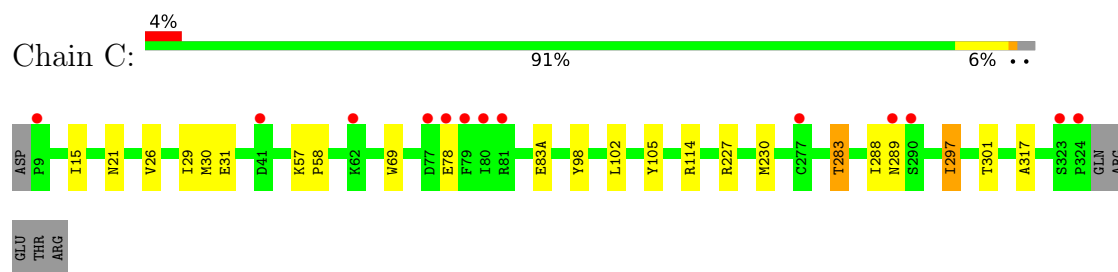
3 Residue-property plots [i](#)

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.

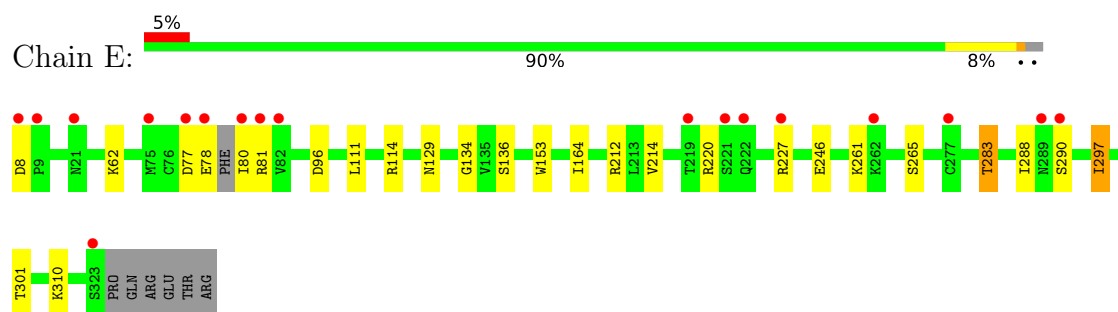
- Molecule 1: Hemagglutinin HA1 chain



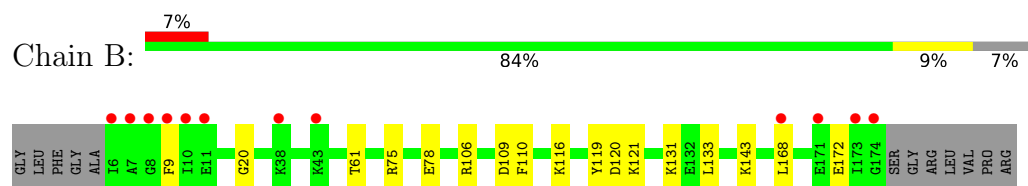
- Molecule 1: Hemagglutinin HA1 chain



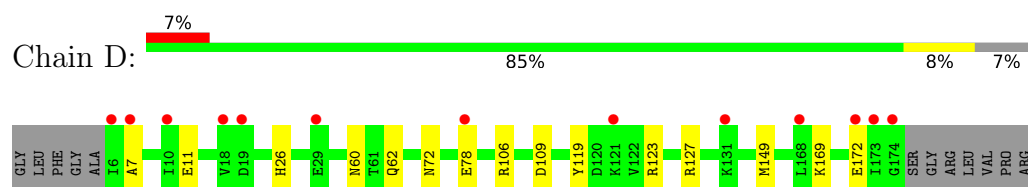
- Molecule 1: Hemagglutinin HA1 chain



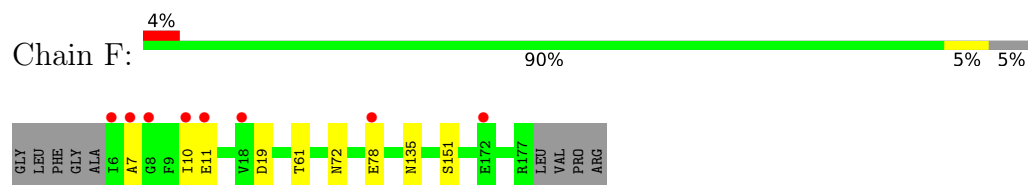
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



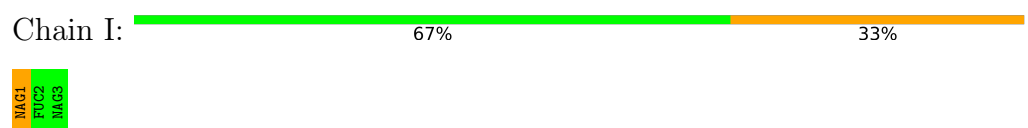
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



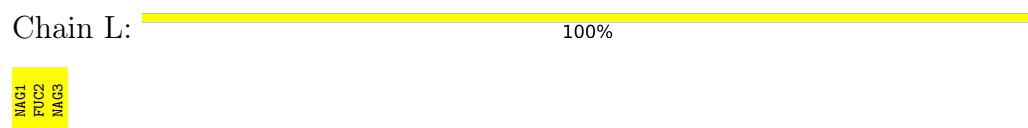
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain J:  100%

MAG1
MAG2
BMA3
MAN4

- Molecule 7: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50%

MAG1
FUC2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33%

MAG1
MAG2
BMA3

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  25%

MAG1
MAG2
BMA3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.38Å 171.60Å 226.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 1.94 45.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.56-1.94) 99.8 (45.56-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.167 , 0.188 (Not available) , 0.181	Depositor DCC
R_{free} test set	13571 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14217	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: EDO, MAN, SO4, PEG, FUC, NAG, 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	A	0.28	0/2599	0.49	0/3533
1	C	0.32	0/2620	0.51	0/3564
1	E	0.33	0/2607	0.51	0/3545
2	B	0.27	0/1404	0.42	0/1887
2	D	0.23	0/1404	0.41	0/1887
2	F	0.27	0/1425	0.43	0/1914
All	All	0.29	0/12059	0.48	0/16330

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	2537	0	2492	22	0
1	C	2555	0	2509	19	0
1	E	2545	0	2495	23	0
2	B	1378	0	1282	12	0
2	D	1378	0	1282	11	0
2	F	1399	0	1303	7	0
3	G	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	38	0	34	0	0
5	I	38	0	34	1	0
5	L	38	0	34	0	0
6	J	50	0	43	0	0
7	K	24	0	22	0	0
8	M	39	0	34	0	0
9	N	49	0	43	1	0
10	A	24	0	36	1	0
10	B	8	0	12	1	0
10	C	24	0	36	5	0
10	D	4	0	6	2	0
10	E	28	0	42	4	0
10	F	12	0	18	2	0
11	A	55	0	0	1	0
11	B	5	0	0	0	0
11	C	50	0	0	1	0
11	D	10	0	0	0	0
11	E	30	0	0	1	0
12	E	14	0	13	0	0
13	E	14	0	20	5	0
14	A	390	0	0	5	0
14	B	187	0	0	2	0
14	C	416	0	0	7	0
14	D	146	0	0	0	0
14	E	433	0	0	6	0
14	F	238	0	0	2	0
All	All	14217	0	11842	92	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 4.

All (92) 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:F:72:ASN:H	10:F:201:EDO:H11	1.47	0.78
1:A:77:ASP:HB2	1:A:80:ILE:HD11	1.73	0.71
1:C:69:TRP:HD1	10:C:405:EDO:H21	1.55	0.71
1:A:80:ILE:HG22	1:A:81:ARG:H	1.55	0.71
1:E:8:ASP:N	14:E:704:HOH:O	2.23	0.70
1:E:111:LEU:HD12	1:E:261:LYS:HD2	1.74	0.70
2:D:72:ASN:H	10:D:301:EDO:H12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:GLU:O	14:E:701:HOH:O	2.11	0.67
1:C:288:ILE:HG21	1:C:297:ILE:HD13	1.77	0.66
1:C:98:TYR:CD1	1:C:230:MET:HG3	2.31	0.66
2:D:106:ARG:NH2	2:D:109:ASP:OD2	2.30	0.65
1:E:212:ARG:NH1	14:E:709:HOH:O	2.29	0.65
2:F:19:ASP:HB2	10:F:203:EDO:H21	1.78	0.64
2:F:10:ILE:HG12	2:F:135:ASN:HA	1.79	0.63
14:A:567:HOH:O	2:B:61:THR:HG22	1.98	0.62
1:E:62:LYS:HB2	10:E:605:EDO:H22	1.82	0.61
1:E:77:ASP:HB3	1:E:80:ILE:HG12	1.82	0.60
1:C:289:ASN:ND2	14:C:508:HOH:O	2.32	0.60
1:A:135:VAL:HG22	1:A:146:SER:HA	1.83	0.60
1:A:111:LEU:HD12	1:A:261:LYS:HD2	1.83	0.60
2:B:75:ARG:NH1	2:B:78:GLU:OE1	2.35	0.60
2:F:7:ALA:HB1	2:F:11:GLU:HG3	1.84	0.59
1:A:288:ILE:HG21	1:A:297:ILE:HD13	1.84	0.58
1:E:77:ASP:O	1:E:78:GLU:C	2.47	0.57
2:D:7:ALA:HB1	2:D:11:GLU:HG3	1.88	0.56
1:E:114:ARG:HB2	1:E:265:SER:HB2	1.86	0.56
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.87	0.56
1:C:105:TYR:CD2	10:C:406:EDO:H12	2.41	0.56
13:E:609:PEG:H21	14:E:884:HOH:O	2.07	0.54
1:A:289:ASN:ND2	14:A:505:HOH:O	2.36	0.54
1:A:150:ASN:HD21	10:A:402:EDO:H12	1.72	0.54
1:C:57:LYS:HG2	1:C:58:PRO:HD2	1.90	0.54
1:E:114:ARG:NH1	11:E:613:SO4:S	2.80	0.53
1:A:227:ARG:NH2	11:A:415:SO4:O3	2.42	0.53
2:B:110:PHE:CD1	1:C:30:MET:HE1	2.44	0.53
1:E:288:ILE:HG21	1:E:297:ILE:HD13	1.90	0.53
2:D:26:HIS:HB2	2:D:149:MET:HE3	1.91	0.53
1:A:240:ASN:HB3	14:A:708:HOH:O	2.09	0.53
2:D:123:ARG:HH11	2:D:123:ARG:HB3	1.74	0.53
2:D:72:ASN:N	10:D:301:EDO:H12	2.23	0.52
1:C:69:TRP:CD1	10:C:405:EDO:H21	2.42	0.51
1:A:114:ARG:HB2	1:A:265:SER:HB2	1.93	0.49
2:B:106:ARG:NH2	2:B:109:ASP:OD2	2.45	0.49
1:E:164:ILE:HG23	13:E:609:PEG:H42	1.93	0.49
2:B:116:LYS:NZ	2:B:120:ASP:OD2	2.43	0.48
1:E:136:SER:HB2	13:E:610:PEG:H41	1.94	0.48
1:C:114:ARG:HD2	14:C:645:HOH:O	2.14	0.48
1:C:21:ASN:ND2	14:C:510:HOH:O	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLU:OE1	14:C:501:HOH:O	2.20	0.47
2:D:123:ARG:HB3	2:D:123:ARG:NH1	2.29	0.47
1:E:96:ASP:H	10:E:602:EDO:H12	1.80	0.47
1:A:62:LYS:HD3	1:A:62:LYS:HA	1.79	0.46
10:C:405:EDO:H12	14:C:518:HOH:O	2.15	0.46
2:B:143:LYS:HE2	2:B:143:LYS:HA	1.97	0.46
1:C:15:ILE:HG13	2:D:119:TYR:HA	1.98	0.46
1:C:283:THR:HG22	1:C:301:THR:HG22	1.98	0.46
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.98	0.46
1:A:15:ILE:HG13	2:B:119:TYR:HA	1.97	0.46
1:C:83(A):GLU:OE1	14:C:503:HOH:O	2.21	0.45
1:C:29:ILE:HG23	1:C:30:MET:HG3	1.98	0.45
2:B:168:LEU:O	2:B:172:GLU:HG3	2.15	0.45
1:E:283:THR:HG22	1:E:301:THR:HG22	1.97	0.45
1:E:164:ILE:O	1:E:246:GLU:HA	2.16	0.45
1:A:289:ASN:HA	14:A:549:HOH:O	2.16	0.45
2:B:9:PHE:CD1	10:B:201:EDO:H12	2.52	0.45
1:C:78:GLU:O	14:C:502:HOH:O	2.21	0.45
1:E:96:ASP:H	10:E:602:EDO:C1	2.29	0.45
2:B:131:LYS:HD2	2:B:133:LEU:HD23	1.99	0.45
2:F:151:SER:HB3	9:N:1:NAG:H62	1.99	0.45
2:D:127:ARG:HD2	14:F:358:HOH:O	2.16	0.45
1:C:102:LEU:HB3	10:C:406:EDO:H11	1.99	0.44
1:E:220:ARG:O	1:E:227:ARG:HD3	2.18	0.44
1:A:135:VAL:HG13	1:A:145:PRO:HB2	2.00	0.43
14:E:883:HOH:O	2:F:61:THR:HG22	2.18	0.43
1:A:283:THR:HG22	1:A:301:THR:HG22	2.00	0.43
1:C:227:ARG:NH2	11:C:410:SO4:O2	2.47	0.43
2:F:78:GLU:HG2	14:F:491:HOH:O	2.18	0.43
1:A:289:ASN:HB2	14:A:574:HOH:O	2.18	0.43
1:E:290:SER:N	14:E:723:HOH:O	2.51	0.43
1:E:214:VAL:HG12	10:E:607:EDO:H12	2.00	0.43
2:D:60:ASN:OD1	1:E:310:LYS:HD3	2.19	0.42
1:E:153:TRP:HH2	13:E:610:PEG:H42	1.84	0.42
2:B:121:LYS:HE3	14:B:316:HOH:O	2.20	0.41
1:A:78:GLU:O	1:A:80:ILE:N	2.53	0.41
2:D:169:LYS:O	2:D:172:GLU:HG2	2.21	0.41
1:A:18:HIS:HB2	2:B:20:GLY:O	2.20	0.41
14:B:466:HOH:O	5:I:1:NAG:H83	2.21	0.41
1:A:80:ILE:HG22	1:A:81:ARG:N	2.31	0.41
1:E:129:ASN:HB2	13:E:609:PEG:H12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.56	0.40
1:C:26:VAL:HG21	1:C:317:ALA:HB2	2.03	0.40
1:A:260:ILE:HD13	1:A:260:ILE:HA	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/329 (96%)	309 (98%)	8 (2%)	0	100	100
1	C	321/329 (98%)	310 (97%)	11 (3%)	0	100	100
1	E	318/329 (97%)	308 (97%)	10 (3%)	0	100	100
2	B	167/181 (92%)	164 (98%)	3 (2%)	0	100	100
2	D	167/181 (92%)	165 (99%)	2 (1%)	0	100	100
2	F	170/181 (94%)	169 (99%)	1 (1%)	0	100	100
All	All	1460/1530 (95%)	1425 (98%)	35 (2%)	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	286/294 (97%)	283 (99%)	3 (1%)	68	64
1	C	288/294 (98%)	286 (99%)	2 (1%)	76	74
1	E	287/294 (98%)	284 (99%)	3 (1%)	68	64
2	B	146/154 (95%)	146 (100%)	0	100	100
2	D	146/154 (95%)	144 (99%)	2 (1%)	59	52
2	F	148/154 (96%)	148 (100%)	0	100	100
All	All	1301/1344 (97%)	1291 (99%)	10 (1%)	73	71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	283	THR
1	A	297	ILE
1	C	283	THR
1	C	297	ILE
2	D	62	GLN
2	D	78	GLU
1	E	81	ARG
1	E	283	THR
1	E	297	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	103	ASN
1	A	158	ASN
1	A	240	ASN
2	B	50	ASN
1	C	12	GLN
1	C	40	GLN
1	C	222	GLN
2	D	25	HIS
2	D	42	GLN
2	D	50	ASN
2	D	95	ASN
1	E	38	HIS
1	E	40	GLN
2	F	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

27 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	G	1	1,3	14,14,15	0.80	0	17,19,21	1.02	1 (5%)
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	1.14	3 (17%)
3	BMA	G	3	3	11,11,12	0.82	0	15,15,17	1.56	2 (13%)
3	MAN	G	4	3	11,11,12	0.68	0	15,15,17	1.07	1 (6%)
3	MAN	G	5	3	11,11,12	0.65	0	15,15,17	1.43	1 (6%)
4	NAG	H	1	4,1	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
4	NAG	H	2	4	14,14,15	0.73	0	17,19,21	0.88	1 (5%)
4	FUC	H	3	4	10,10,11	0.73	0	14,14,16	0.97	0
5	NAG	I	1	5,2	14,14,15	0.88	1 (7%)	17,19,21	1.45	2 (11%)
5	FUC	I	2	5	10,10,11	0.80	0	14,14,16	1.03	0
5	NAG	I	3	5	14,14,15	0.71	0	17,19,21	0.79	0
6	NAG	J	1	6,1	14,14,15	0.77	0	17,19,21	1.43	1 (5%)
6	NAG	J	2	6	14,14,15	0.65	0	17,19,21	1.59	4 (23%)
6	BMA	J	3	6	11,11,12	0.84	0	15,15,17	1.49	3 (20%)
6	MAN	J	4	6	11,11,12	0.69	0	15,15,17	1.33	1 (6%)
7	NAG	K	1	7,1	14,14,15	0.75	0	17,19,21	1.07	1 (5%)
7	FUC	K	2	7	10,10,11	0.74	0	14,14,16	1.03	0
5	NAG	L	1	5,2	14,14,15	0.69	0	17,19,21	1.08	2 (11%)
5	FUC	L	2	5	10,10,11	0.66	0	14,14,16	1.24	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	L	3	5	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
8	NAG	M	1	1,8	14,14,15	0.74	0	17,19,21	1.18	1 (5%)
8	NAG	M	2	8	14,14,15	0.66	0	17,19,21	0.99	0
8	BMA	M	3	8	11,11,12	0.77	0	15,15,17	1.48	1 (6%)
9	NAG	N	1	9,2	14,14,15	0.76	0	17,19,21	0.80	0
9	NAG	N	2	9	14,14,15	0.71	0	17,19,21	0.98	0
9	BMA	N	3	9	11,11,12	0.80	0	15,15,17	1.90	2 (13%)
9	FUC	N	4	9	10,10,11	0.70	0	14,14,16	1.14	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1
5	NAG	I	1	5,2	-	0/6/23/26	0/1/1/1
5	FUC	I	2	5	-	-	0/1/1/1
5	NAG	I	3	5	-	1/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	FUC	K	2	7	-	-	0/1/1/1
5	NAG	L	1	5,2	-	0/6/23/26	0/1/1/1
5	FUC	L	2	5	-	-	0/1/1/1
5	NAG	L	3	5	-	2/6/23/26	0/1/1/1
8	NAG	M	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
8	BMA	M	3	8	-	0/2/19/22	0/1/1/1
9	NAG	N	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	N	3	9	-	1/2/19/22	0/1/1/1
9	FUC	N	4	9	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	C1-C2	2.11	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	3	BMA	C1-O5-C5	5.67	119.78	112.19
6	J	2	NAG	C1-O5-C5	4.77	118.58	112.19
6	J	1	NAG	C1-O5-C5	4.49	118.20	112.19
3	G	5	MAN	C1-O5-C5	4.38	118.06	112.19
8	M	3	BMA	C1-O5-C5	4.09	117.66	112.19
6	J	4	MAN	C1-O5-C5	4.08	117.65	112.19
5	I	1	NAG	C1-O5-C5	3.67	117.10	112.19
3	G	3	BMA	C1-O5-C5	3.49	116.86	112.19
5	I	1	NAG	C2-N2-C7	3.38	127.43	122.90
6	J	3	BMA	O5-C5-C6	3.22	113.94	107.66
3	G	4	MAN	C1-O5-C5	3.19	116.47	112.19
6	J	3	BMA	C1-O5-C5	2.95	116.14	112.19
5	L	2	FUC	C1-O5-C5	2.87	119.73	112.97
8	M	1	NAG	C2-N2-C7	2.79	126.64	122.90
7	K	1	NAG	C1-O5-C5	2.71	115.82	112.19
4	H	1	NAG	C1-O5-C5	2.64	115.72	112.19
3	G	1	NAG	C1-O5-C5	2.62	115.70	112.19
5	L	1	NAG	O4-C4-C3	-2.62	104.20	110.38
3	G	3	BMA	O5-C5-C6	2.45	112.42	107.66
6	J	2	NAG	O4-C4-C3	-2.39	104.75	110.38
9	N	3	BMA	C3-C4-C5	2.38	114.54	110.23
3	G	2	NAG	O4-C4-C3	-2.36	104.81	110.38
6	J	3	BMA	O3-C3-C2	-2.28	105.40	110.05
4	H	2	NAG	O5-C1-C2	-2.27	107.77	111.29
5	L	3	NAG	O5-C1-C2	-2.27	107.78	111.29
9	N	4	FUC	C1-O5-C5	2.26	118.30	112.97
3	G	2	NAG	C4-C3-C2	2.24	114.31	111.02
3	G	2	NAG	C1-O5-C5	2.10	115.00	112.19
5	L	1	NAG	O5-C1-C2	-2.05	108.12	111.29
6	J	2	NAG	O3-C3-C2	-2.05	105.15	109.40
6	J	2	NAG	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (18) torsion outliers are listed below:

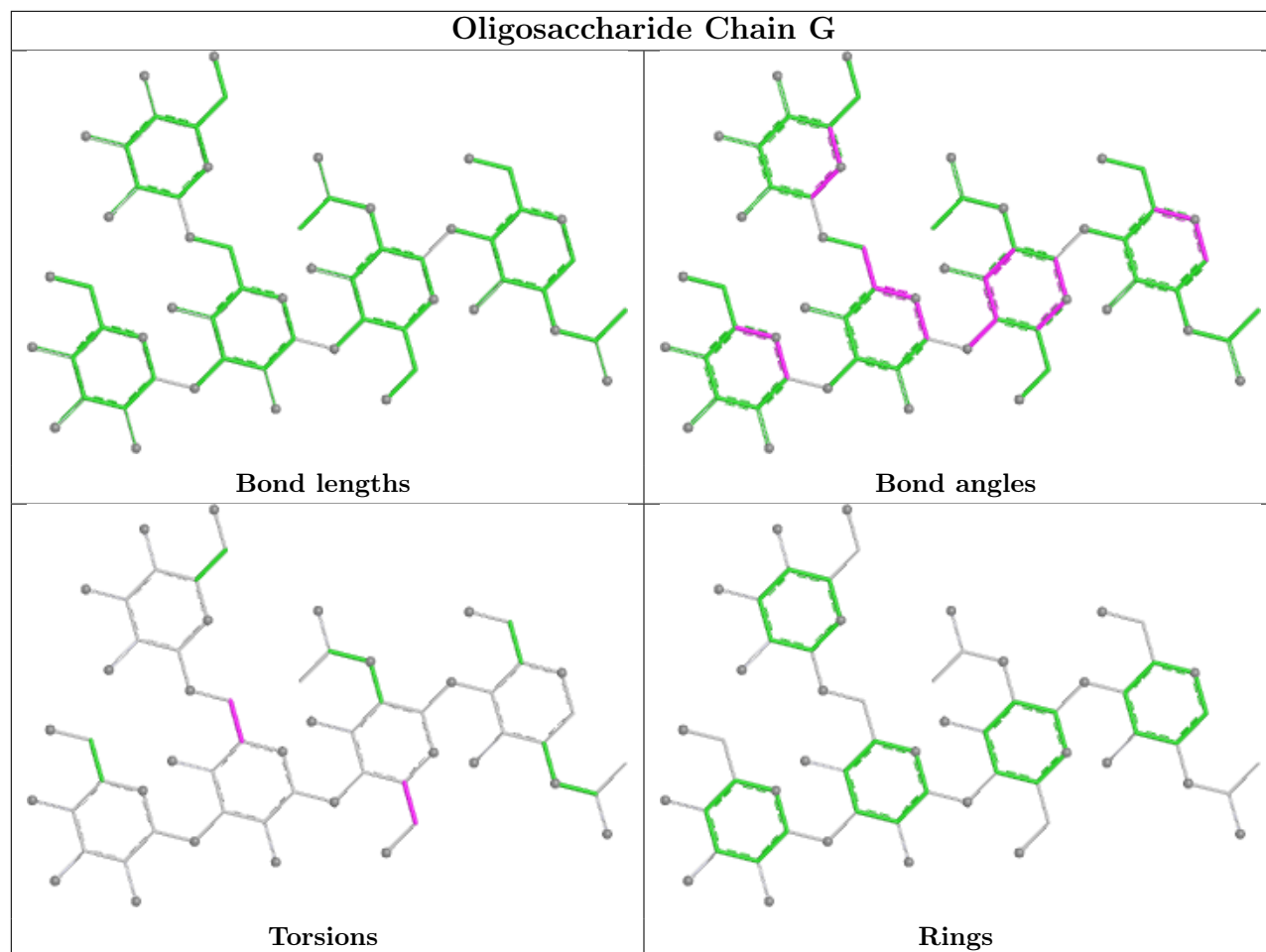
Mol	Chain	Res	Type	Atoms
5	L	3	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
5	L	3	NAG	C4-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
8	M	2	NAG	C4-C5-C6-O6
9	N	3	BMA	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
8	M	2	NAG	O5-C5-C6-O6
5	I	3	NAG	C1-C2-N2-C7
9	N	1	NAG	C1-C2-N2-C7

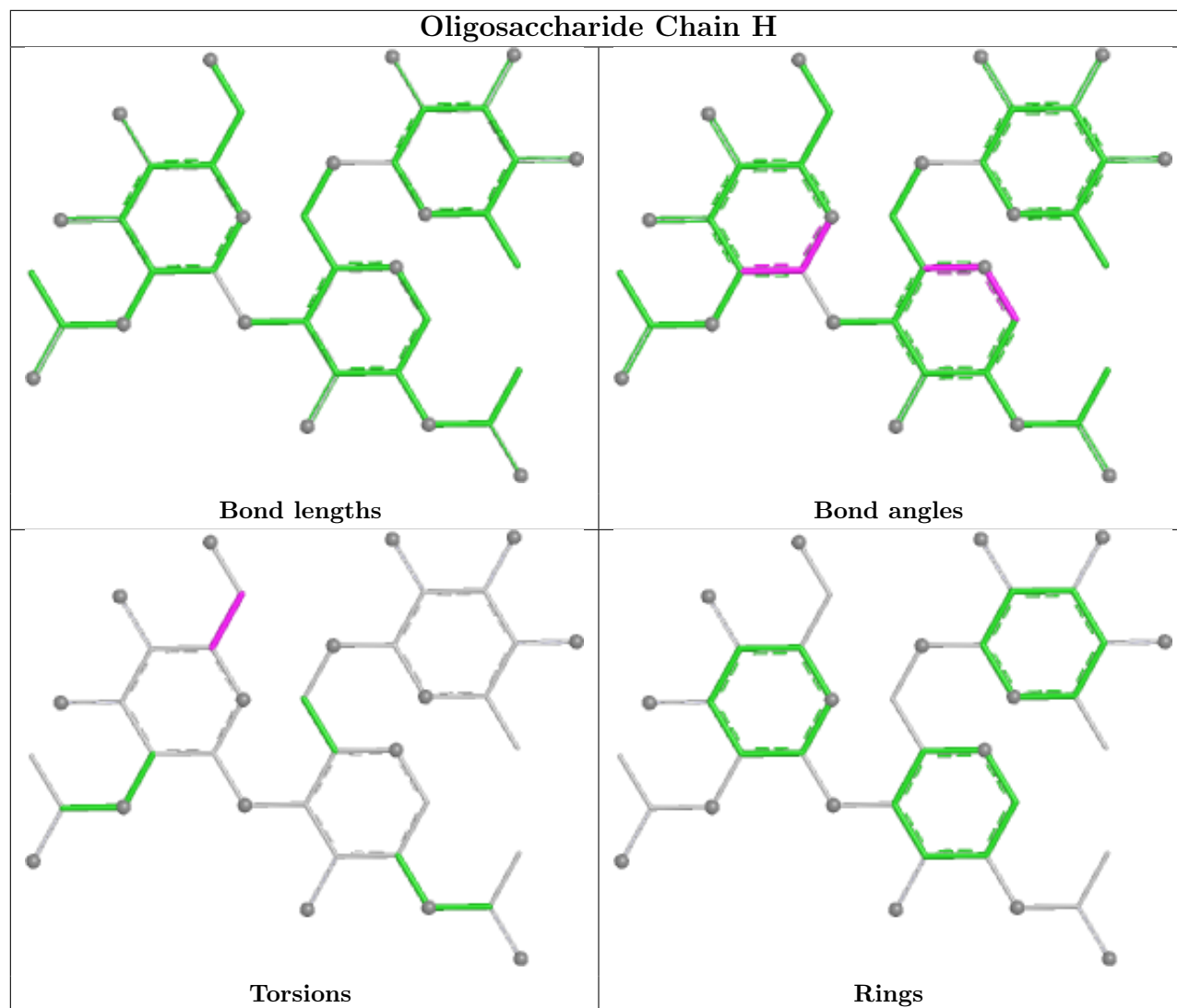
There are no ring outliers.

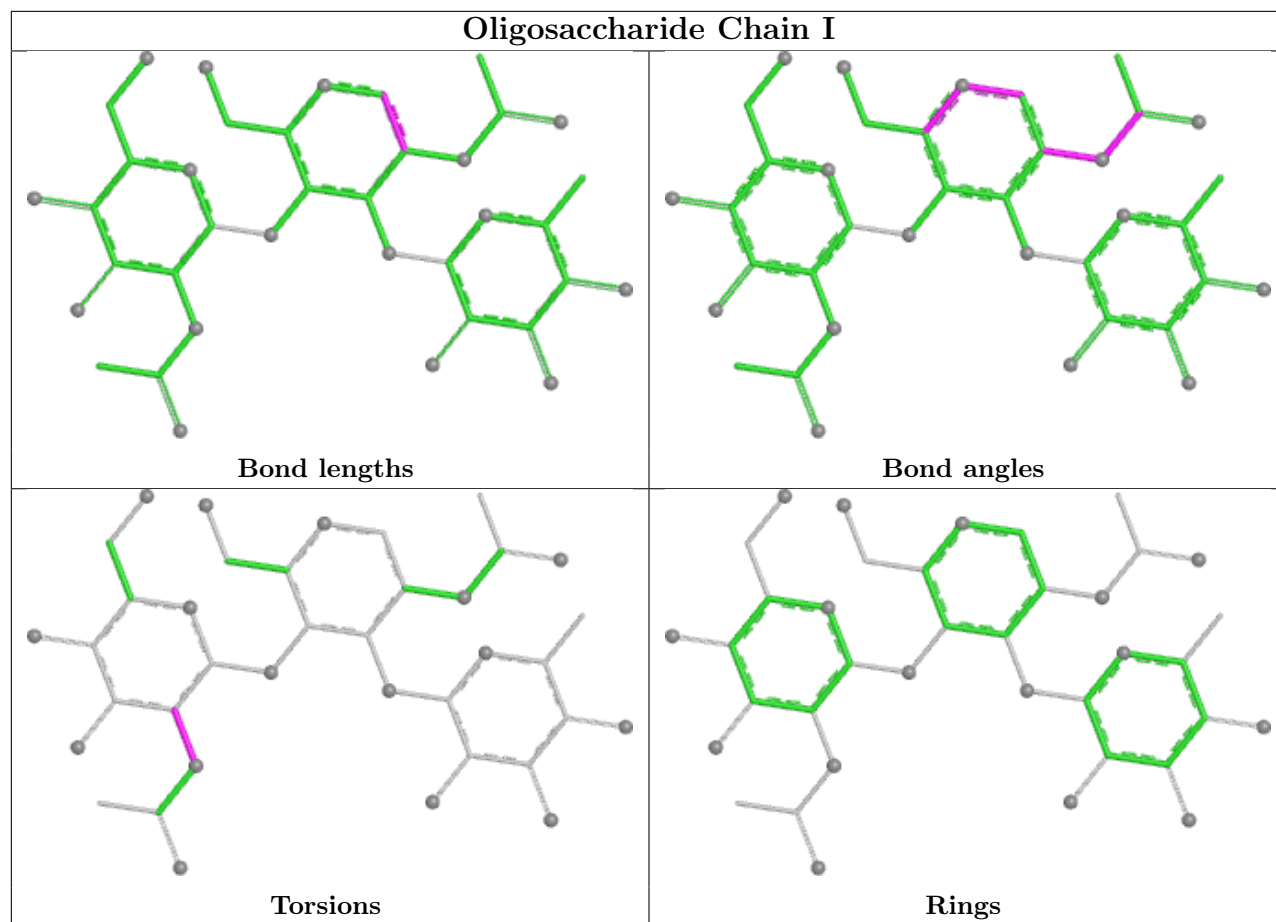
2 monomers are involved in 2 short contacts:

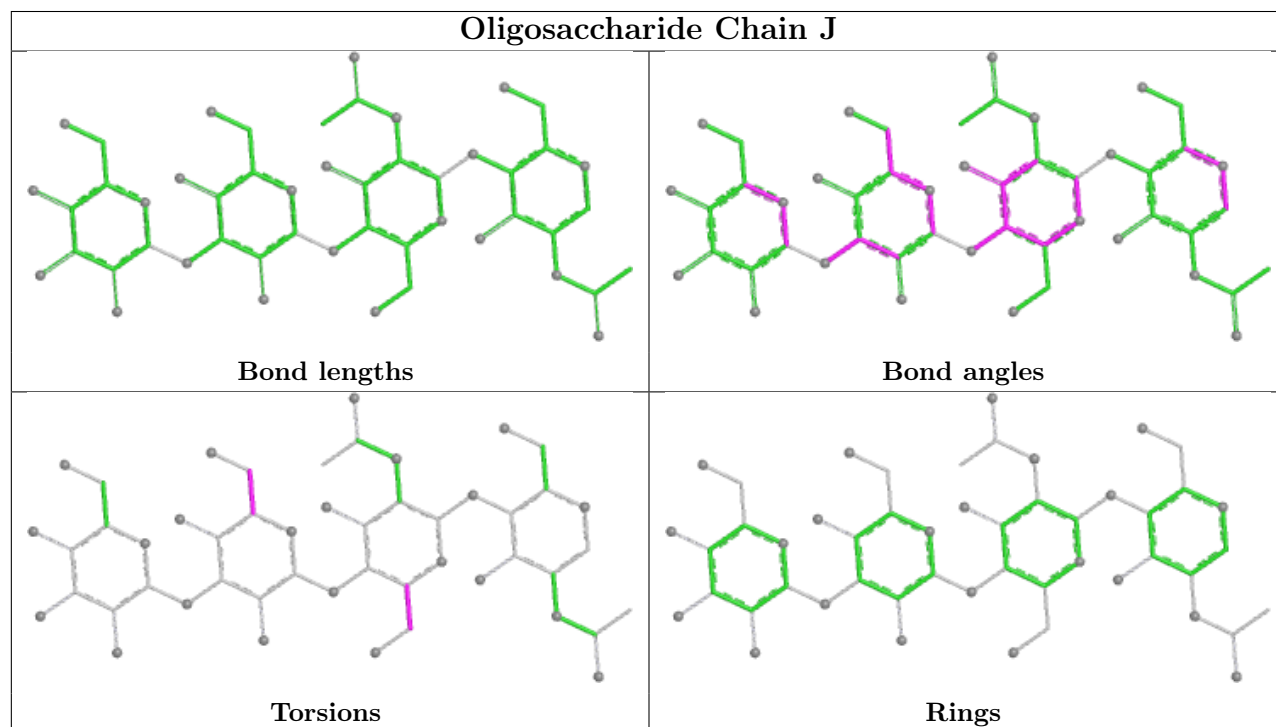
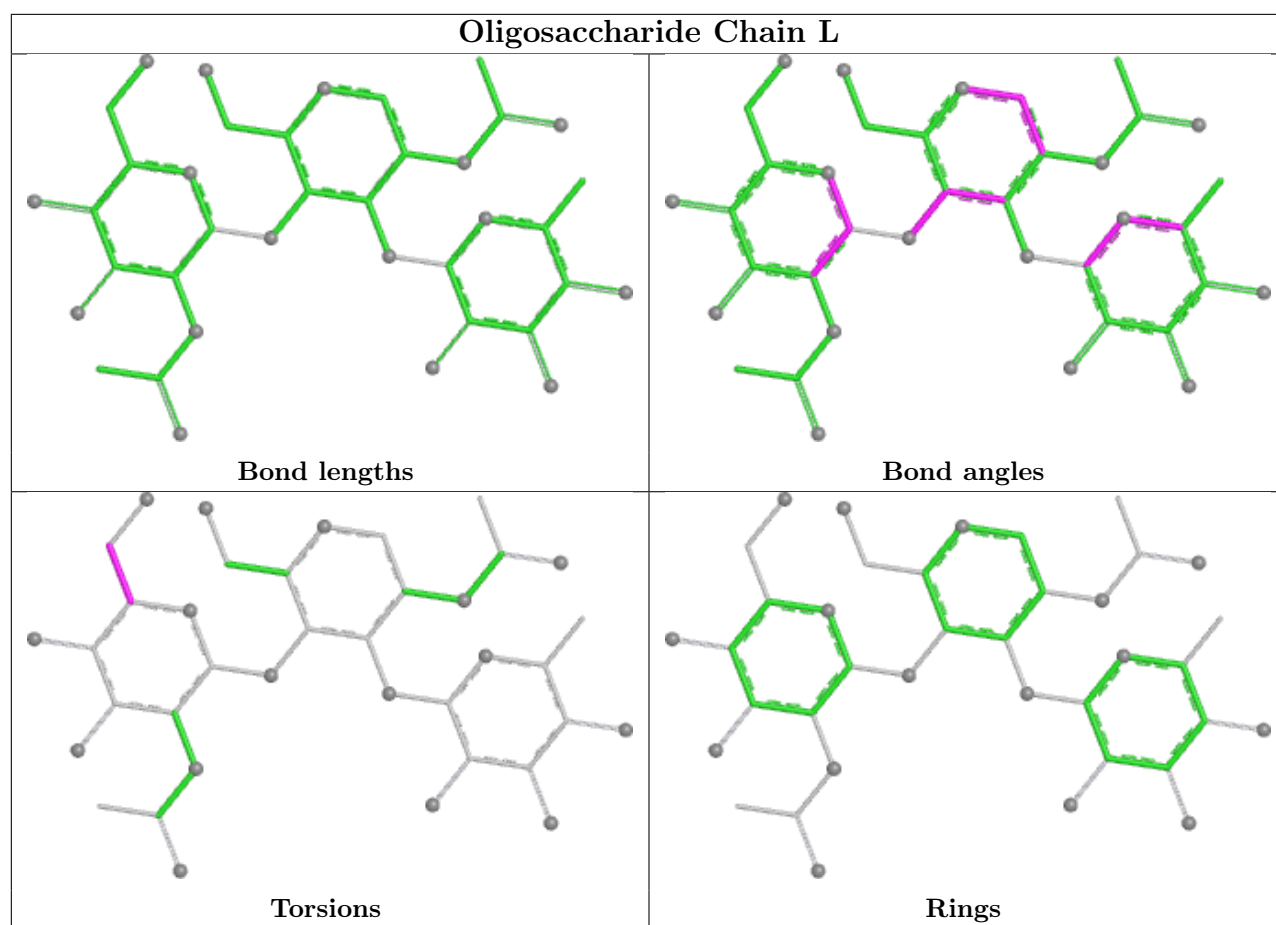
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	1	NAG	1	0
5	I	1	NAG	1	0

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

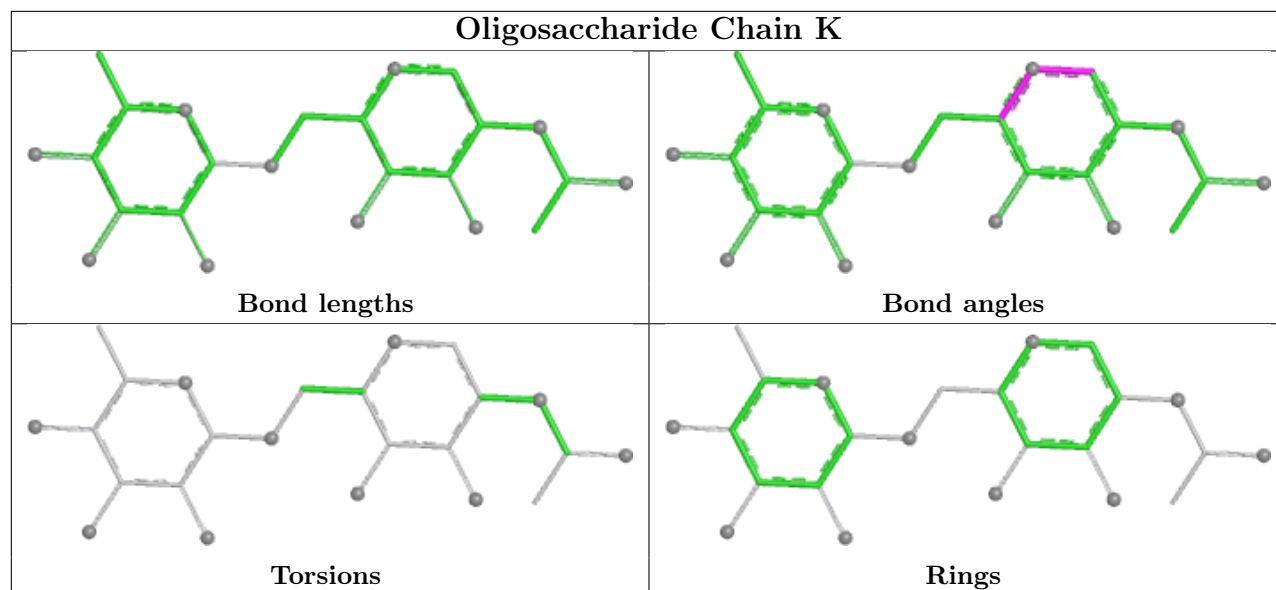




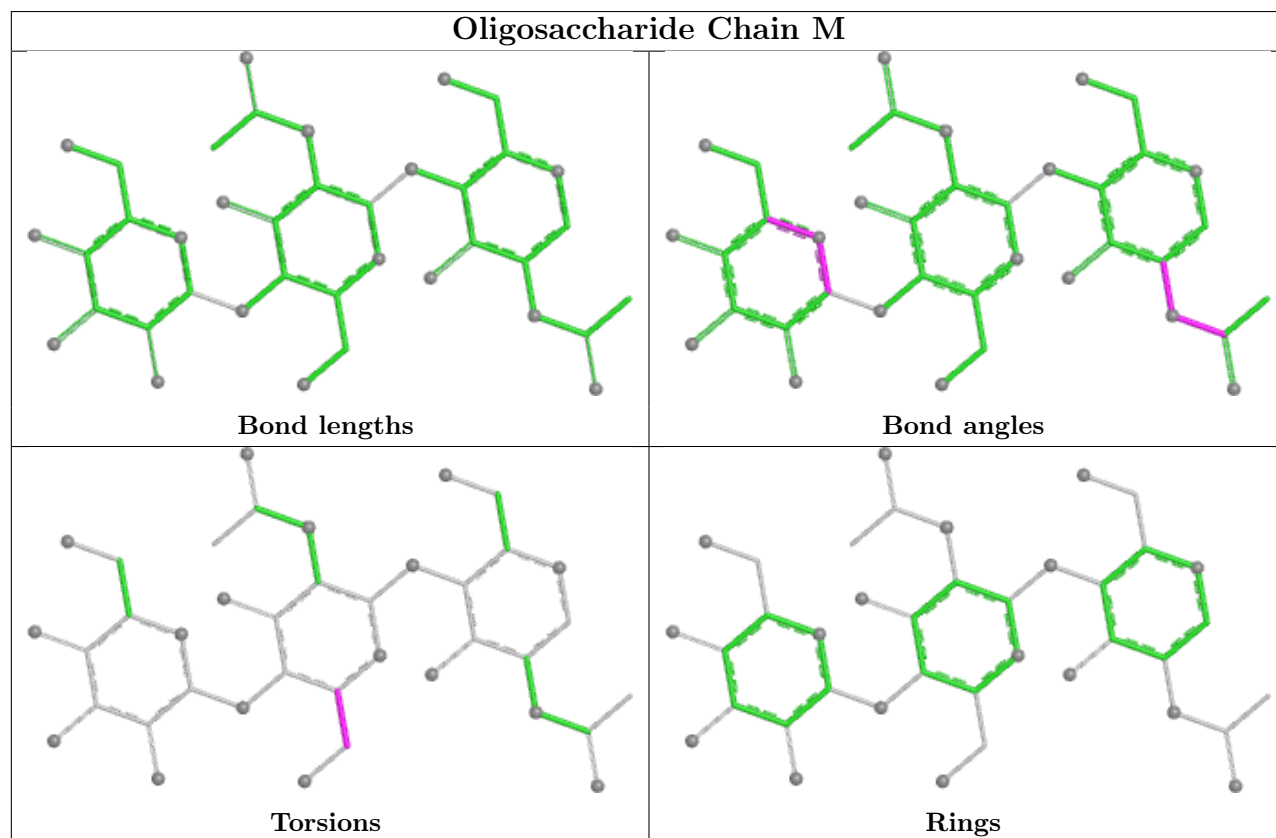


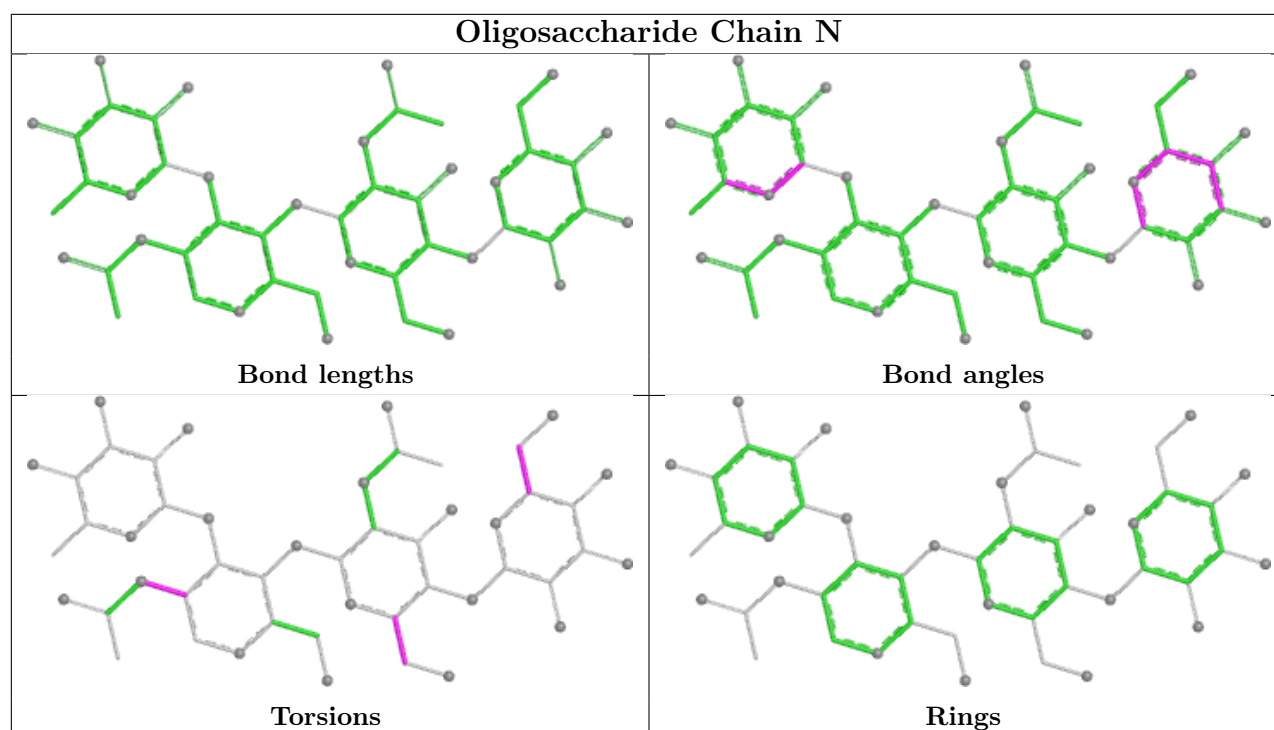


Oligosaccharide Chain K



Oligosaccharide Chain M





5.6 Ligand geometry [i](#)

58 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	$\# Z > 2$
11	SO4	E	612	-	4,4,4	0.69	0	6,6,6	0.10	0
11	SO4	A	412	-	4,4,4	0.69	0	6,6,6	0.07	0
13	PEG	E	609	-	6,6,6	0.31	0	5,5,5	0.78	0
10	EDO	A	405	-	3,3,3	0.24	0	2,2,2	0.30	0
10	EDO	E	604	-	3,3,3	0.26	0	2,2,2	0.33	0
10	EDO	F	202	-	3,3,3	0.25	0	2,2,2	0.29	0
11	SO4	C	413	-	4,4,4	0.69	0	6,6,6	0.14	0
12	NAG	E	601	1	14,14,15	0.64	0	17,19,21	1.18	1 (5%)
11	SO4	A	410	-	4,4,4	0.71	0	6,6,6	0.08	0
11	SO4	C	414	-	4,4,4	0.69	0	6,6,6	0.07	0
10	EDO	F	201	-	3,3,3	0.27	0	2,2,2	0.26	0
11	SO4	A	409	-	4,4,4	0.72	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SO4	D	303	-	4,4,4	0.70	0	6,6,6	0.10	0
10	EDO	C	403	-	3,3,3	0.27	0	2,2,2	0.15	0
11	SO4	E	611	-	4,4,4	0.69	0	6,6,6	0.12	0
10	EDO	E	602	-	3,3,3	0.24	0	2,2,2	0.36	0
10	EDO	E	608	-	3,3,3	0.25	0	2,2,2	0.19	0
11	SO4	E	613	-	4,4,4	0.71	0	6,6,6	0.08	0
11	SO4	E	615	-	4,4,4	0.67	0	6,6,6	0.34	0
10	EDO	C	401	-	3,3,3	0.25	0	2,2,2	0.22	0
11	SO4	A	411	-	4,4,4	0.70	0	6,6,6	0.09	0
10	EDO	C	405	-	3,3,3	0.29	0	2,2,2	0.16	0
10	EDO	B	202	-	3,3,3	0.25	0	2,2,2	0.36	0
11	SO4	A	414	-	4,4,4	0.67	0	6,6,6	0.15	0
11	SO4	C	410	-	4,4,4	0.90	0	6,6,6	0.61	0
11	SO4	C	411	-	4,4,4	0.73	0	6,6,6	0.45	0
11	SO4	C	409	-	4,4,4	0.74	0	6,6,6	0.18	0
10	EDO	D	301	-	3,3,3	0.24	0	2,2,2	0.33	0
10	EDO	E	603	-	3,3,3	0.29	0	2,2,2	0.25	0
11	SO4	A	416	-	4,4,4	0.69	0	6,6,6	0.09	0
10	EDO	E	607	-	3,3,3	0.27	0	2,2,2	0.40	0
11	SO4	C	416	-	4,4,4	0.66	0	6,6,6	0.10	0
11	SO4	E	614	-	4,4,4	0.72	0	6,6,6	0.07	0
10	EDO	E	605	-	3,3,3	0.25	0	2,2,2	0.29	0
10	EDO	A	403	-	3,3,3	0.26	0	2,2,2	0.16	0
10	EDO	C	402	-	3,3,3	0.24	0	2,2,2	0.32	0
10	EDO	E	606	-	3,3,3	0.25	0	2,2,2	0.29	0
11	SO4	A	407	-	4,4,4	0.70	0	6,6,6	0.22	0
10	EDO	C	406	-	3,3,3	0.29	0	2,2,2	0.15	0
10	EDO	B	201	-	3,3,3	0.24	0	2,2,2	0.07	0
11	SO4	A	415	-	4,4,4	0.69	0	6,6,6	0.26	0
10	EDO	A	404	-	3,3,3	0.26	0	2,2,2	0.24	0
11	SO4	E	616	-	4,4,4	0.73	0	6,6,6	0.37	0
11	SO4	C	412	-	4,4,4	0.72	0	6,6,6	0.28	0
11	SO4	A	408	-	4,4,4	0.70	0	6,6,6	0.12	0
11	SO4	B	203	-	4,4,4	0.71	0	6,6,6	0.12	0
11	SO4	C	407	-	4,4,4	0.67	0	6,6,6	0.31	0
11	SO4	D	302	-	4,4,4	0.70	0	6,6,6	0.08	0
10	EDO	F	203	-	3,3,3	0.24	0	2,2,2	0.28	0
11	SO4	A	413	-	4,4,4	0.70	0	6,6,6	0.07	0
13	PEG	E	610	-	6,6,6	0.24	0	5,5,5	0.45	0
10	EDO	A	402	-	3,3,3	0.26	0	2,2,2	0.19	0
11	SO4	A	417	-	4,4,4	0.74	0	6,6,6	0.18	0
11	SO4	C	415	-	4,4,4	0.71	0	6,6,6	0.14	0
10	EDO	A	406	-	3,3,3	0.26	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SO4	C	408	-	4,4,4	0.69	0	6,6,6	0.09	0
10	EDO	C	404	-	3,3,3	0.24	0	2,2,2	0.33	0
10	EDO	A	401	-	3,3,3	0.21	0	2,2,2	0.46	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
13	PEG	E	609	-	-	2/4/4/4	-
10	EDO	A	405	-	-	0/1/1/1	-
10	EDO	E	604	-	-	0/1/1/1	-
10	EDO	F	202	-	-	1/1/1/1	-
12	NAG	E	601	1	-	0/6/23/26	0/1/1/1
10	EDO	F	201	-	-	0/1/1/1	-
10	EDO	C	403	-	-	1/1/1/1	-
10	EDO	E	602	-	-	0/1/1/1	-
10	EDO	E	608	-	-	1/1/1/1	-
10	EDO	C	401	-	-	0/1/1/1	-
10	EDO	C	405	-	-	0/1/1/1	-
10	EDO	B	202	-	-	1/1/1/1	-
10	EDO	D	301	-	-	0/1/1/1	-
10	EDO	E	603	-	-	0/1/1/1	-
10	EDO	E	607	-	-	0/1/1/1	-
10	EDO	E	605	-	-	0/1/1/1	-
10	EDO	A	403	-	-	1/1/1/1	-
10	EDO	C	402	-	-	1/1/1/1	-
10	EDO	E	606	-	-	0/1/1/1	-
10	EDO	C	406	-	-	1/1/1/1	-
10	EDO	B	201	-	-	0/1/1/1	-
10	EDO	A	404	-	-	1/1/1/1	-
10	EDO	F	203	-	-	0/1/1/1	-
13	PEG	E	610	-	-	2/4/4/4	-
10	EDO	A	402	-	-	1/1/1/1	-
10	EDO	A	406	-	-	0/1/1/1	-
10	EDO	C	404	-	-	0/1/1/1	-
10	EDO	A	401	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	E	601	NAG	C1-O5-C5	3.91	117.43	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	E	609	PEG	C4-C3-O2-C2
13	E	609	PEG	O1-C1-C2-O2
13	E	610	PEG	O1-C1-C2-O2
10	C	403	EDO	O1-C1-C2-O2
10	E	608	EDO	O1-C1-C2-O2
10	F	202	EDO	O1-C1-C2-O2
10	B	202	EDO	O1-C1-C2-O2
10	A	404	EDO	O1-C1-C2-O2
13	E	610	PEG	C4-C3-O2-C2
10	A	402	EDO	O1-C1-C2-O2
10	A	403	EDO	O1-C1-C2-O2
10	C	406	EDO	O1-C1-C2-O2
10	C	402	EDO	O1-C1-C2-O2
10	A	401	EDO	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	609	PEG	3	0
10	F	201	EDO	1	0
10	E	602	EDO	2	0
11	E	613	SO4	1	0
10	C	405	EDO	3	0
11	C	410	SO4	1	0
10	D	301	EDO	2	0
10	E	607	EDO	1	0
10	E	605	EDO	1	0
10	C	406	EDO	2	0
10	B	201	EDO	1	0
11	A	415	SO4	1	0
10	F	203	EDO	1	0
13	E	610	PEG	2	0
10	A	402	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/329 (97%)	0.05	19 (5%) 28 31	20, 34, 59, 126	0
1	C	323/329 (98%)	-0.05	13 (4%) 42 47	16, 31, 60, 117	0
1	E	322/329 (97%)	-0.03	18 (5%) 30 33	17, 30, 54, 123	0
2	B	169/181 (93%)	0.30	12 (7%) 22 25	21, 38, 81, 123	0
2	D	169/181 (93%)	0.56	13 (7%) 19 22	22, 48, 76, 101	0
2	F	172/181 (95%)	0.02	8 (4%) 36 41	22, 35, 53, 74	0
All	All	1476/1530 (96%)	0.10	83 (5%) 30 33	16, 35, 66, 126	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	6	ILE	10.6
2	D	6	ILE	10.2
2	D	173	ILE	9.6
1	A	80	ILE	9.0
1	A	81	ARG	8.8
2	D	174	GLY	8.8
2	B	174	GLY	8.7
2	B	7	ALA	8.6
1	E	80	ILE	7.9
1	C	9	PRO	7.5
1	E	78	GLU	6.8
2	B	8	GLY	6.8
2	B	10	ILE	6.6
1	A	9	PRO	6.2
2	B	9	PHE	5.8
1	A	78	GLU	5.7
1	C	79	PHE	5.6
1	A	323	SER	4.7
1	C	289	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	323	SER	4.4
1	C	277	CYS	4.4
1	C	324	PRO	4.3
1	E	77	ASP	4.2
1	E	81	ARG	4.2
1	A	290	SER	4.1
1	A	277	CYS	4.1
2	F	6	ILE	3.8
1	E	82	VAL	3.7
2	D	168	LEU	3.6
1	A	77	ASP	3.6
1	E	277	CYS	3.4
2	F	10	ILE	3.4
1	E	290	SER	3.3
1	C	290	SER	3.3
1	C	80	ILE	3.2
1	E	222	GLN	3.2
1	E	8	ASP	3.2
2	D	172	GLU	3.2
2	B	173	ILE	3.1
1	C	81	ARG	3.1
2	D	18	VAL	3.0
2	B	11	GLU	3.0
1	C	78	GLU	2.9
2	F	7	ALA	2.8
1	A	264	ASP	2.8
1	E	21	ASN	2.8
2	F	8	GLY	2.8
2	B	171	GLU	2.8
1	C	323	SER	2.7
2	D	121	LYS	2.7
1	A	289	ASN	2.7
1	E	221	SER	2.7
1	E	227	ARG	2.6
2	D	29	GLU	2.6
1	E	75	MET	2.6
2	F	11	GLU	2.6
1	A	291	SER	2.6
1	E	289	ASN	2.6
1	E	9	PRO	2.5
2	D	78	GLU	2.5
1	A	82	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	262	LYS	2.5
1	A	262	LYS	2.5
1	E	219	THR	2.4
2	F	18	VAL	2.4
1	A	64	CYS	2.4
1	A	62	LYS	2.3
2	B	43	LYS	2.3
2	D	7	ALA	2.3
1	C	62	LYS	2.3
2	D	10	ILE	2.2
2	F	172	GLU	2.2
1	A	142	GLN	2.2
1	A	189	GLU	2.2
1	A	141	TYR	2.1
1	C	77	ASP	2.1
2	D	19	ASP	2.1
2	F	78	GLU	2.1
1	A	260	ILE	2.1
2	B	168	LEU	2.1
2	B	38	LYS	2.0
1	C	41	ASP	2.0
2	D	131	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	2	14/15	0.32	0.19	94,119,131,137	0
5	FUC	L	2	10/11	0.35	0.22	121,139,141,143	0
8	BMA	M	3	11/12	0.44	0.16	111,140,148,150	0
4	FUC	H	3	10/11	0.53	0.20	95,117,124,127	0
7	FUC	K	2	10/11	0.57	0.20	92,106,118,119	0
9	BMA	N	3	11/12	0.57	0.15	87,97,111,113	0

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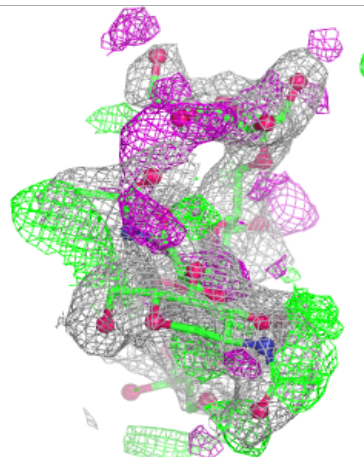
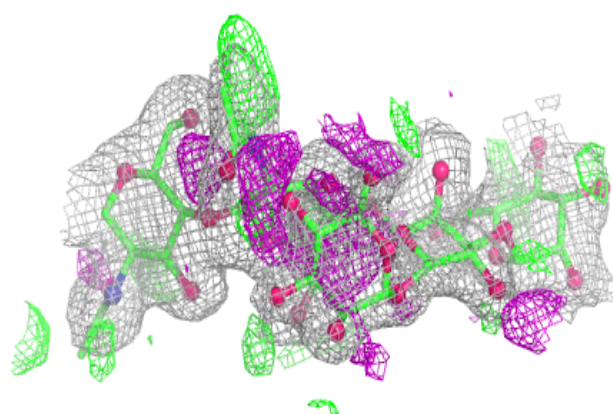
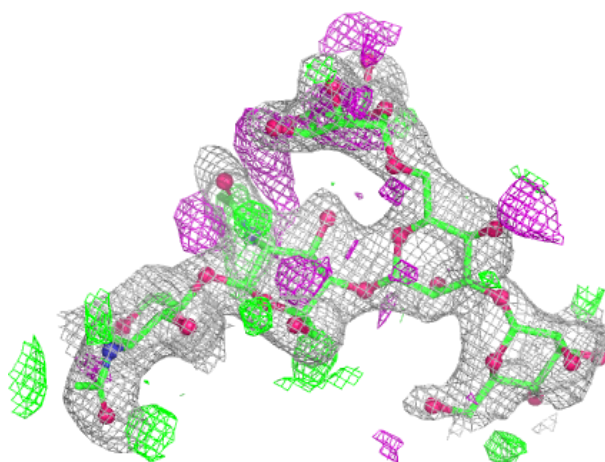
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	L	3	14/15	0.68	0.20	104,123,129,135	0
8	NAG	M	2	14/15	0.69	0.17	50,103,117,137	0
5	NAG	I	3	14/15	0.70	0.18	89,105,114,117	0
3	MAN	G	4	11/12	0.71	0.18	84,91,103,103	0
3	NAG	G	2	14/15	0.73	0.20	50,64,73,76	0
7	NAG	K	1	14/15	0.73	0.16	79,93,98,99	0
5	NAG	I	1	14/15	0.73	0.18	36,84,103,105	0
4	NAG	H	1	14/15	0.78	0.14	72,98,114,122	0
5	FUC	I	2	10/11	0.78	0.20	74,97,103,103	0
5	NAG	L	1	14/15	0.79	0.16	72,109,120,134	0
9	FUC	N	4	10/11	0.79	0.16	73,83,87,90	0
3	BMA	G	3	11/12	0.83	0.15	68,74,91,92	0
8	NAG	M	1	14/15	0.83	0.15	50,66,79,98	0
3	MAN	G	5	11/12	0.83	0.20	41,69,77,87	0
6	BMA	J	3	11/12	0.85	0.13	42,53,65,77	0
6	NAG	J	1	14/15	0.90	0.13	38,48,60,62	0
3	NAG	G	1	14/15	0.92	0.11	29,45,58,66	0
6	MAN	J	4	11/12	0.93	0.12	37,44,57,80	0
6	NAG	J	2	14/15	0.94	0.11	38,46,62,68	0
9	NAG	N	1	14/15	0.94	0.10	35,56,59,68	0
9	NAG	N	2	14/15	0.95	0.08	47,58,81,81	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.

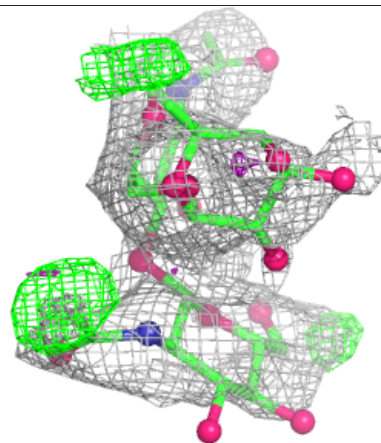
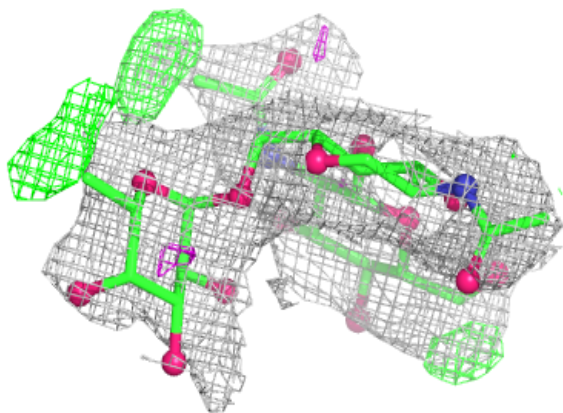
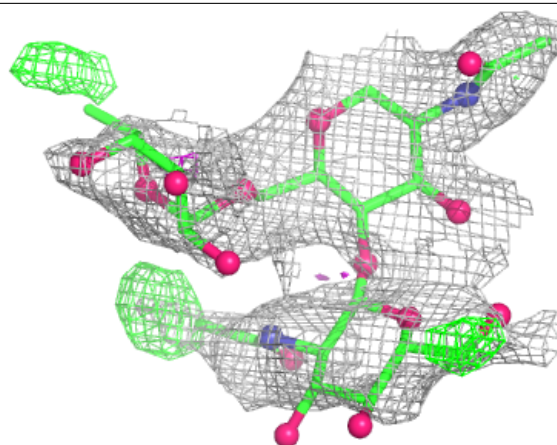
Electron density around Chain G:

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



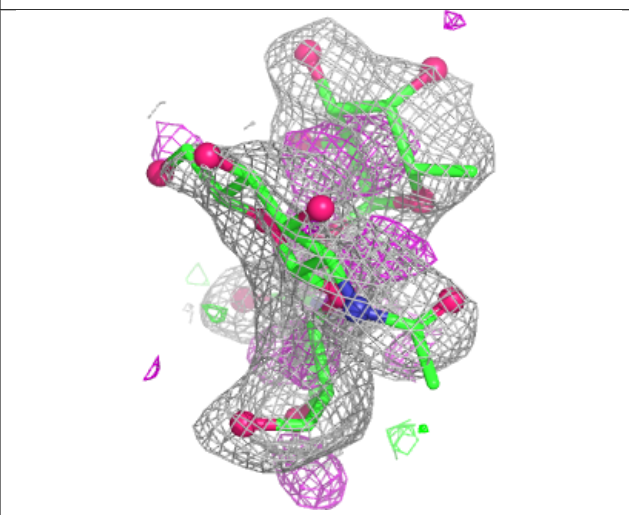
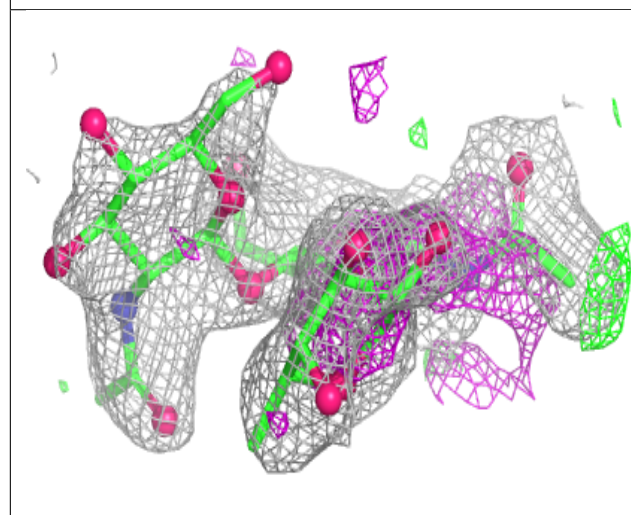
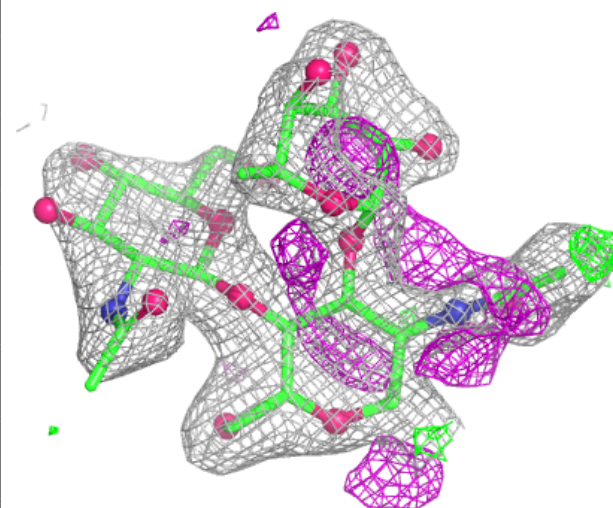
Electron density around Chain H:

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



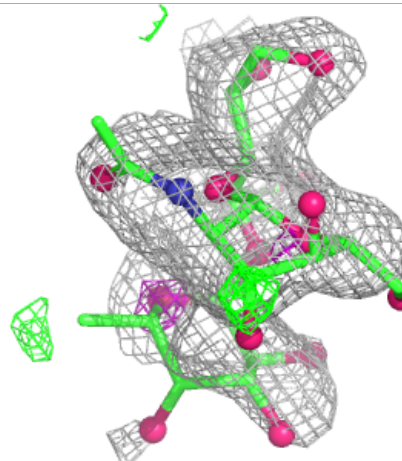
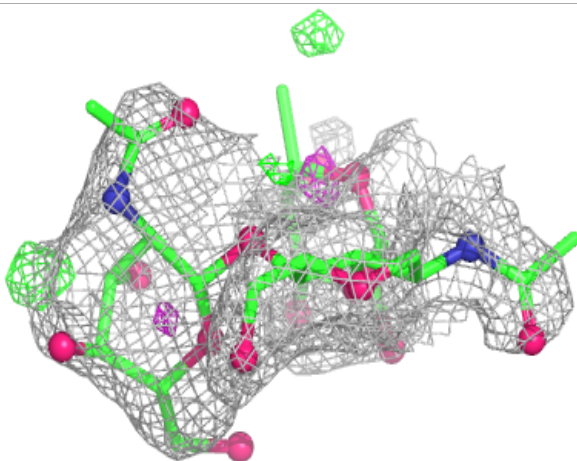
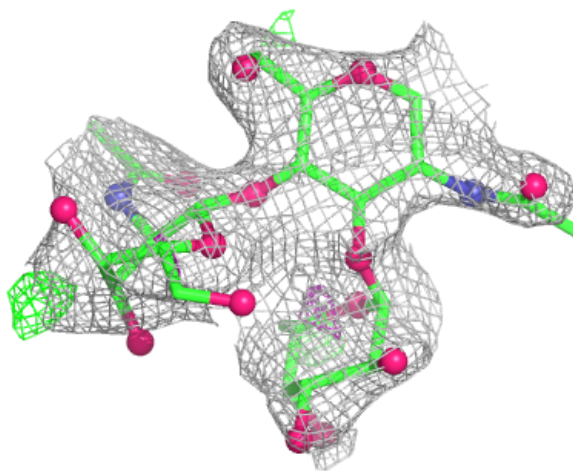
Electron density around Chain I:

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



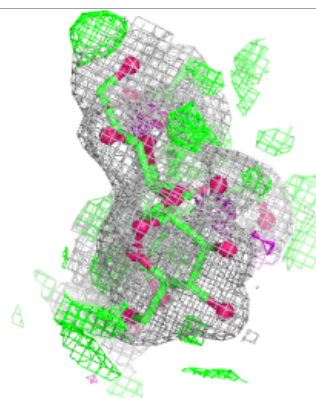
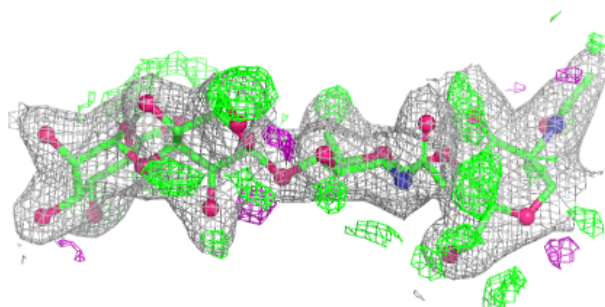
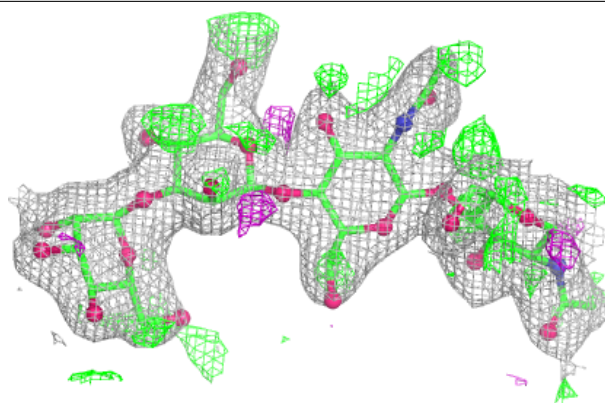
Electron density around Chain L:

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

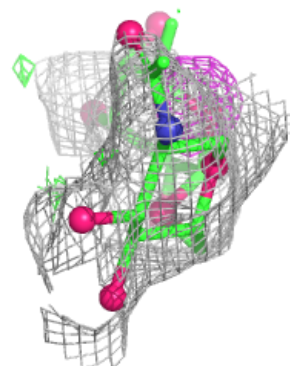
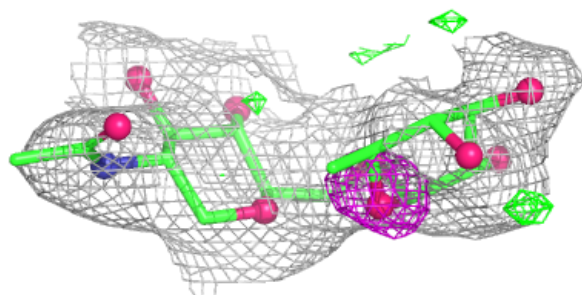
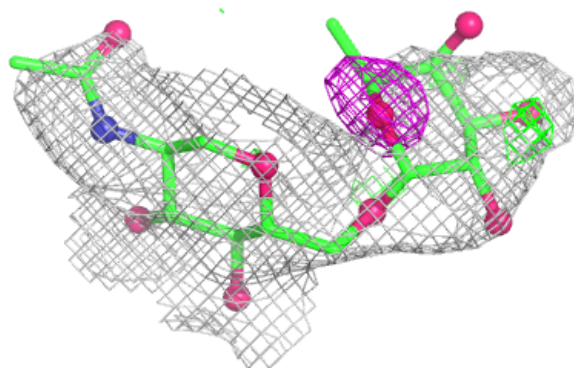


Electron density around Chain J:

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

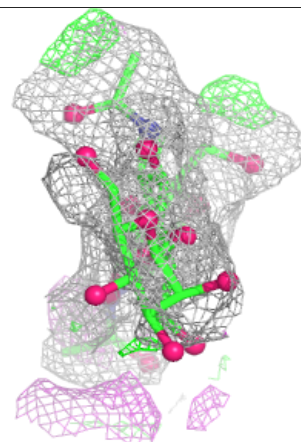
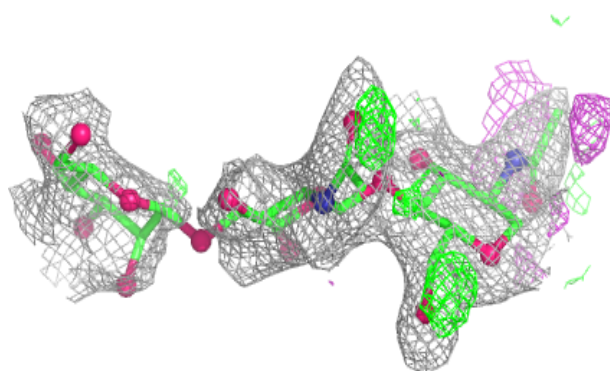
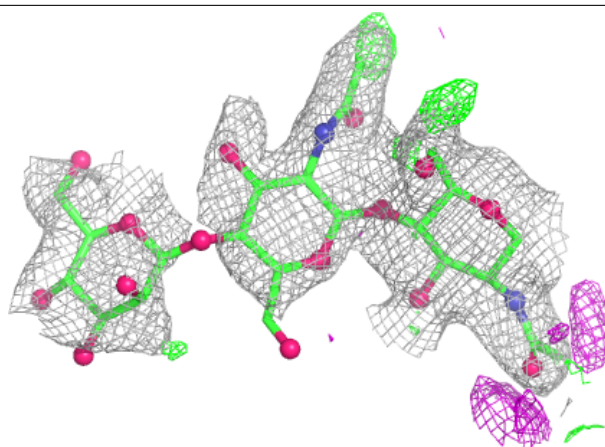
**Electron density around Chain K:**

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

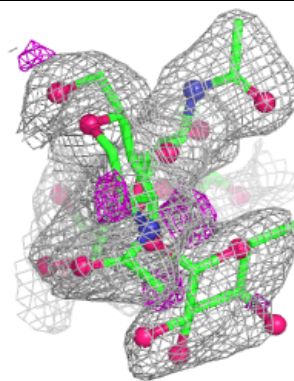
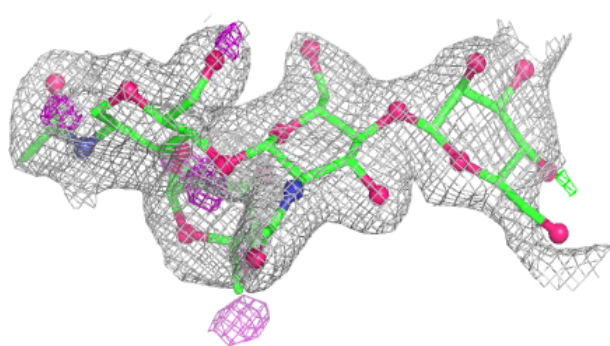
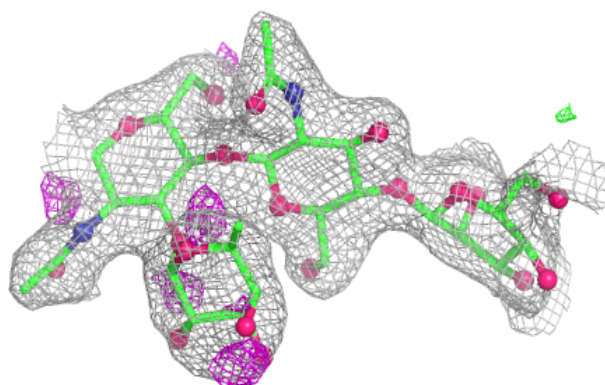


Electron density around Chain M:

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

**Electron density around Chain N:**

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	SO4	A	409	5/5	0.44	0.21	91,111,132,142	0
11	SO4	C	408	5/5	0.52	0.15	79,107,134,137	0
11	SO4	A	408	5/5	0.55	0.15	100,105,111,135	0
11	SO4	A	415	5/5	0.67	0.21	78,85,106,117	0
11	SO4	C	410	5/5	0.67	0.20	42,44,57,91	0
11	SO4	A	413	5/5	0.71	0.13	86,91,123,125	0
11	SO4	D	302	5/5	0.72	0.15	77,107,125,135	0
11	SO4	D	303	5/5	0.73	0.15	81,100,110,117	0
11	SO4	A	414	5/5	0.74	0.16	69,90,117,128	0
11	SO4	C	415	5/5	0.75	0.16	60,90,97,117	0
11	SO4	A	412	5/5	0.75	0.10	91,110,132,135	0
11	SO4	B	203	5/5	0.75	0.14	76,92,100,112	0
10	EDO	E	608	4/4	0.76	0.24	52,69,77,83	0
11	SO4	A	410	5/5	0.76	0.12	72,91,122,125	0
10	EDO	A	402	4/4	0.76	0.30	50,55,68,83	0
12	NAG	E	601	14/15	0.76	0.15	74,79,93,98	0
11	SO4	E	614	5/5	0.78	0.17	84,85,98,112	0
11	SO4	C	413	5/5	0.79	0.12	73,80,105,122	0
10	EDO	C	403	4/4	0.79	0.27	45,53,67,72	0
11	SO4	E	613	5/5	0.80	0.12	69,88,114,115	0
10	EDO	C	405	4/4	0.80	0.25	43,60,62,66	0
10	EDO	F	202	4/4	0.80	0.20	66,72,77,78	0
11	SO4	E	611	5/5	0.81	0.14	45,77,110,126	0
11	SO4	C	416	5/5	0.81	0.14	57,70,89,93	0
11	SO4	A	417	5/5	0.81	0.16	57,71,93,107	0
11	SO4	A	411	5/5	0.81	0.14	87,88,112,115	0
10	EDO	B	201	4/4	0.84	0.24	55,68,73,75	0
11	SO4	C	409	5/5	0.84	0.14	42,60,73,83	0
11	SO4	E	612	5/5	0.85	0.10	104,105,120,134	0
10	EDO	E	605	4/4	0.85	0.21	54,68,68,76	0
10	EDO	B	202	4/4	0.86	0.19	56,57,59,67	0
11	SO4	C	412	5/5	0.86	0.15	32,63,70,70	0
10	EDO	D	301	4/4	0.87	0.19	54,57,58,71	0
10	EDO	C	404	4/4	0.87	0.16	55,70,73,78	0
10	EDO	C	401	4/4	0.88	0.17	43,45,64,72	0
10	EDO	A	405	4/4	0.88	0.17	47,55,69,73	0
11	SO4	C	414	5/5	0.88	0.12	50,65,80,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	EDO	E	604	4/4	0.88	0.20	42,50,65,74	0
10	EDO	A	406	4/4	0.88	0.20	36,43,44,68	0
10	EDO	E	606	4/4	0.88	0.17	61,61,63,73	0
10	EDO	E	607	4/4	0.89	0.19	38,41,43,61	0
10	EDO	F	203	4/4	0.89	0.15	57,63,63,70	0
11	SO4	A	416	5/5	0.89	0.11	42,83,94,95	0
10	EDO	A	401	4/4	0.89	0.17	37,43,49,53	0
10	EDO	F	201	4/4	0.89	0.19	41,57,62,79	0
13	PEG	E	609	7/7	0.89	0.17	29,37,53,72	0
10	EDO	A	404	4/4	0.90	0.20	32,56,62,76	0
10	EDO	E	602	4/4	0.91	0.16	35,43,54,55	0
13	PEG	E	610	7/7	0.91	0.17	36,46,57,60	0
10	EDO	C	402	4/4	0.92	0.15	38,38,65,66	0
10	EDO	A	403	4/4	0.94	0.17	33,35,36,43	0
11	SO4	E	616	5/5	0.95	0.17	32,34,45,49	0
11	SO4	C	407	5/5	0.95	0.10	50,59,78,78	0
11	SO4	C	411	5/5	0.97	0.14	33,34,42,48	0
11	SO4	A	407	5/5	0.97	0.08	44,51,63,68	0
10	EDO	E	603	4/4	0.97	0.07	28,28,30,31	0
11	SO4	E	615	5/5	0.97	0.09	42,42,50,65	0
10	EDO	C	406	4/4	0.98	0.06	27,30,31,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.