wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2025 – 11:18 PM EDT

PDB ID	:	7U4E / pdb_00007u4e
Title	:	Neuraminidase from influenza virus A/Bilthoven/17938/1969(H3N2)
Authors	:	Lei, R.; Hernandez Garcia, A.
Deposited on	:	2022-02-28
Resolution	:	1.54 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 (i) 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 (i)) were used in the production of this report:

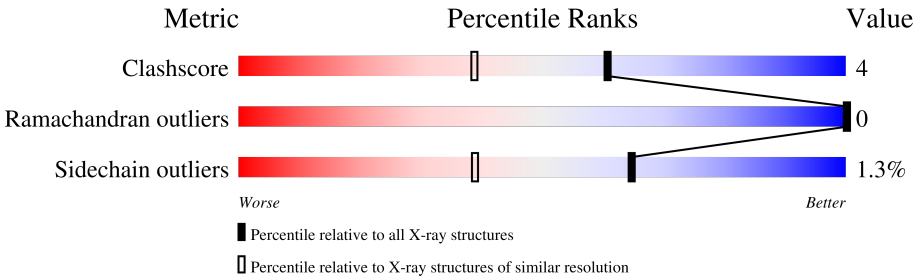
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.54 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))
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	469	75% 7% 17%
1	B	469	75% 7% 17%
1	C	469	76% 7% 17%
1	D	469	76% 6% 17%
2	F	6	83% 17%
2	G	6	100%
2	H	6	100%
2	K	6	50% 33% 17%

2 Entry composition (i)

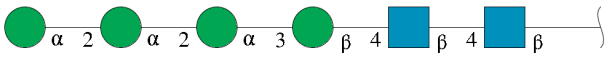
There are 6 unique types of molecules in this entry. The entry contains 14568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

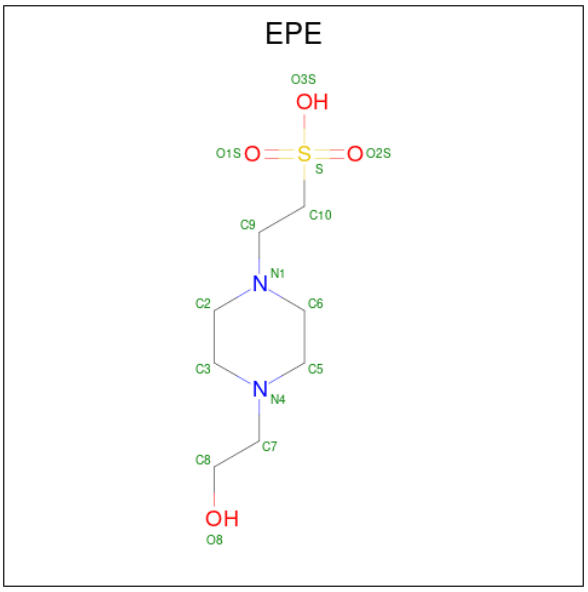
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	1	0
			3033	1872	549	589	23			
1	B	388	Total	C	N	O	S	0	3	0
			3041	1879	549	590	23			
1	C	388	Total	C	N	O	S	0	4	0
			3044	1879	550	592	23			
1	D	388	Total	C	N	O	S	0	2	0
			3038	1875	550	590	23			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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.



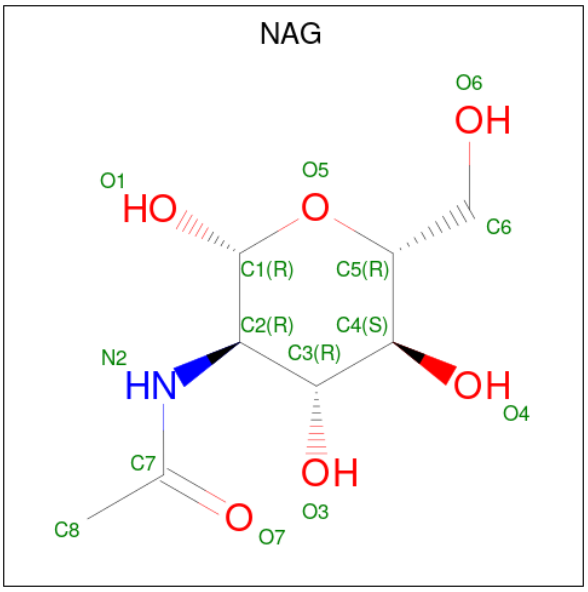
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	G	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	H	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 15 8 2 4 1	0	0
3	B	1	Total C N O S 15 8 2 4 1	0	0
3	C	1	Total C N O S 15 8 2 4 1	0	0
3	D	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	495	Total O 495 495	0	0
6	B	518	Total O 518 518	0	0
6	C	493	Total O 493 493	0	0
6	D	498	Total O 498 498	0	0

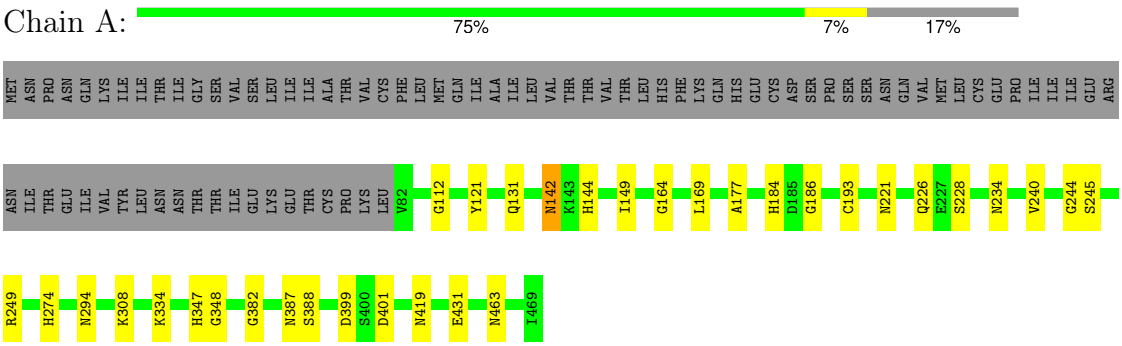
3 Residue-property plots (i)

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.

Note EDS failed to run properly.

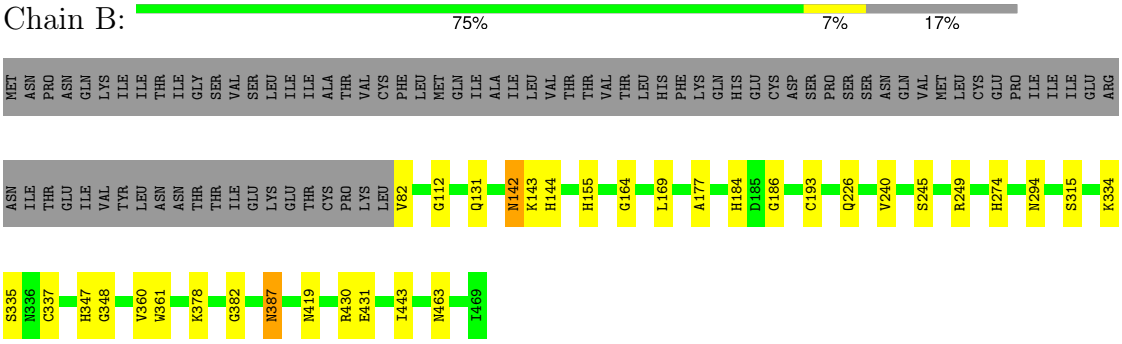
- Molecule 1: Neuraminidase

Chain A:



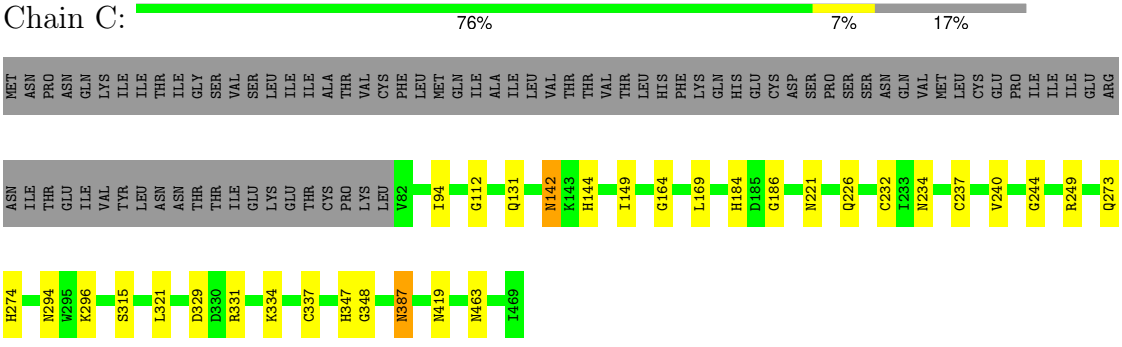
- Molecule 1: Neuraminidase

Chain B:



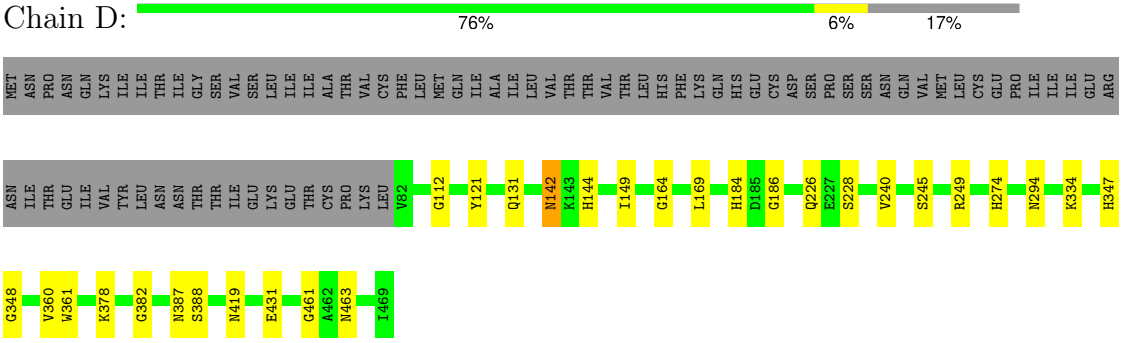
- Molecule 1: Neuraminidase

Chain C:



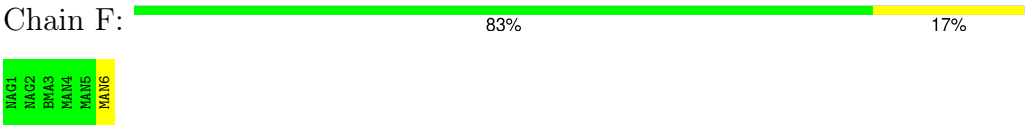
- Molecule 1: Neuraminidase

Chain D:



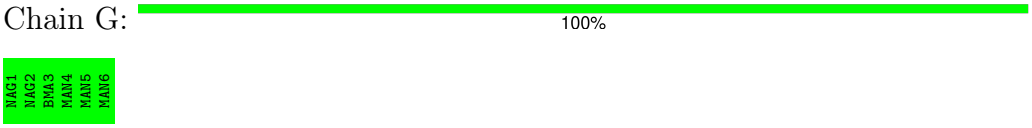
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



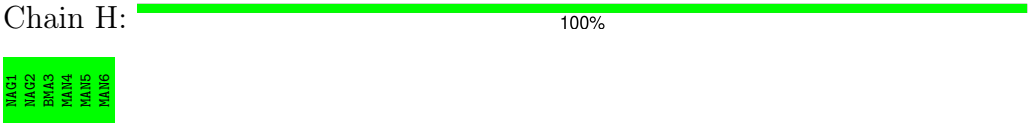
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 H:



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 K:

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.34Å 137.94Å 138.25Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	25.00 – 1.54	Depositor
% Data completeness (in resolution range)	100.0 (25.00-1.54)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.180	Depositor
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.618	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.079 for -h,-k,l	Xtriage
Total number of atoms	14568	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.26	0/3104	0.57	0/4207
1	B	0.26	0/3118	0.58	0/4226
1	C	0.26	0/3124	0.57	0/4234
1	D	0.26	0/3112	0.57	0/4218
All	All	0.26	0/12458	0.57	0/16885

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

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	3033	0	2865	29	0
1	B	3041	0	2881	26	0
1	C	3044	0	2881	27	0
1	D	3038	0	2871	27	0
2	F	72	0	61	0	0
2	G	72	0	61	0	0
2	H	72	0	61	0	0
2	K	72	0	61	5	0
3	A	15	0	17	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	18	0	0
3	C	15	0	17	0	0
3	D	15	0	17	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	495	0	0	5	0
6	B	518	0	0	1	0
6	C	493	0	0	2	0
6	D	498	0	0	3	0
All	All	14568	0	11863	100	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.

The worst 5 of 100 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:A:463:ASN:H	1:C:144:HIS:HE2	1.22	0.86
1:B:144:HIS:HE2	1:D:463:ASN:H	1.26	0.83
1:A:144:HIS:HE2	1:B:463:ASN:H	1.24	0.82
1:C:463:ASN:H	1:D:144:HIS:HE2	1.24	0.81
1:D:226:GLN:HE21	1:D:240:VAL:H	1.29	0.81

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	387/469 (82%)	370 (96%)	17 (4%)	0	100	100
1	B	389/469 (83%)	372 (96%)	17 (4%)	0	100	100
1	C	390/469 (83%)	373 (96%)	17 (4%)	0	100	100
1	D	388/469 (83%)	372 (96%)	16 (4%)	0	100	100
All	All	1554/1876 (83%)	1487 (96%)	67 (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	340/417 (82%)	337 (99%)	3 (1%)	75	56
1	B	342/417 (82%)	335 (98%)	7 (2%)	50	20
1	C	343/417 (82%)	335 (98%)	8 (2%)	45	16
1	D	341/417 (82%)	339 (99%)	2 (1%)	84	71
All	All	1366/1668 (82%)	1346 (98%)	20 (2%)	65	33

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	329	ASP
1	C	419	ASN
1	D	419	ASN
1	D	142	ASN
1	B	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	86	ASN
1	C	264	HIS
1	D	273	GLN

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Mol	Chain	Res	Type
1	C	104	ASN
1	C	161	ASN

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)

24 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	F	1	1,2	14,14,15	0.32	0	17,19,21	0.71	0
2	NAG	F	2	2	14,14,15	0.38	0	17,19,21	0.51	0
2	BMA	F	3	2	11,11,12	0.28	0	15,15,17	0.49	0
2	MAN	F	4	2	11,11,12	0.30	0	15,15,17	0.72	0
2	MAN	F	5	2	11,11,12	0.29	0	15,15,17	0.72	0
2	MAN	F	6	2	11,11,12	0.32	0	15,15,17	0.73	1 (6%)
2	NAG	G	1	1,2	14,14,15	0.36	0	17,19,21	0.53	0
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.59	0
2	BMA	G	3	2	11,11,12	0.27	0	15,15,17	0.53	0
2	MAN	G	4	2	11,11,12	0.28	0	15,15,17	0.72	0
2	MAN	G	5	2	11,11,12	0.36	0	15,15,17	0.64	0
2	MAN	G	6	2	11,11,12	0.47	0	15,15,17	0.82	0
2	NAG	H	1	1,2	14,14,15	0.41	0	17,19,21	0.74	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.59	0
2	BMA	H	3	2	11,11,12	0.33	0	15,15,17	0.47	0
2	MAN	H	4	2	11,11,12	0.25	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	H	5	2	11,11,12	0.31	0	15,15,17	0.65	0
2	MAN	H	6	2	11,11,12	0.43	0	15,15,17	0.72	0
2	NAG	K	1	1,2	14,14,15	0.35	0	17,19,21	0.91	1 (5%)
2	NAG	K	2	2	14,14,15	0.27	0	17,19,21	0.46	0
2	BMA	K	3	2	11,11,12	0.27	0	15,15,17	0.48	0
2	MAN	K	4	2	11,11,12	0.28	0	15,15,17	0.75	0
2	MAN	K	5	2	11,11,12	0.33	0	15,15,17	0.83	1 (6%)
2	MAN	K	6	2	11,11,12	0.36	0	15,15,17	1.03	1 (6%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	6	MAN	C1-O5-C5	2.99	116.20	112.19
2	K	5	MAN	C1-O5-C5	2.87	116.03	112.19
2	F	6	MAN	C1-O5-C5	2.13	115.04	112.19
2	K	1	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	5	MAN	C4-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
2	K	5	MAN	O5-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
2	K	1	NAG	O7-C7-N2-C2

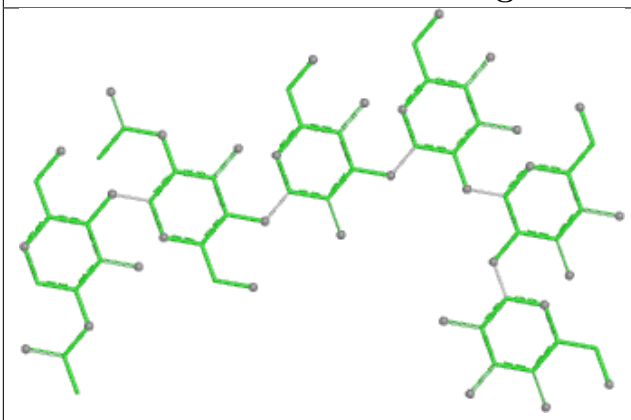
There are no ring outliers.

1 monomer is involved in 5 short contacts:

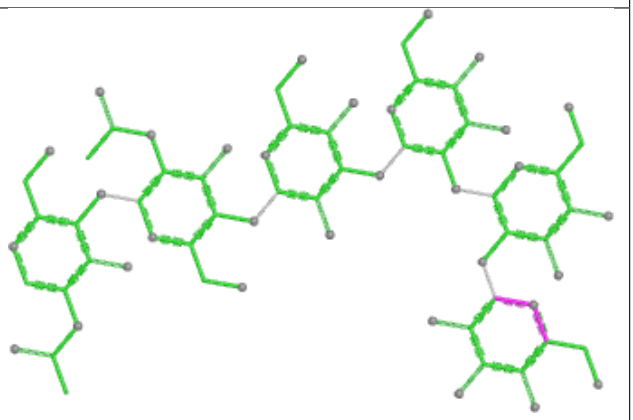
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	6	MAN	5	0

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

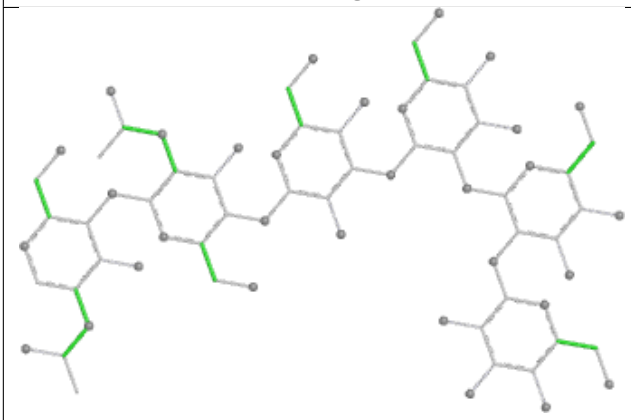
Oligosaccharide Chain F



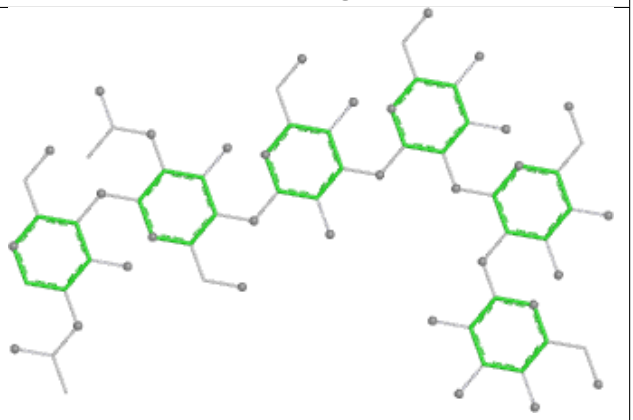
Bond lengths



Bond angles

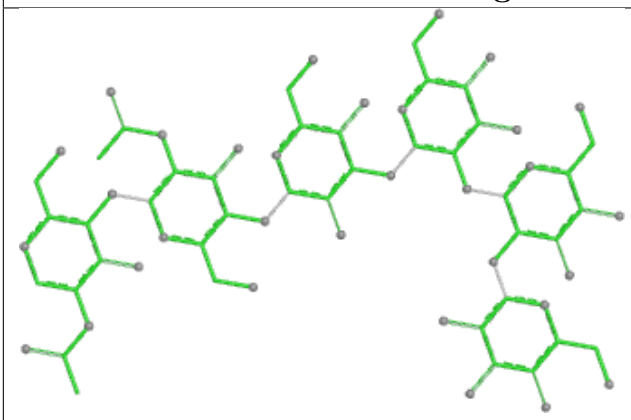


Torsions

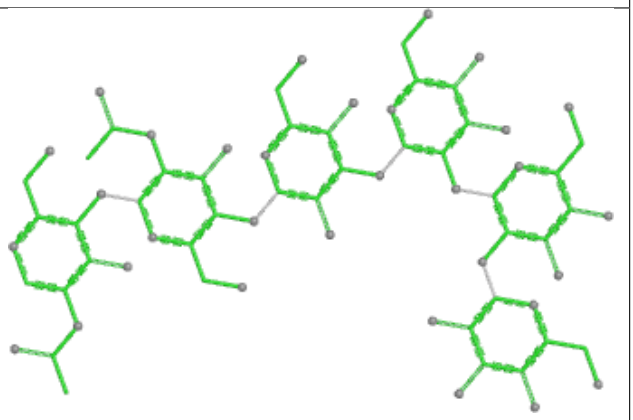


Rings

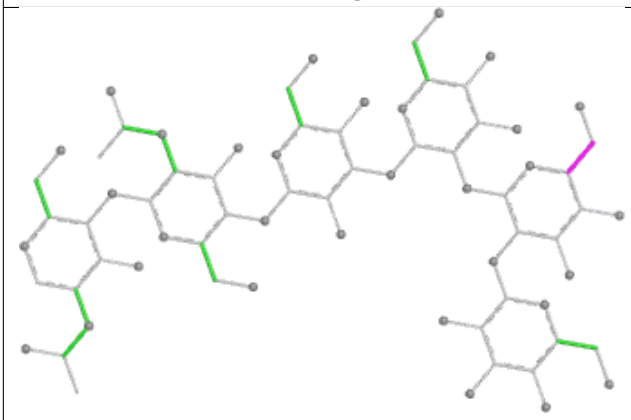
Oligosaccharide Chain G



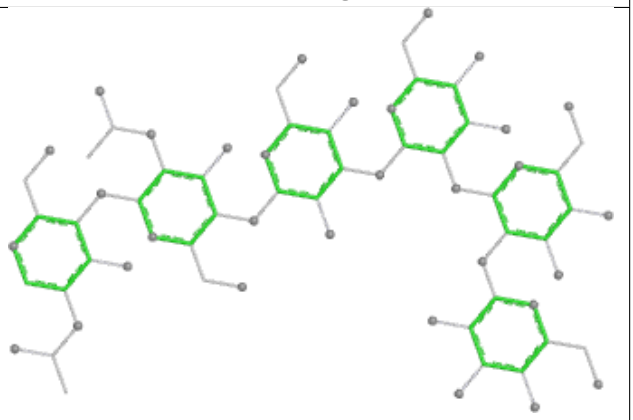
Bond lengths



Bond angles

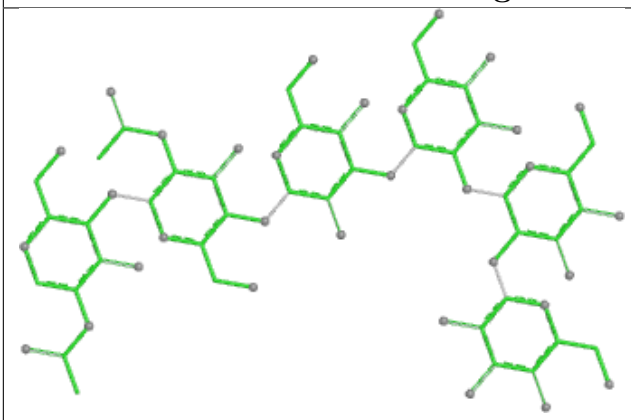


Torsions

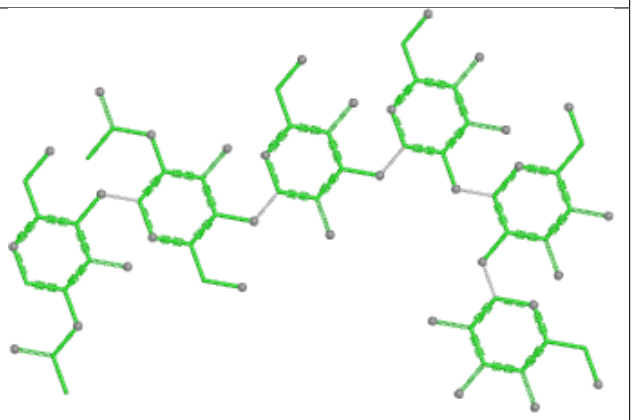


Rings

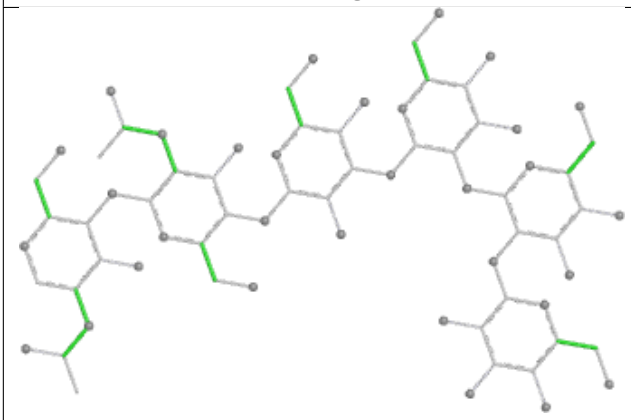
Oligosaccharide Chain H



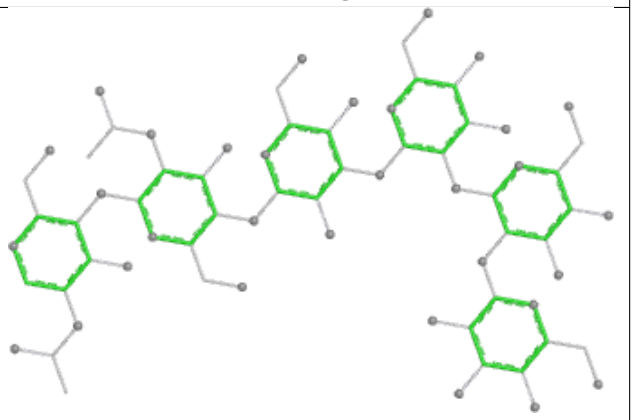
Bond lengths



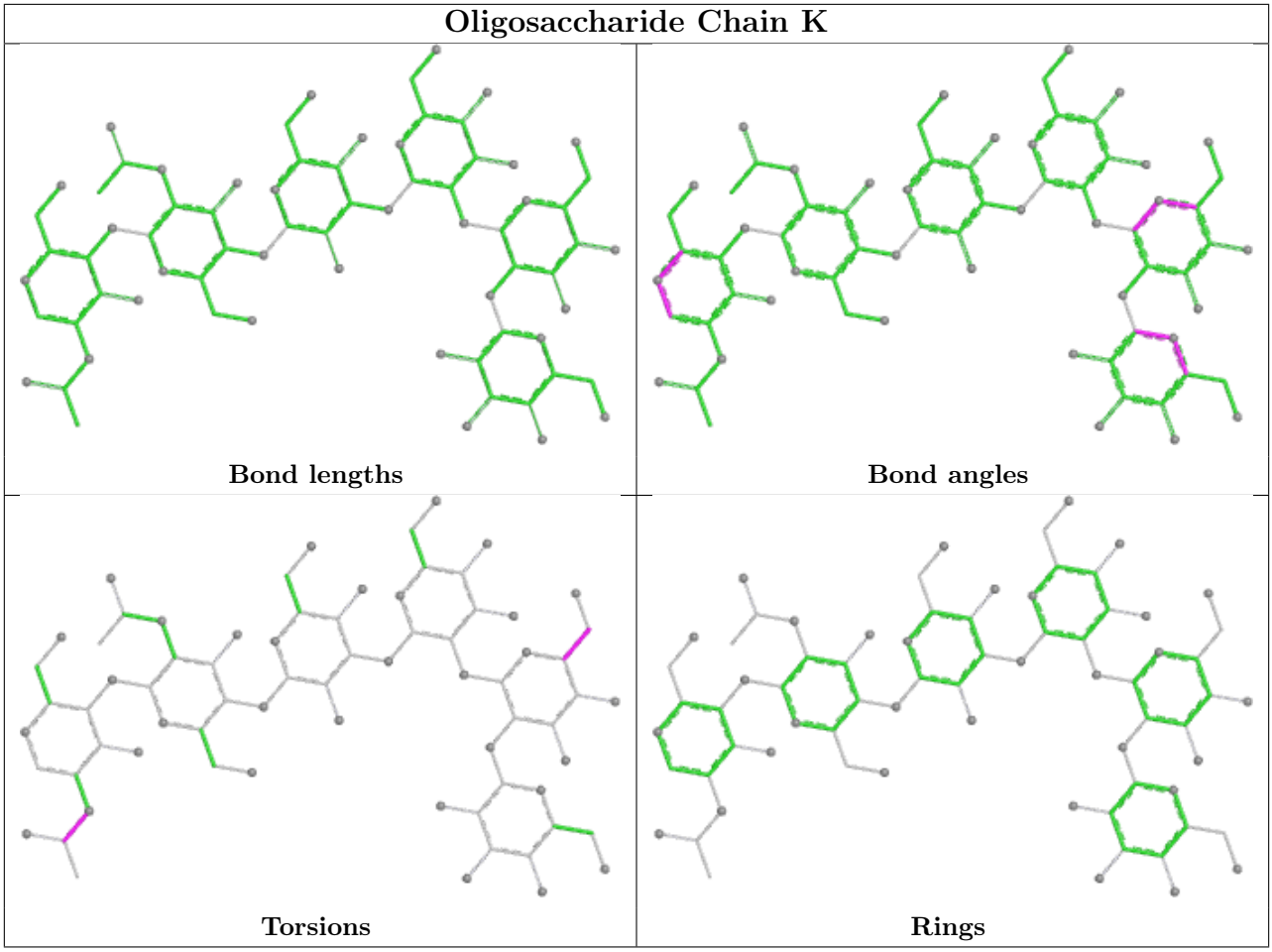
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
4	NAG	A	502	1	14,14,15	0.33	0	17,19,21	0.63	0
3	EPE	B	502	-	15,15,15	0.60	1 (6%)	19,20,20	0.55	0
4	NAG	D	502	1	14,14,15	0.36	0	17,19,21	0.56	0
4	NAG	B	501	1	14,14,15	0.38	0	17,19,21	0.75	1 (5%)
3	EPE	A	501	-	15,15,15	0.91	1 (6%)	19,20,20	1.00	2 (10%)
3	EPE	C	501	-	15,15,15	0.95	1 (6%)	19,20,20	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	502	1	14,14,15	0.37	0	17,19,21	0.42	0
3	EPE	D	501	-	15,15,15	0.94	1 (6%)	19,20,20	0.95	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	EPE	B	502	-	-	1/9/19/19	0/1/1/1
4	NAG	D	502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
3	EPE	A	501	-	-	3/9/19/19	0/1/1/1
3	EPE	C	501	-	-	5/9/19/19	0/1/1/1
4	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	EPE	D	501	-	-	3/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	EPE	O1S-S	3.52	1.55	1.45
3	D	501	EPE	O1S-S	3.45	1.54	1.45
3	A	501	EPE	O2S-S	3.37	1.54	1.45
3	B	502	EPE	O3S-S	2.13	1.55	1.47

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	EPE	O2S-S-C10	-2.84	102.43	106.73
3	C	501	EPE	O3S-S-O2S	2.75	118.28	111.40
3	A	501	EPE	O3S-S-O1S	2.68	118.11	111.40
3	D	501	EPE	O1S-S-C10	-2.57	102.85	106.73
3	D	501	EPE	O3S-S-O2S	2.46	117.55	111.40

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
3	A	501	EPE	S-C10-C9-N1
3	D	501	EPE	C10-C9-N1-C2
3	C	501	EPE	N4-C7-C8-O8
3	C	501	EPE	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	EPE	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

EDS failed to run properly - this section is therefore empty.

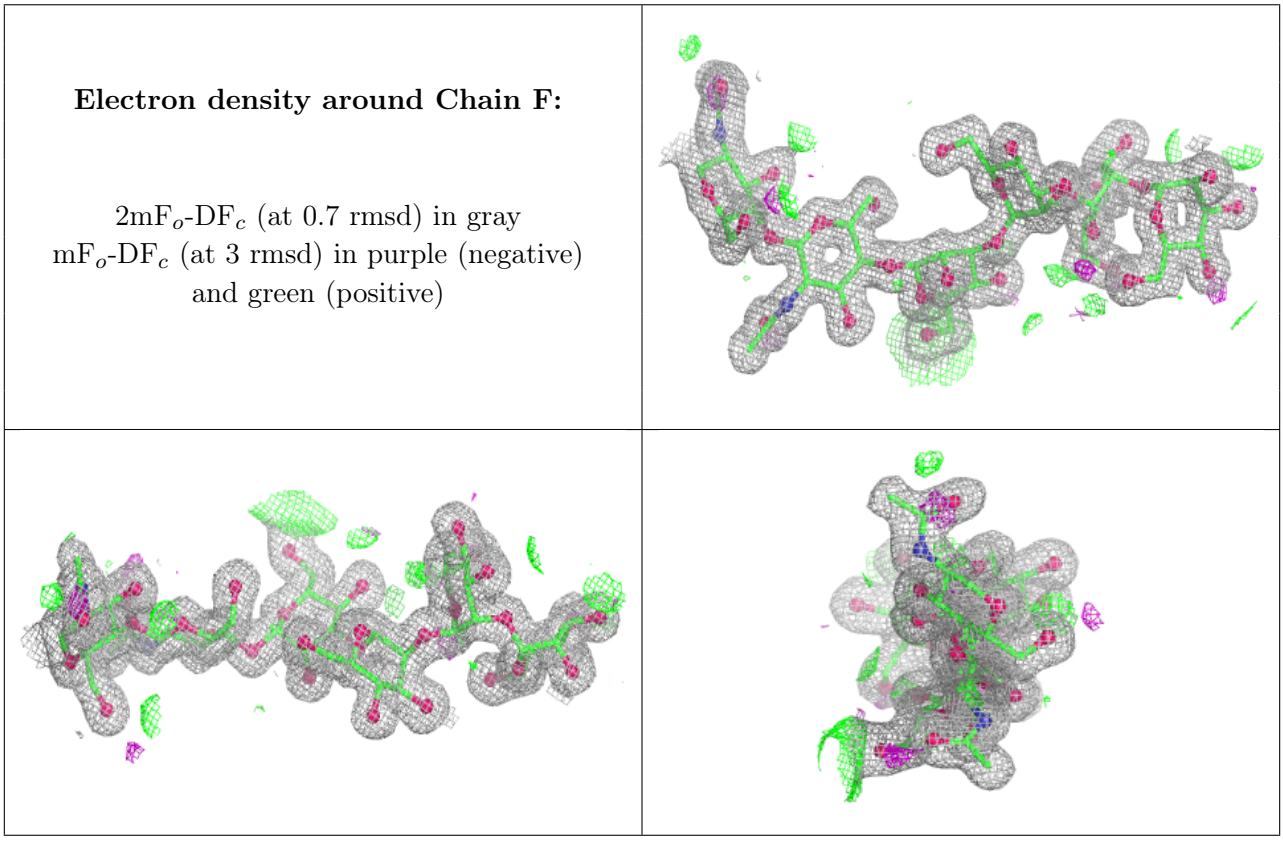
6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

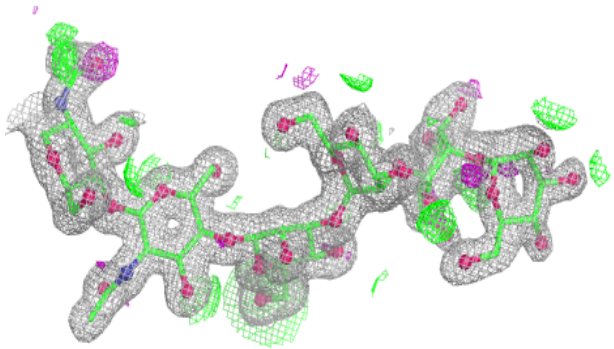
EDS failed to run properly - this section is therefore empty.

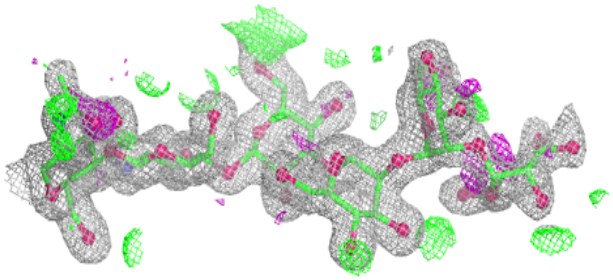
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

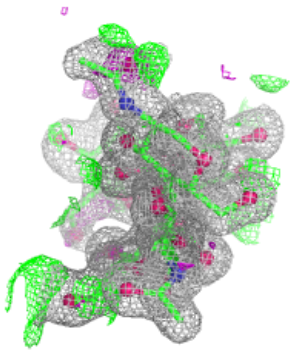


Electron density around Chain G:

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

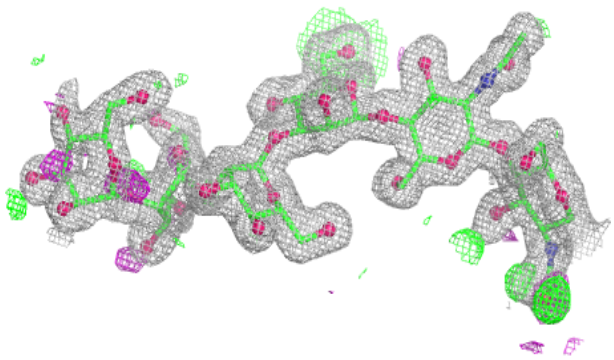


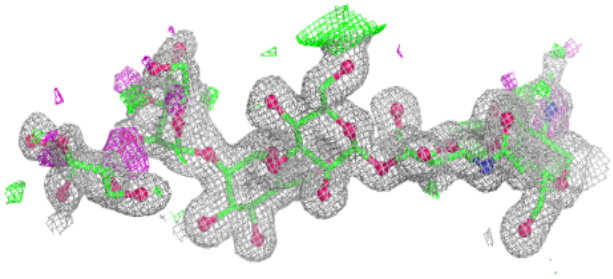


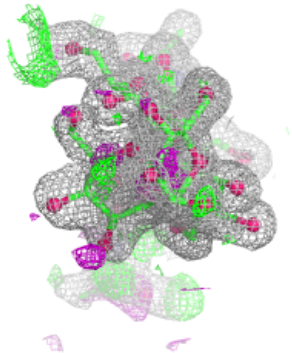


Electron density around Chain H:

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

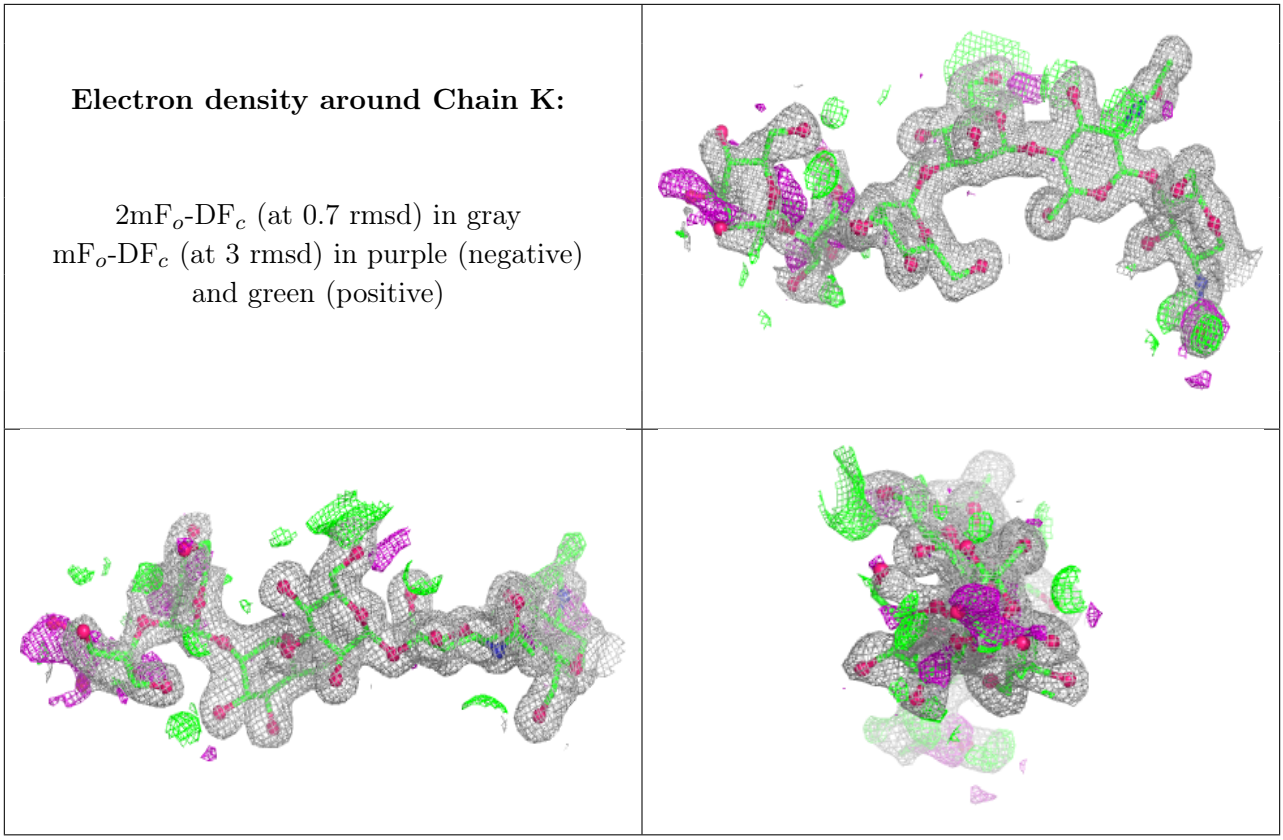






Electron density around Chain K:

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



6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.