wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2023 – 06:51 PM EDT

PDB ID	:	5V5X
Title	:	Protocadherin gammaB7 EC3-6 cis-dimer structure
Authors	:	Goodman, K.M.; Mannepalli, S.; Bahna, F.; Honig, B.; Shapiro, L.
Deposited on	:	2017-03-15
Resolution	:	3.50 Å(reported)

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

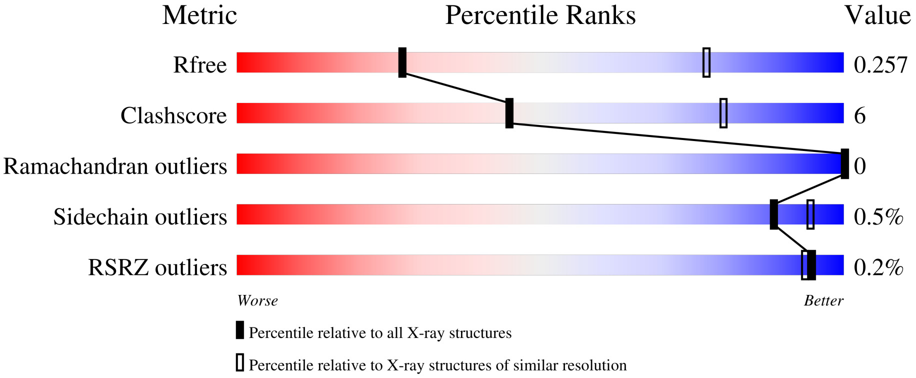
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

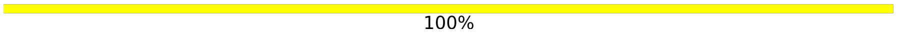
The reported resolution of this entry is 3.50 Å.

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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 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	439	
1	B	439	
1	C	439	
1	D	439	
2	E	3	

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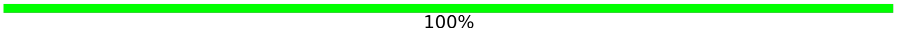
Mol	Chain	Length	Quality of chain
3	F	2	
4	G	3	
5	H	2	

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
2	NAG	E	2	-	-	-	X
4	BMA	G	3	-	-	-	X
8	NAG	C	719	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13104 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 MCG133388, isoform CRA_y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total 3197	C 1988	N 550	O 653	S 6	0	0	0
1	B	415	Total 3102	C 1938	N 532	O 628	S 4	0	1	0
1	C	415	Total 3111	C 1943	N 527	O 636	S 5	0	0	0
1	D	427	Total 3209	C 1994	N 554	O 656	S 5	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	HIS	-	expression tag	UNP Q91XX3
A	640	HIS	-	expression tag	UNP Q91XX3
A	641	HIS	-	expression tag	UNP Q91XX3
A	642	HIS	-	expression tag	UNP Q91XX3
A	643	HIS	-	expression tag	UNP Q91XX3
A	644	HIS	-	expression tag	UNP Q91XX3
A	645	HIS	-	expression tag	UNP Q91XX3
A	646	HIS	-	expression tag	UNP Q91XX3
B	639	HIS	-	expression tag	UNP Q91XX3
B	640	HIS	-	expression tag	UNP Q91XX3
B	641	HIS	-	expression tag	UNP Q91XX3
B	642	HIS	-	expression tag	UNP Q91XX3
B	643	HIS	-	expression tag	UNP Q91XX3
B	644	HIS	-	expression tag	UNP Q91XX3
B	645	HIS	-	expression tag	UNP Q91XX3
B	646	HIS	-	expression tag	UNP Q91XX3
C	639	HIS	-	expression tag	UNP Q91XX3
C	640	HIS	-	expression tag	UNP Q91XX3
C	641	HIS	-	expression tag	UNP Q91XX3
C	642	HIS	-	expression tag	UNP Q91XX3
C	643	HIS	-	expression tag	UNP Q91XX3

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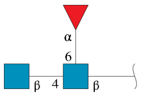
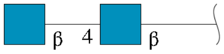
Chain	Residue	Modelled	Actual	Comment	Reference
C	644	HIS	-	expression tag	UNP Q91XX3
C	645	HIS	-	expression tag	UNP Q91XX3
C	646	HIS	-	expression tag	UNP Q91XX3
D	639	HIS	-	expression tag	UNP Q91XX3
D	640	HIS	-	expression tag	UNP Q91XX3
D	641	HIS	-	expression tag	UNP Q91XX3
D	642	HIS	-	expression tag	UNP Q91XX3
D	643	HIS	-	expression tag	UNP Q91XX3
D	644	HIS	-	expression tag	UNP Q91XX3
D	645	HIS	-	expression tag	UNP Q91XX3
D	646	HIS	-	expression tag	UNP Q91XX3

- Molecule 2 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.



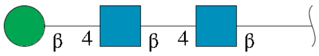
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	38	22	2	14	0	0	0

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



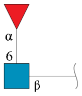
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0

- Molecule 4 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
4	G	3	Total C N O 39 22 2 15	0	0	0

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

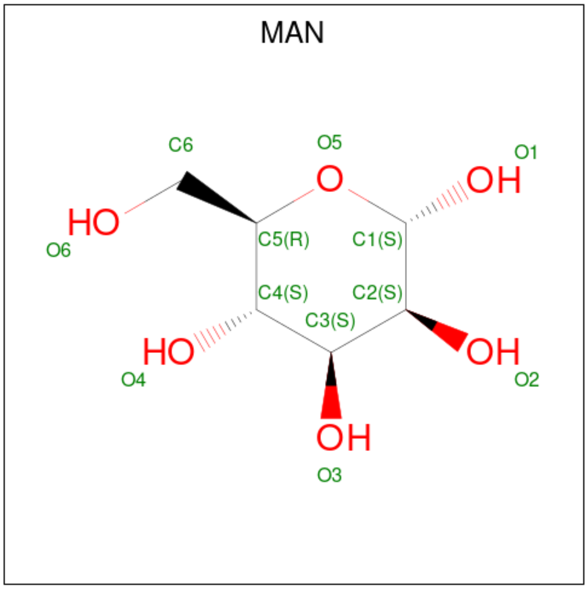


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	2	Total C N O 24 14 1 9	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total Ca 9 9	0	0
6	B	9	Total Ca 9 9	0	0
6	C	9	Total Ca 9 9	0	0
6	D	9	Total Ca 9 9	0	0

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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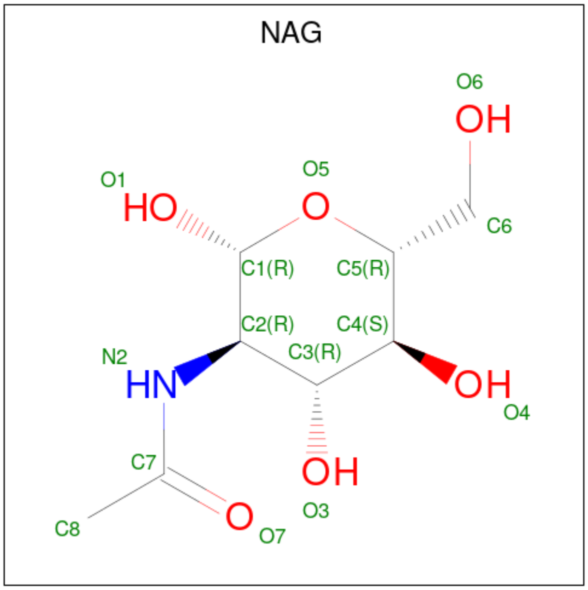
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 11 6 5	0	0
7	D	1	Total C O 11 6 5	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



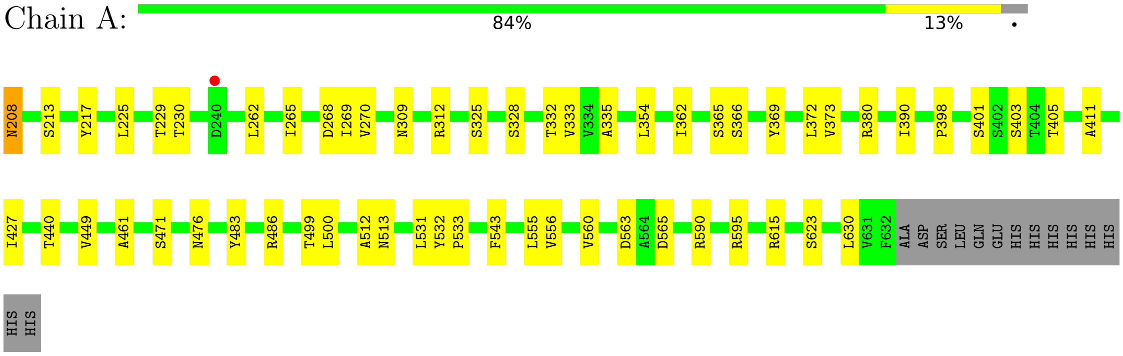
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots

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.

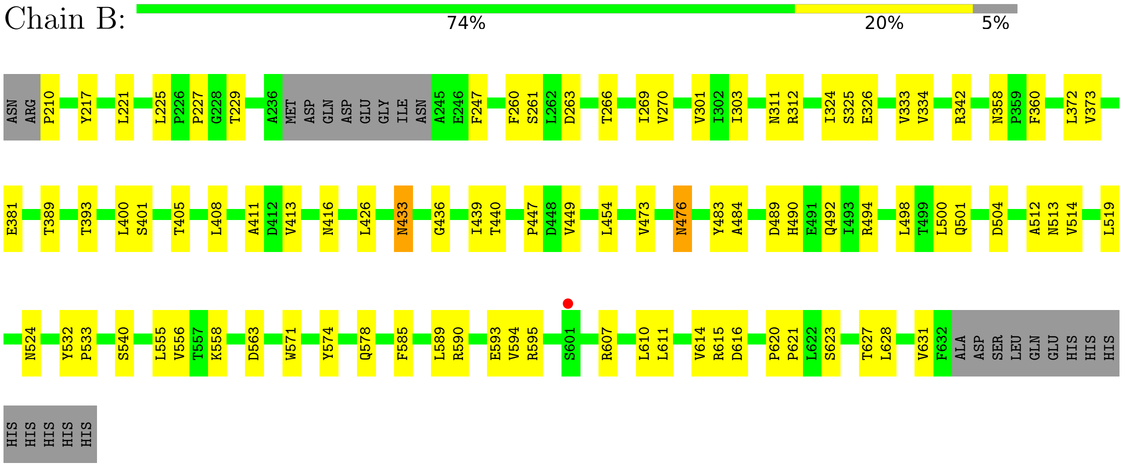
- Molecule 1: MCG133388, isoform CRA_y

Chain A:



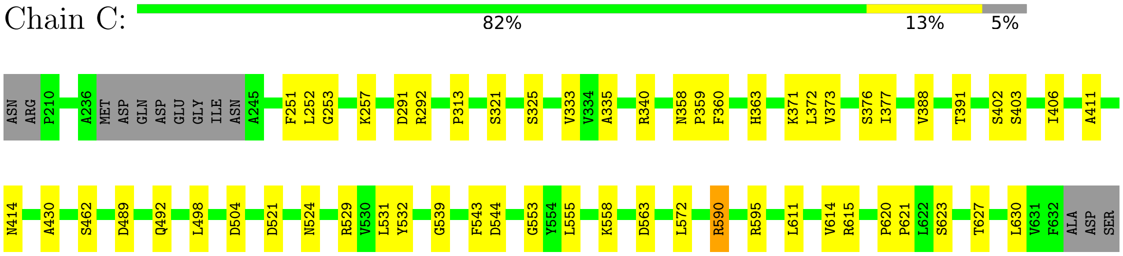
- Molecule 1: MCG133388, isoform CRA_y

Chain B:



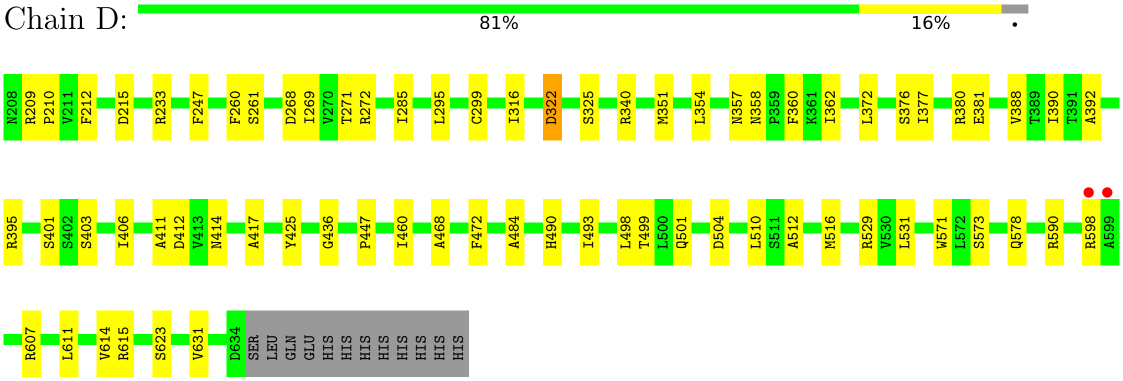
- Molecule 1: MCG133388, isoform CRA_y

Chain C:



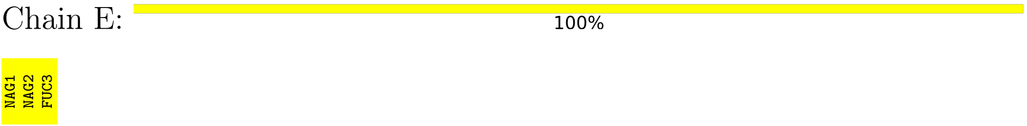
- Molecule 1: MCG133388, isoform CRA_y

Chain D:



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

Chain E:

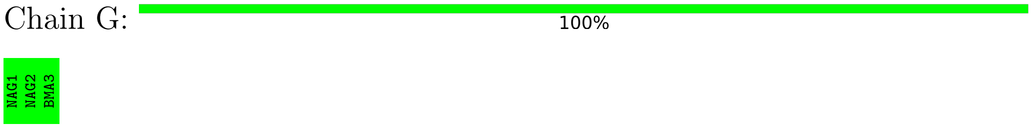


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.24Å 91.76Å 452.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.50 19.96 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.96-3.50) 98.0 (19.96-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.52Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.208 , 0.257 0.208 , 0.257	Depositor DCC
R_{free} test set	1781 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	77.7	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13104	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CA, BMA, MAN, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/3254	0.46	0/4447
1	B	0.27	0/3161	0.46	0/4326
1	C	0.26	0/3167	0.44	0/4332
1	D	0.26	0/3266	0.46	0/4466
All	All	0.26	0/12848	0.46	0/17571

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	3197	0	3058	36	0
1	B	3102	0	2960	61	0
1	C	3111	0	2978	39	0
1	D	3209	0	3062	42	0
2	E	38	0	34	2	0
3	F	28	0	25	0	0
4	G	39	0	34	0	0
5	H	24	0	22	0	0
6	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	0	0
6	C	9	0	0	0	0
6	D	9	0	0	0	0
7	A	66	0	60	0	0
7	B	66	0	60	0	0
7	C	66	0	60	0	0
7	D	66	0	60	0	0
8	A	28	0	26	1	0
8	C	14	0	13	0	0
8	D	14	0	13	0	0
All	All	13104	0	12465	165	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 6.

The worst 5 of 165 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:461:ALA:HB3	1:A:499:THR:HB	1.60	0.81
1:B:490:HIS:O	1:C:590:ARG:NH1	2.24	0.70
1:A:230:THR:HA	1:A:270:VAL:HG22	1.74	0.70
1:D:351:MET:SD	1:D:395:ARG:NH2	2.65	0.69
1:C:555:LEU:HA	1:C:595:ARG:HG2	1.76	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/439 (96%)	410 (97%)	13 (3%)	0	100	100
1	B	412/439 (94%)	396 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	411/439 (94%)	395 (96%)	16 (4%)	0	100	100
1	D	425/439 (97%)	413 (97%)	12 (3%)	0	100	100
All	All	1671/1756 (95%)	1614 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/380 (92%)	350 (100%)	1 (0%)	92	97
1	B	336/380 (88%)	334 (99%)	2 (1%)	86	94
1	C	342/380 (90%)	341 (100%)	1 (0%)	92	97
1	D	351/380 (92%)	348 (99%)	3 (1%)	78	90
All	All	1380/1520 (91%)	1373 (100%)	7 (0%)	88	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	590	ARG
1	D	215	ASP
1	D	598	ARG
1	D	322	ASP
1	B	476	ASN

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

Mol	Chain	Res	Type
1	A	497	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	1,2	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.38	0
2	FUC	E	3	2	10,10,11	0.79	1 (10%)	14,14,16	0.98	1 (7%)
3	NAG	F	1	1,3	14,14,15	0.36	0	17,19,21	0.77	1 (5%)
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	0.40	0
4	NAG	G	1	4,1	14,14,15	0.49	0	17,19,21	0.52	0
4	NAG	G	2	4	14,14,15	0.33	0	17,19,21	0.49	0
4	BMA	G	3	4	11,11,12	0.72	0	15,15,17	0.76	0
5	NAG	H	1	1,5	14,14,15	0.22	0	17,19,21	0.36	0
5	FUC	H	2	5	10,10,11	0.83	0	14,14,16	1.04	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
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	4/6/23/26	0/1/1/1
5	FUC	H	2	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	FUC	C1-C2	2.04	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	2.70	115.85	112.19
5	H	2	FUC	C1-O5-C5	2.37	118.15	112.78
2	E	3	FUC	O2-C2-C1	2.08	113.40	109.15

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

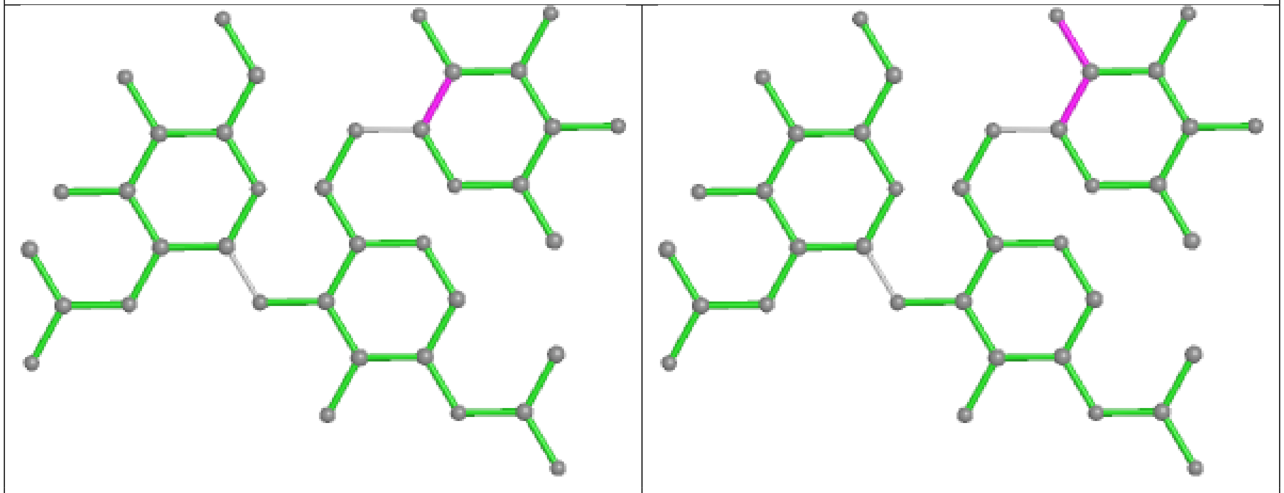
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

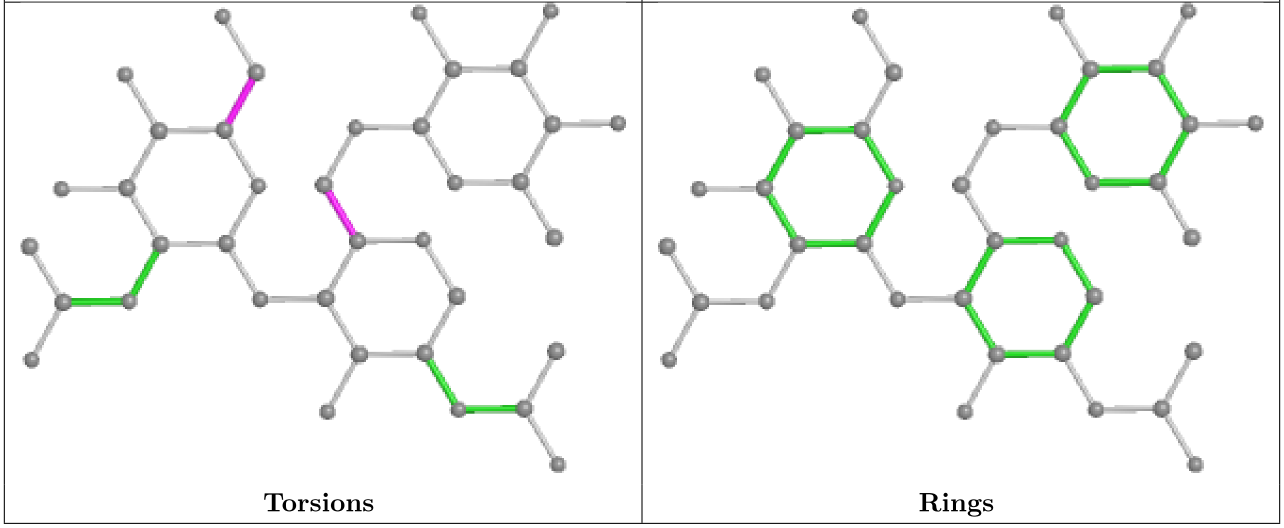
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Bond lengths

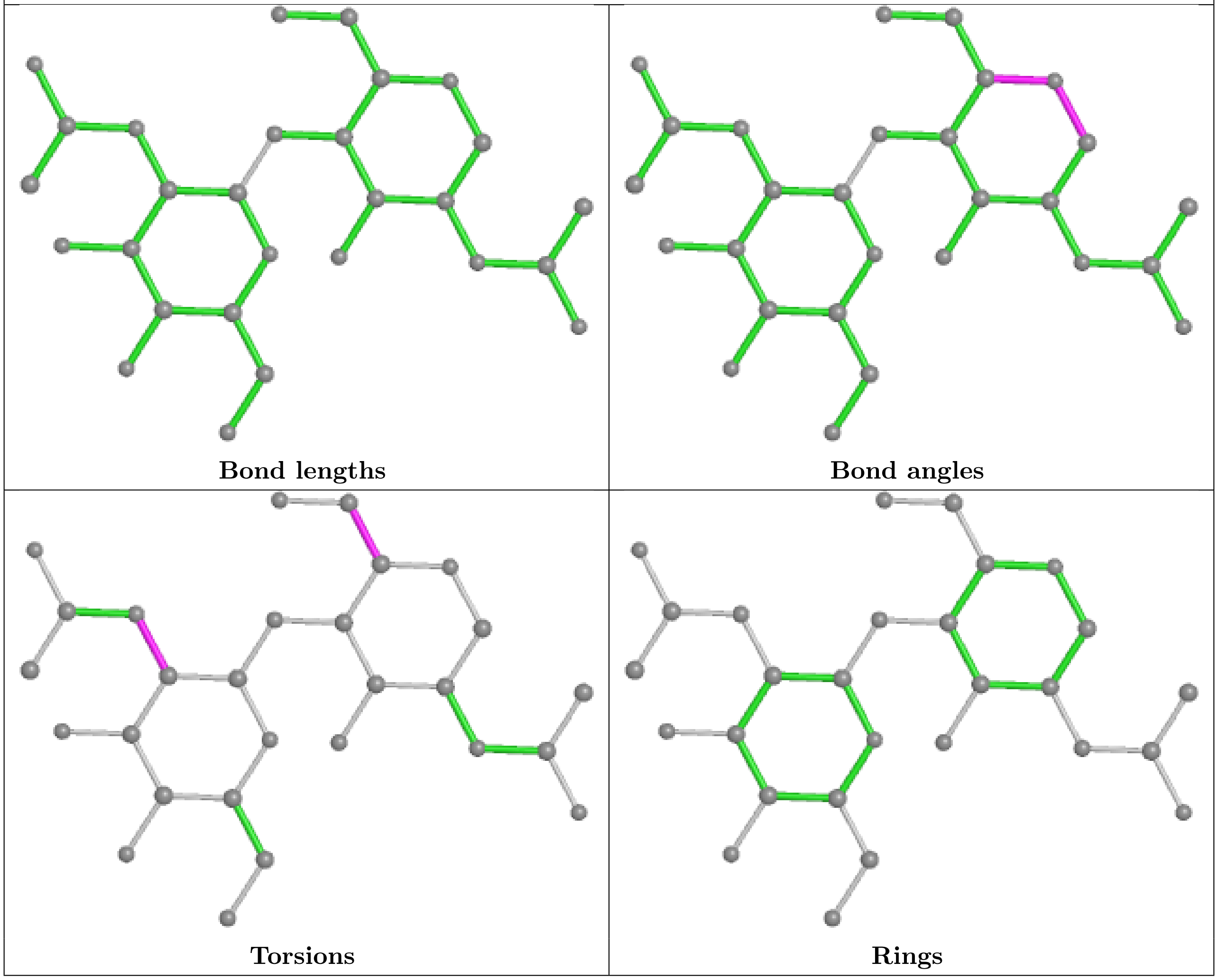
Bond angles



Torsions

Rings

Oligosaccharide Chain F

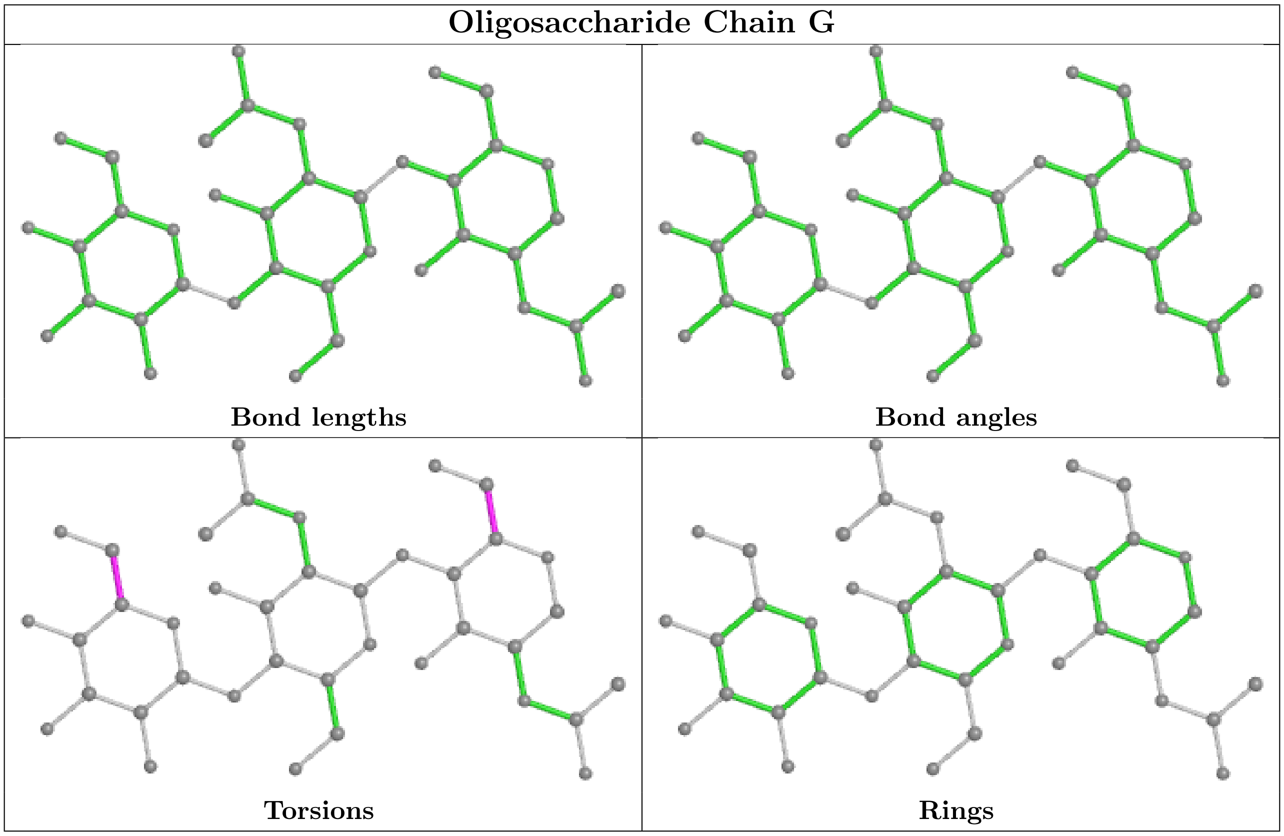


Bond lengths

Bond angles

Torsions

Rings



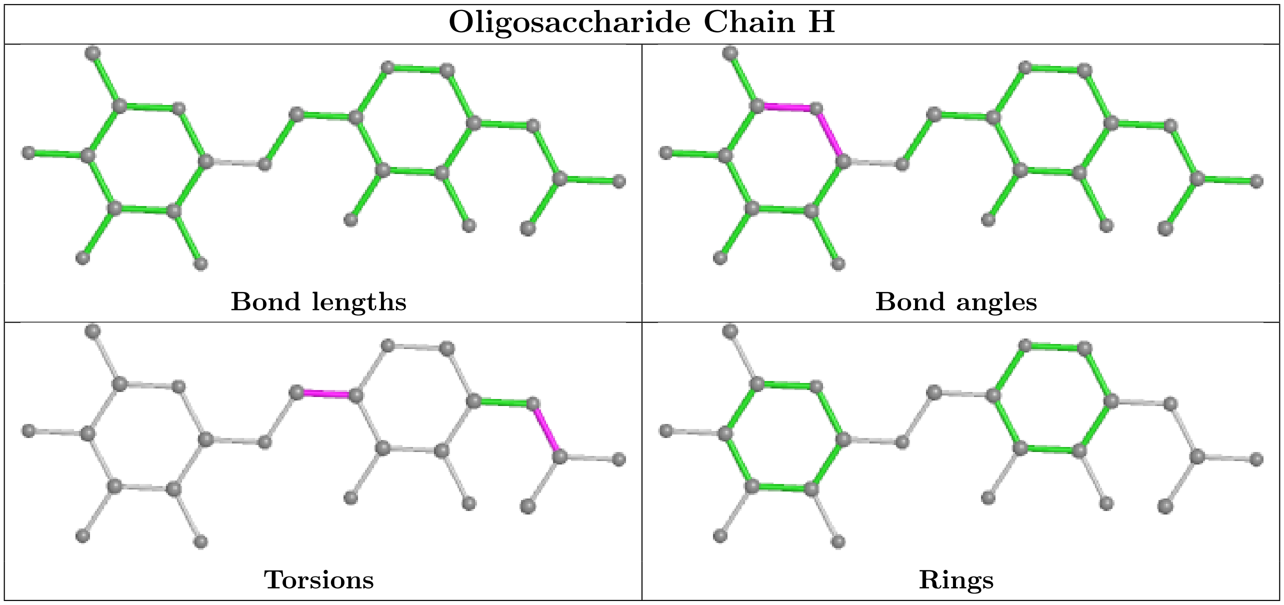
Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings



Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 36 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
7	MAN	B	711	1	11,11,12	0.76	0	15,15,17	1.01	2 (13%)
7	MAN	C	715	1	11,11,12	0.89	0	15,15,17	1.13	1 (6%)
7	MAN	A	712	1	11,11,12	0.68	0	15,15,17	1.36	3 (20%)
7	MAN	D	713	1	11,11,12	0.80	0	15,15,17	1.14	2 (13%)
7	MAN	D	710	1	11,11,12	0.86	0	15,15,17	1.12	2 (13%)
7	MAN	C	713	1	11,11,12	0.72	0	15,15,17	1.21	3 (20%)
7	MAN	A	714	1	11,11,12	0.74	0	15,15,17	1.07	2 (13%)
8	NAG	D	716	1	14,14,15	0.32	0	17,19,21	0.58	0
7	MAN	A	715	1	11,11,12	0.71	0	15,15,17	0.94	1 (6%)
7	MAN	D	714	1	11,11,12	0.76	0	15,15,17	1.08	2 (13%)
7	MAN	B	712	1	11,11,12	0.64	0	15,15,17	1.19	2 (13%)
7	MAN	B	710	1	11,11,12	0.76	0	15,15,17	1.16	2 (13%)
7	MAN	C	710	1	11,11,12	0.93	0	15,15,17	1.09	2 (13%)
7	MAN	D	715	1	11,11,12	0.64	0	15,15,17	1.07	2 (13%)
7	MAN	B	715	1	11,11,12	0.76	0	15,15,17	1.00	2 (13%)
7	MAN	A	713	1	11,11,12	0.83	0	15,15,17	1.08	2 (13%)
8	NAG	A	716	1	14,14,15	0.16	0	17,19,21	0.38	0
7	MAN	A	711	1	11,11,12	0.74	0	15,15,17	1.05	2 (13%)
7	MAN	A	710	1	11,11,12	0.81	1 (9%)	15,15,17	1.00	2 (13%)
8	NAG	A	717	1	14,14,15	0.45	0	17,19,21	0.60	0
7	MAN	C	712	1	11,11,12	0.64	0	15,15,17	1.30	2 (13%)
7	MAN	B	713	1	11,11,12	0.67	0	15,15,17	1.31	3 (20%)
7	MAN	D	711	1	11,11,12	0.94	0	15,15,17	0.98	1 (6%)
7	MAN	D	712	1	11,11,12	0.61	0	15,15,17	1.22	2 (13%)
8	NAG	C	719	1	14,14,15	0.27	0	17,19,21	0.40	0
7	MAN	C	714	1	11,11,12	0.79	0	15,15,17	1.04	2 (13%)
7	MAN	C	711	1	11,11,12	0.78	0	15,15,17	1.16	2 (13%)
7	MAN	B	714	1	11,11,12	0.82	0	15,15,17	1.19	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
7	MAN	B	711	1	-	0/2/19/22	0/1/1/1
7	MAN	C	715	1	-	2/2/19/22	0/1/1/1
7	MAN	A	712	1	-	2/2/19/22	0/1/1/1
7	MAN	D	713	1	-	0/2/19/22	0/1/1/1
7	MAN	D	710	1	-	1/2/19/22	0/1/1/1
7	MAN	C	713	1	-	0/2/19/22	0/1/1/1
7	MAN	A	714	1	-	0/2/19/22	0/1/1/1
8	NAG	D	716	1	-	2/6/23/26	0/1/1/1
7	MAN	A	715	1	-	0/2/19/22	0/1/1/1
7	MAN	D	714	1	-	0/2/19/22	0/1/1/1
7	MAN	B	712	1	-	0/2/19/22	0/1/1/1
7	MAN	B	710	1	-	1/2/19/22	0/1/1/1
7	MAN	C	710	1	-	0/2/19/22	0/1/1/1
7	MAN	D	715	1	-	1/2/19/22	0/1/1/1
7	MAN	B	715	1	-	2/2/19/22	0/1/1/1
7	MAN	A	713	1	-	0/2/19/22	0/1/1/1
8	NAG	A	716	1	-	2/6/23/26	0/1/1/1
7	MAN	A	711	1	-	0/2/19/22	0/1/1/1
7	MAN	A	710	1	-	0/2/19/22	0/1/1/1
8	NAG	A	717	1	-	0/6/23/26	0/1/1/1
7	MAN	C	712	1	-	0/2/19/22	0/1/1/1
7	MAN	B	713	1	-	2/2/19/22	0/1/1/1
7	MAN	D	711	1	-	2/2/19/22	0/1/1/1
7	MAN	D	712	1	-	0/2/19/22	0/1/1/1
8	NAG	C	719	1	-	0/6/23/26	0/1/1/1
7	MAN	C	714	1	-	0/2/19/22	0/1/1/1
7	MAN	C	711	1	-	0/2/19/22	0/1/1/1
7	MAN	B	714	1	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	710	MAN	O5-C1	-2.16	1.40	1.43

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	712	MAN	C1-O5-C5	3.59	117.06	112.19
7	B	713	MAN	C1-O5-C5	3.27	116.62	112.19
7	C	712	MAN	C1-O5-C5	3.22	116.56	112.19
7	C	711	MAN	C1-O5-C5	3.11	116.41	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	712	MAN	C1-O5-C5	2.99	116.24	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	715	MAN	O5-C5-C6-O6
7	B	713	MAN	O5-C5-C6-O6
8	A	716	NAG	O5-C5-C6-O6
7	B	715	MAN	O5-C5-C6-O6
7	A	712	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	716	NAG	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	425/439 (96%)	-0.53	1 (0%)	95	93	47, 92, 148, 183	0
1	B	415/439 (94%)	-0.50	1 (0%)	95	93	43, 90, 175, 219	0
1	C	415/439 (94%)	-0.50	0	100	100	55, 99, 151, 209	0
1	D	427/439 (97%)	-0.52	2 (0%)	91	88	44, 88, 154, 187	0
All	All	1682/1756 (95%)	-0.51	4 (0%)	95	93	43, 93, 157, 219	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ASP	2.8
1	D	599	ALA	2.5
1	D	598	ARG	2.1
1	B	601	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	G	3	11/12	0.73	0.43	125,159,166,167	0
2	NAG	E	2	14/15	0.80	0.46	126,155,163,168	0
5	FUC	H	2	10/11	0.81	0.36	126,142,147,149	0

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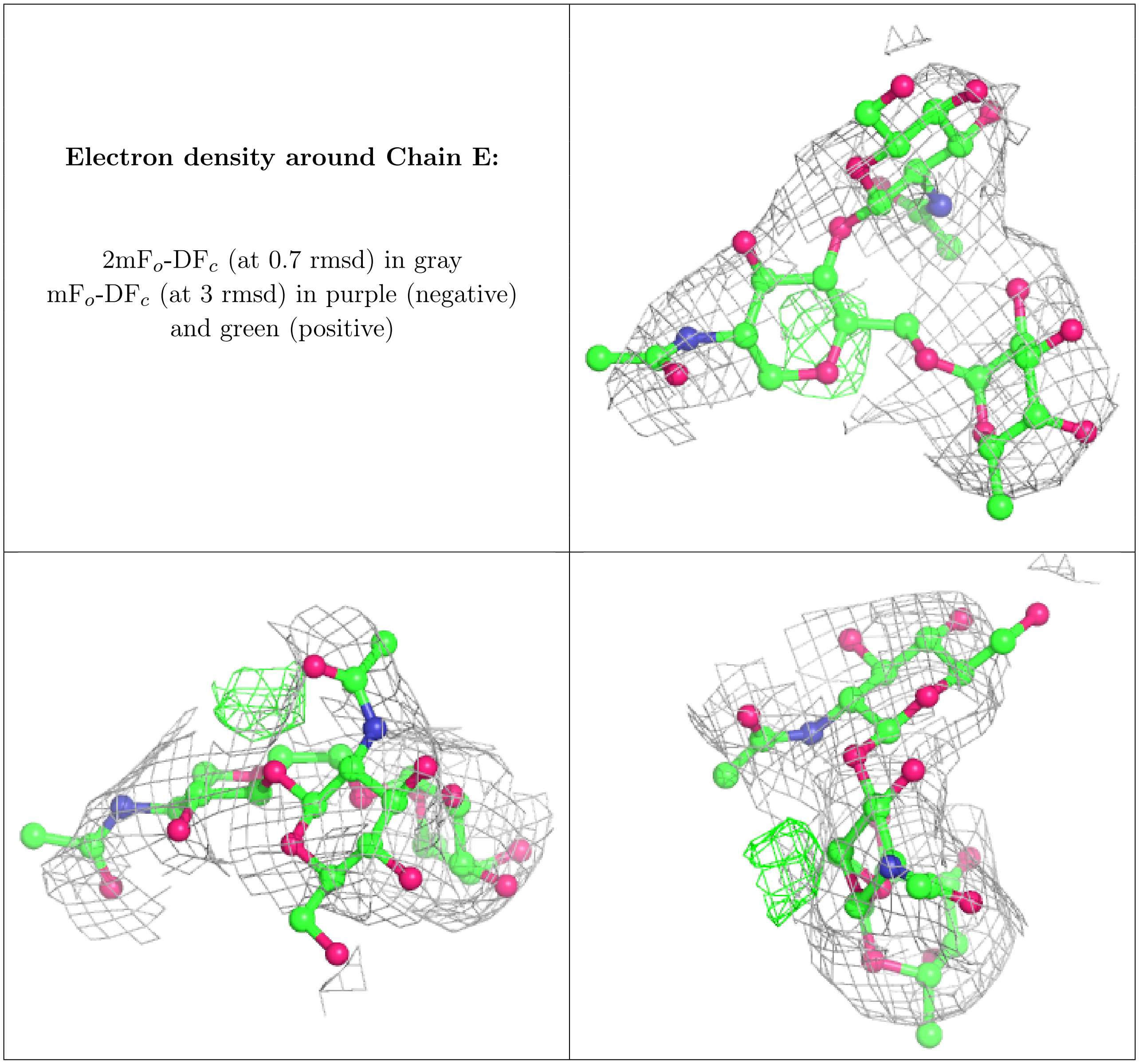
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	F	2	14/15	0.82	0.56	147,153,163,170	0
3	NAG	F	1	14/15	0.85	0.25	80,109,126,138	0
5	NAG	H	1	14/15	0.86	0.30	111,125,145,147	0
4	NAG	G	2	14/15	0.86	0.40	117,144,154,157	0
2	NAG	E	1	14/15	0.87	0.26	112,127,149,156	0
4	NAG	G	1	14/15	0.89	0.25	63,94,129,148	0
2	FUC	E	3	10/11	0.93	0.31	130,143,150,157	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.

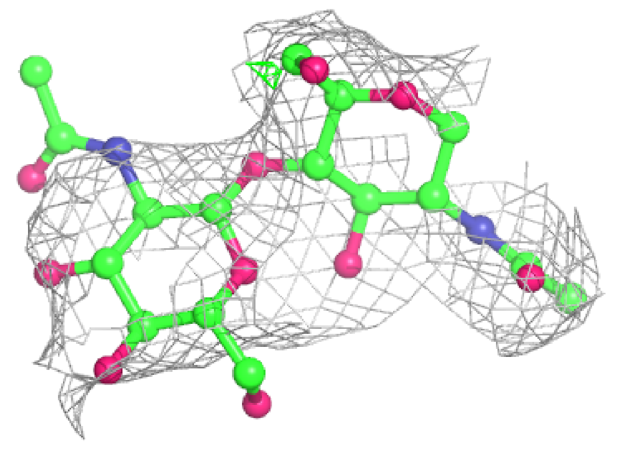


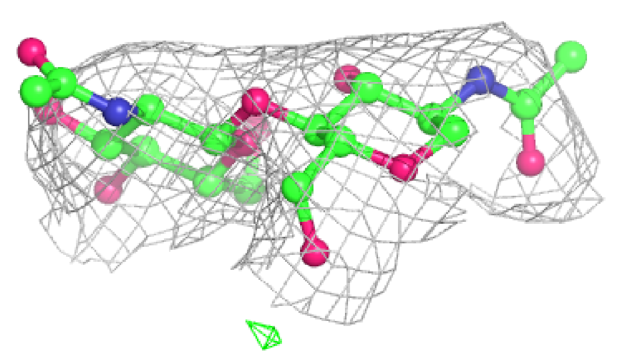
Electron density around Chain E:

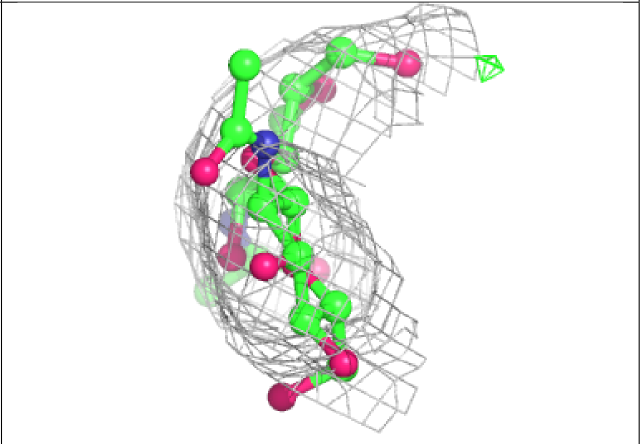
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain F:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

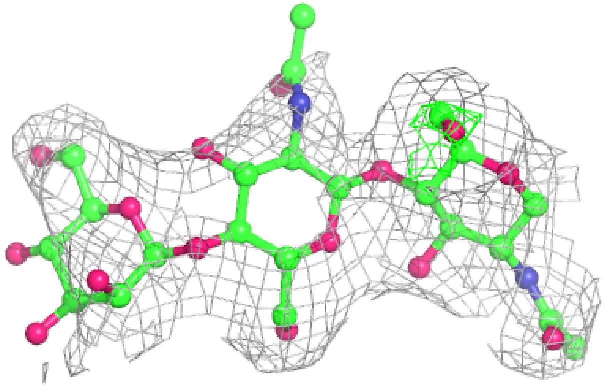


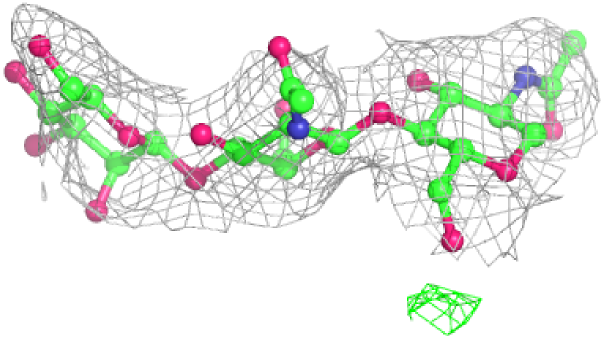


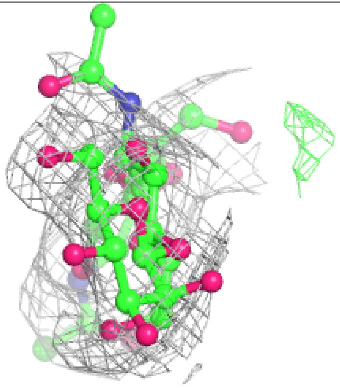


Electron density around Chain G:

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:

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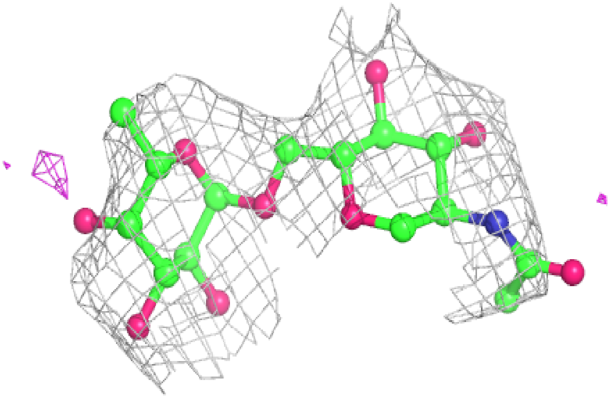
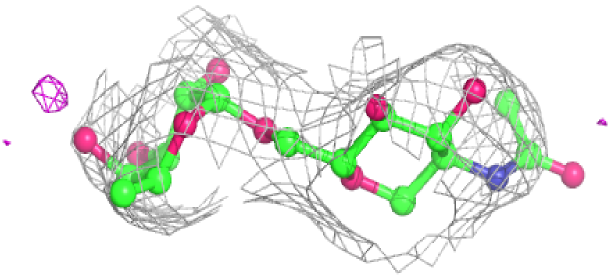
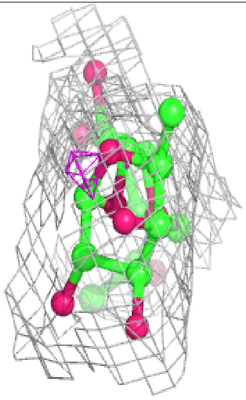
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
8	NAG	A	716	14/15	0.72	0.33	114,142,153,155	0
8	NAG	C	719	14/15	0.77	0.47	121,135,154,158	0
7	MAN	B	713	11/12	0.81	0.27	100,120,138,140	0
7	MAN	B	714	11/12	0.83	0.39	71,111,124,130	0
8	NAG	D	716	14/15	0.83	0.48	115,126,135,137	0
7	MAN	A	713	11/12	0.84	0.27	81,106,124,125	0
7	MAN	D	714	11/12	0.86	0.40	100,122,127,128	0
8	NAG	A	717	14/15	0.87	0.36	71,100,125,128	0
7	MAN	C	714	11/12	0.88	0.38	105,117,128,137	0
7	MAN	A	715	11/12	0.88	0.37	91,109,124,146	0
7	MAN	A	714	11/12	0.89	0.37	104,130,144,145	0
7	MAN	C	713	11/12	0.89	0.30	87,112,122,122	0
7	MAN	D	711	11/12	0.90	0.26	84,95,105,107	0
7	MAN	D	715	11/12	0.90	0.26	98,106,133,145	0
7	MAN	C	715	11/12	0.91	0.43	79,97,115,120	0
7	MAN	C	712	11/12	0.91	0.23	47,68,88,90	0
7	MAN	A	712	11/12	0.91	0.26	60,90,100,107	0
7	MAN	A	710	11/12	0.91	0.19	67,93,110,111	0
7	MAN	C	710	11/12	0.92	0.21	59,91,125,141	0
7	MAN	D	713	11/12	0.92	0.21	77,97,123,124	0
7	MAN	B	712	11/12	0.93	0.19	69,87,103,115	0
7	MAN	B	715	11/12	0.93	0.28	88,115,129,136	0
7	MAN	B	710	11/12	0.93	0.24	51,70,79,89	0
7	MAN	D	710	11/12	0.94	0.19	56,79,92,101	0
6	CA	C	704	1/1	0.94	0.13	96,96,96,96	0
7	MAN	D	712	11/12	0.94	0.16	55,79,90,95	0
6	CA	C	707	1/1	0.94	0.12	91,91,91,91	0
7	MAN	B	711	11/12	0.94	0.34	73,87,103,107	0
7	MAN	C	711	11/12	0.95	0.35	59,83,97,102	0
7	MAN	A	711	11/12	0.95	0.31	74,105,116,117	0
6	CA	B	703	1/1	0.95	0.13	48,48,48,48	0
6	CA	A	709	1/1	0.96	0.16	98,98,98,98	0
6	CA	A	703	1/1	0.96	0.11	53,53,53,53	0
6	CA	B	708	1/1	0.96	0.10	86,86,86,86	0
6	CA	B	707	1/1	0.97	0.07	87,87,87,87	0
6	CA	C	708	1/1	0.97	0.09	72,72,72,72	0
6	CA	D	702	1/1	0.97	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
6	CA	D	705	1/1	0.97	0.09	56,56,56,56	0
6	CA	D	707	1/1	0.97	0.06	93,93,93,93	0
6	CA	D	708	1/1	0.97	0.10	87,87,87,87	0
6	CA	D	709	1/1	0.97	0.15	74,74,74,74	0
6	CA	C	702	1/1	0.98	0.08	30,30,30,30	0
6	CA	B	704	1/1	0.98	0.08	66,66,66,66	0
6	CA	B	705	1/1	0.98	0.12	49,49,49,49	0
6	CA	B	709	1/1	0.98	0.10	92,92,92,92	0
6	CA	C	709	1/1	0.98	0.11	93,93,93,93	0
6	CA	D	701	1/1	0.98	0.11	43,43,43,43	0
6	CA	C	701	1/1	0.98	0.10	43,43,43,43	0
6	CA	D	704	1/1	0.98	0.12	52,52,52,52	0
6	CA	A	705	1/1	0.99	0.11	62,62,62,62	0
6	CA	B	706	1/1	0.99	0.11	46,46,46,46	0
6	CA	A	706	1/1	0.99	0.10	49,49,49,49	0
6	CA	A	708	1/1	0.99	0.11	80,80,80,80	0
6	CA	D	703	1/1	0.99	0.12	58,58,58,58	0
6	CA	A	702	1/1	0.99	0.06	39,39,39,39	0
6	CA	B	701	1/1	0.99	0.10	58,58,58,58	0
6	CA	D	706	1/1	0.99	0.13	39,39,39,39	0
6	CA	B	702	1/1	0.99	0.10	44,44,44,44	0
6	CA	A	701	1/1	0.99	0.11	44,44,44,44	0
6	CA	C	705	1/1	0.99	0.14	65,65,65,65	0
6	CA	C	706	1/1	0.99	0.18	75,75,75,75	0
6	CA	A	704	1/1	0.99	0.14	63,63,63,63	0
6	CA	C	703	1/1	1.00	0.12	40,40,40,40	0
6	CA	A	707	1/1	1.00	0.14	98,98,98,98	0

6.5 Other polymers ⓘ

There are no such residues in this entry.