W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 01:09 AM EDT

PDB ID	:	1NMC
Title	:	COMPLEX BETWEEN NC10 ANTI-INFLUENZA VIRUS NEU-RAMINIDASE SINGLE CHAIN ANTIBODY WITH A 15 RESIDUE LINKER AND INFLUENZA VIRUS NEURAMINIDASE
Authors	:	Malby, R.L.; Mccoy, A.J.; Kortt, A.A.; Hudson, P.J.; Colman, P.M.
Deposited on	:	1997-12-21
Resolution	:	2.50 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:

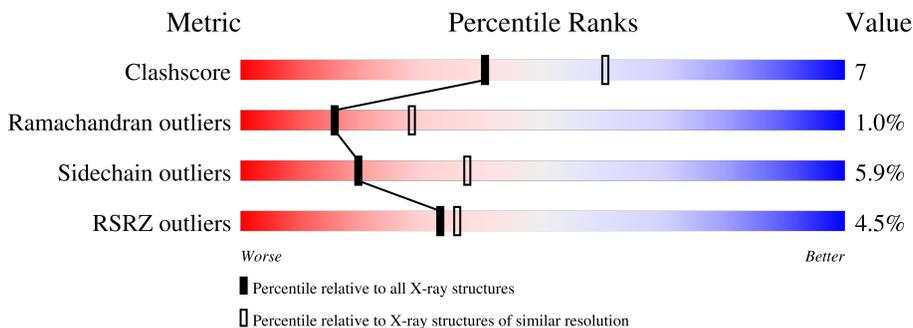|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.50 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.
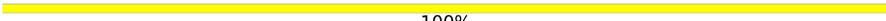
Metric	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		1.0%
Sidechain outliers		5.9%
RSRZ outliers		4.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	388	2% · 87% · 11% ·
1	N	388	88% · 10% ·
2	B	122	2% · 75% · 19% · 6%
2	H	122	2% · 75% · 19% · 6%
3	C	109	19% · 71% · 28% ·
3	L	109	21% · 71% · 28% ·

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Mol	Chain	Length	Quality of chain
4	D	6	100%
4	E	6	100%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 10138 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	N	388	Total 3067	C 1914	N 538	O 592	S 23	0	0	0
1	A	388	Total 3067	C 1914	N 538	O 592	S 23	0	0	0

- Molecule 2 is a protein called SINGLE CHAIN ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	122	Total 943	C 591	N 155	O 192	S 5	0	0	0
2	B	122	Total 943	C 591	N 155	O 192	S 5	0	0	0

- Molecule 3 is a protein called SINGLE CHAIN ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	109	Total 857	C 535	N 138	O 182	S 2	0	0	0
3	C	109	Total 857	C 535	N 138	O 182	S 2	0	0	0

- Molecule 4 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.
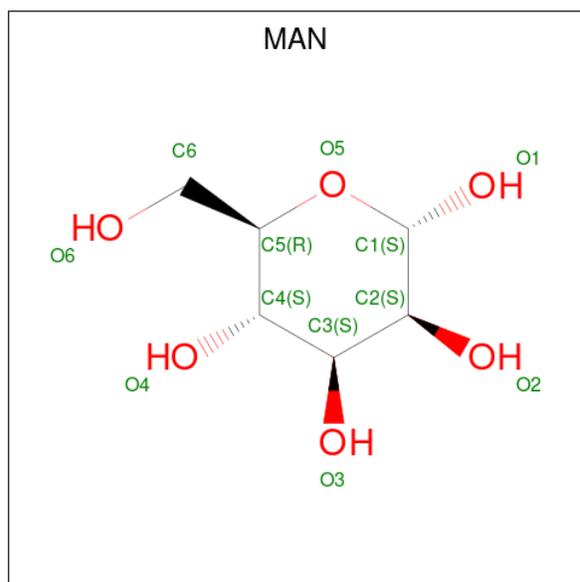

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total 72	C 40	N 2	O 30	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	6	72	40	2	30	0	0	0

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	N	1	11	6	5	0	0
5	A	1	11	6	5	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	81	Total	O	0	0
			81	81		
8	H	6	Total	O	0	0
			6	6		
8	L	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	81	Total 81	O 81	0	0
8	B	6	Total 6	O 6	0	0
8	C	3	Total 3	O 3	0	0

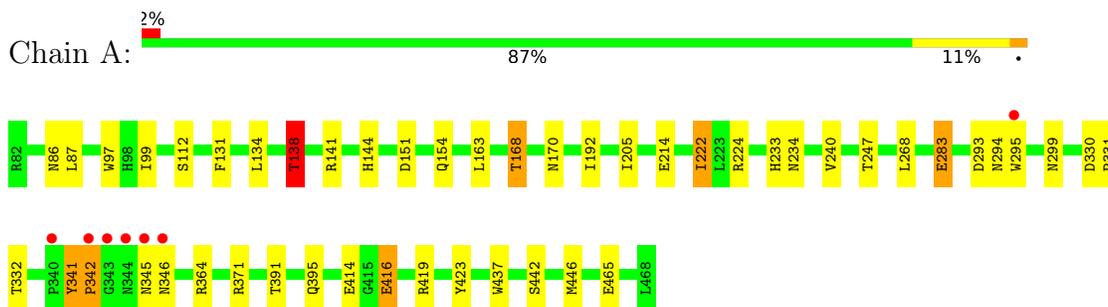# 3 Residue-property plots ⓘ

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.
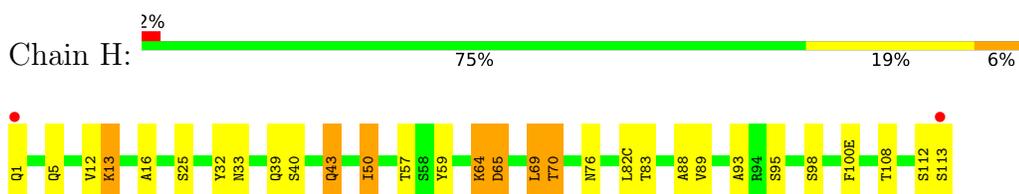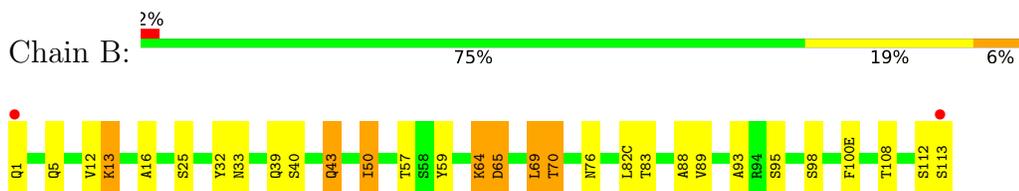
- Molecule 1: NEURAMINIDASE
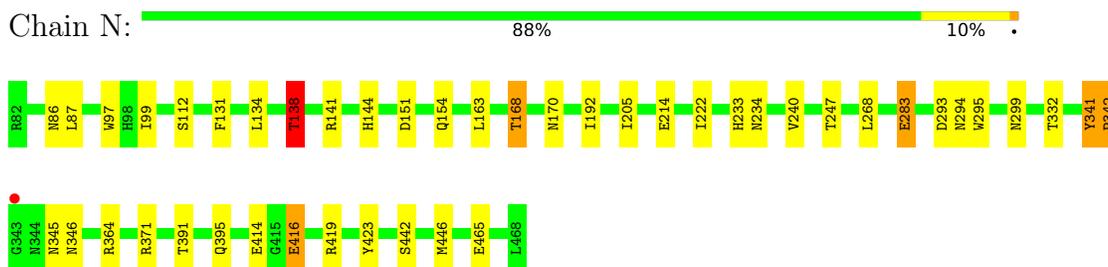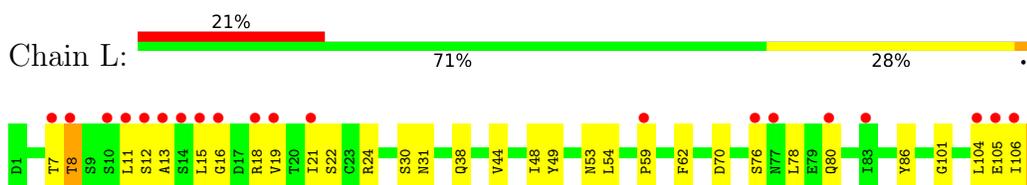
Chain N:

- Molecule 1: NEURAMINIDASE

Chain A:

- Molecule 2: SINGLE CHAIN ANTIBODY

Chain H:

- Molecule 2: SINGLE CHAIN ANTIBODY

Chain B:

- Molecule 3: SINGLE CHAIN ANTIBODY

Chain L:

21%

71%

28%

D1 T7 T8 S9 S10 L11 S12 A13 S14 L15 G16 D17 R18 V19 T20 I21 S22 C23 R24 S30 N31 Q38 V44 I48 Y49 N53 L54 P59 F62 D70 S76 N77 L78 E79 Q80 I83 Y86 G101 L104 E105 I106 R107 D108 Y109

• Molecule 3: SINGLE CHAIN ANTIBODY

Chain C:

19%

71%

28%

D1 T7 T8 S9 S10 L11 S12 A13 S14 L15 G16 D17 R18 V19 T20 I21 S22 C23 R24 S30 N31 Q38 V44 I48 Y49 N53 L54 P59 F62 D70 I75 S76 N77 L78 E79 Q80 I83 Y86 G101 L104 E105 I106 R107 D108 Y109

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

Chain D:					100%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6
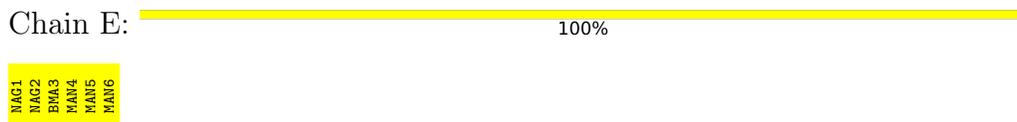
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam ido-2-deoxy-beta-D-glucopyranose

Chain E:					100%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.40Å 144.40Å 227.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50 64.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	80.0 (7.00-2.50) 80.7 (64.58-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	185.30 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.260 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4472e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: MAN, CA, BMA, 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	0.56	0/3150	0.83	1/4290 (0.0%)
1	N	0.56	0/3150	0.83	1/4290 (0.0%)
2	B	0.47	0/966	0.73	0/1306
2	H	0.47	0/966	0.73	0/1306
3	C	0.47	0/874	0.68	0/1187
3	L	0.47	0/874	0.68	0/1187
All	All	0.53	0/9980	0.78	2/13566 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	138	THR	CB-CA-C	-5.50	96.76	111.60
1	A	138	THR	CB-CA-C	-5.49	96.77	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	TYR	Sidechain
1	N	423	TYR	Sidechain

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	3067	0	2893	27	1
1	N	3067	0	2893	24	1
2	B	943	0	880	21	0
2	H	943	0	880	21	0
3	C	857	0	805	23	0
3	L	857	0	805	23	0
4	D	72	0	61	0	0
4	E	72	0	61	0	0
5	A	11	0	10	0	0
5	N	11	0	10	0	0
6	A	28	0	26	1	0
6	N	28	0	26	0	0
7	A	1	0	0	0	0
7	N	1	0	0	0	0
8	A	81	0	0	3	0
8	B	6	0	0	1	0
8	C	3	0	0	0	0
8	H	6	0	0	1	0
8	L	3	0	0	0	0
8	N	81	0	0	3	0
All	All	10138	0	9350	139	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 139 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:B:89:VAL:HG22	2:B:108:THR:HG22	1.57	0.87
2:H:89:VAL:HG22	2:H:108:THR:HG22	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:168:THR:HB	1:N:170:ASN:OD1	1.85	0.77
1:A:168:THR:HB	1:A:170:ASN:OD1	1.85	0.77
1:A:168:THR:HG22	1:A:170:ASN:H	1.49	0.77

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:214:GLU:OE2	1:N:419:ARG:NH2[4_555]	2.09	0.11
1:A:214:GLU:OE2	1:A:419:ARG:NH2[4_555]	2.09	0.11

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	386/388 (100%)	357 (92%)	26 (7%)	3 (1%)	19	35
1	N	386/388 (100%)	357 (92%)	26 (7%)	3 (1%)	19	35
2	B	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9	16
2	H	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9	16
3	C	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	17	31
3	L	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	17	31
All	All	1226/1238 (99%)	1132 (92%)	82 (7%)	12 (1%)	15	28

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	294	ASN
3	L	8	THR
1	A	294	ASN
3	C	8	THR

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Mol	Chain	Res	Type
2	H	43	GLN

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	341/341 (100%)	321 (94%)	20 (6%)	19	37
1	N	341/341 (100%)	321 (94%)	20 (6%)	19	37
2	B	100/100 (100%)	89 (89%)	11 (11%)	6	12
2	H	100/100 (100%)	89 (89%)	11 (11%)	6	12
3	C	98/98 (100%)	97 (99%)	1 (1%)	76	90
3	L	98/98 (100%)	97 (99%)	1 (1%)	76	90
All	All	1078/1078 (100%)	1014 (94%)	64 (6%)	19	37

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	69	LEU
2	B	76	ASN
2	H	64	LYS
2	H	50	ILE
2	B	82(C)	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	296	GLN
3	C	53	ASN
2	B	43	GLN
2	B	76	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 ⓘ

12 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	$\#|Z| > 2$
4	NAG	D	1	1,4	14,14,15	1.43	3 (21%)	17,19,21	3.90	7 (41%)
4	NAG	D	2	4	14,14,15	1.27	2 (14%)	17,19,21	1.44	3 (17%)
4	BMA	D	3	4	11,11,12	1.12	1 (9%)	15,15,17	1.50	2 (13%)
4	MAN	D	4	4	11,11,12	0.95	0	15,15,17	1.43	2 (13%)
4	MAN	D	5	4	11,11,12	1.40	1 (9%)	15,15,17	1.53	3 (20%)
4	MAN	D	6	4	11,11,12	1.88	2 (18%)	15,15,17	1.63	2 (13%)
4	NAG	E	1	1,4	14,14,15	1.43	3 (21%)	17,19,21	3.90	7 (41%)
4	NAG	E	2	4	14,14,15	1.26	2 (14%)	17,19,21	1.44	3 (17%)
4	BMA	E	3	4	11,11,12	1.13	1 (9%)	15,15,17	1.49	2 (13%)
4	MAN	E	4	4	11,11,12	0.94	0	15,15,17	1.44	2 (13%)
4	MAN	E	5	4	11,11,12	1.39	1 (9%)	15,15,17	1.54	3 (20%)
4	MAN	E	6	4	11,11,12	1.88	2 (18%)	15,15,17	1.63	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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	2/2/19/22	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	MAN	O5-C5	4.71	1.53	1.43
4	E	6	MAN	O5-C5	4.70	1.53	1.43
4	D	5	MAN	C2-C3	-2.91	1.48	1.52
4	E	5	MAN	C2-C3	-2.90	1.48	1.52
4	D	1	NAG	C6-C5	2.60	1.60	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	11.75	128.11	112.19
4	D	1	NAG	C1-O5-C5	11.73	128.09	112.19
4	E	1	NAG	C2-N2-C7	6.71	132.45	122.90
4	D	1	NAG	C2-N2-C7	6.69	132.43	122.90
4	D	1	NAG	C1-C2-N2	-5.64	100.86	110.49

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6	MAN	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
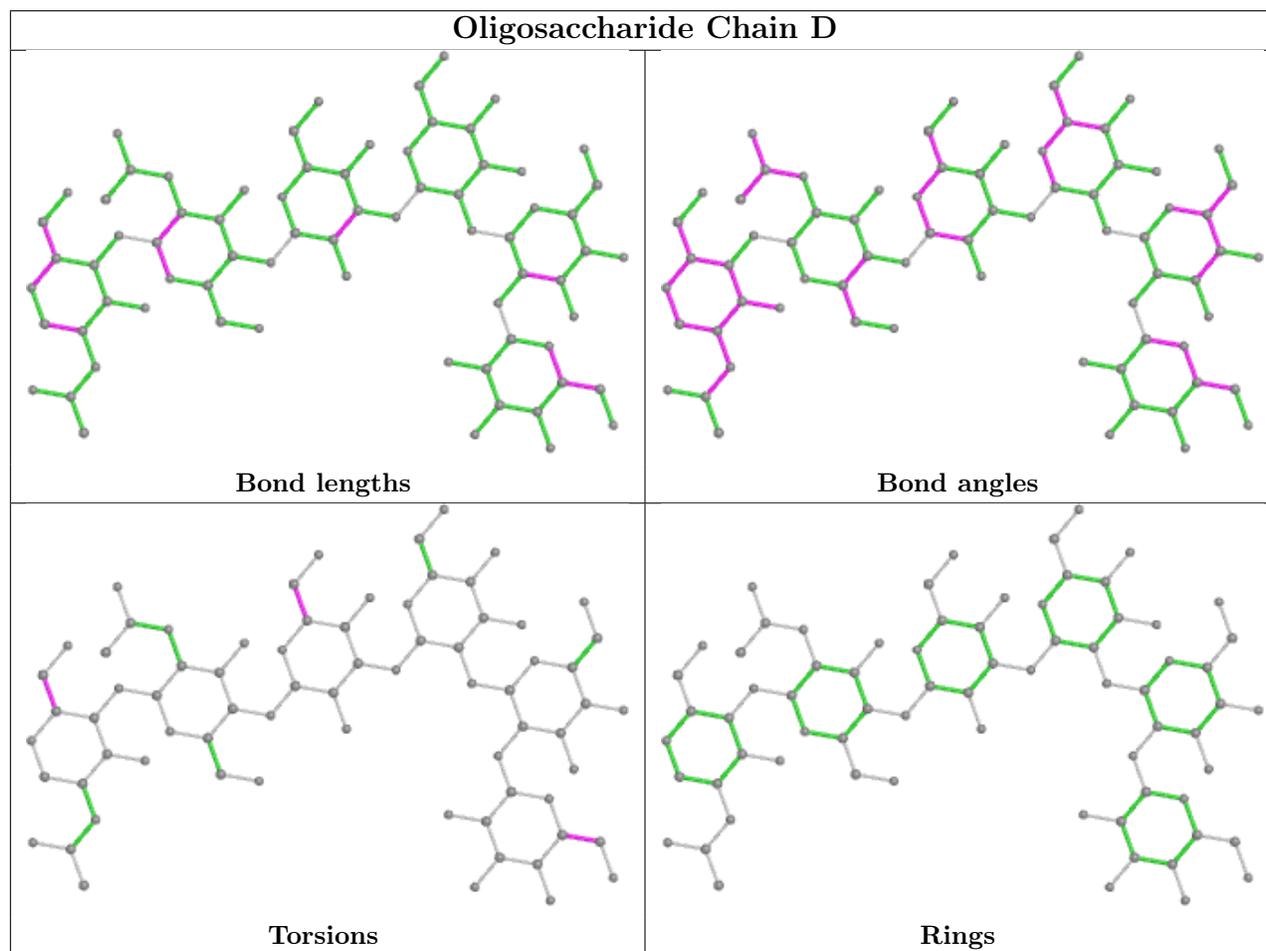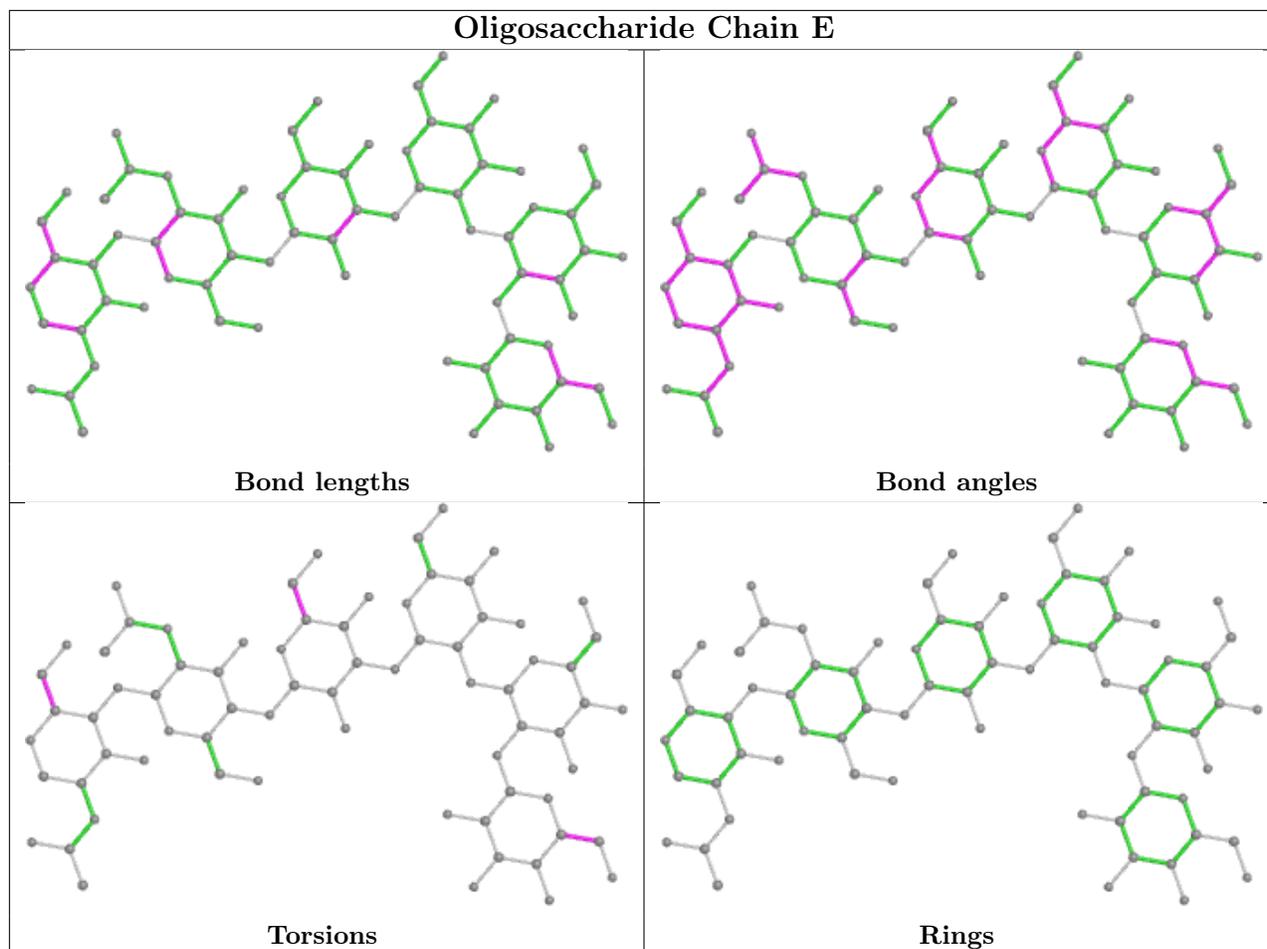
5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	MAN	N	475(G)	-	11,11,12	1.85	3 (27%)	15,15,17	2.71	7 (46%)
6	NAG	A	477(A)	1	14,14,15	1.14	3 (21%)	17,19,21	1.56	6 (35%)
5	MAN	A	475(G)	-	11,11,12	1.85	3 (27%)	15,15,17	2.72	7 (46%)
6	NAG	A	476(A)	1	14,14,15	1.37	3 (21%)	17,19,21	0.81	0
6	NAG	N	476(A)	1	14,14,15	1.37	3 (21%)	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
6	NAG	N	477(A)	1	14,14,15	1.14	3 (21%)	17,19,21	1.56	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	N	475(G)	-	-	0/2/19/22	0/1/1/1
6	NAG	A	477(A)	1	-	1/6/23/26	0/1/1/1
5	MAN	A	475(G)	-	-	0/2/19/22	0/1/1/1
6	NAG	A	476(A)	1	-	0/6/23/26	0/1/1/1
6	NAG	N	476(A)	1	-	0/6/23/26	0/1/1/1
6	NAG	N	477(A)	1	-	1/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	475(G)	MAN	C4-C5	-4.34	1.43	1.53
5	N	475(G)	MAN	C4-C5	-4.33	1.43	1.53
6	N	476(A)	NAG	C1-C2	-2.77	1.48	1.52
6	A	476(A)	NAG	C1-C2	-2.76	1.48	1.52
6	N	476(A)	NAG	O5-C5	2.67	1.48	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	475(G)	MAN	O2-C2-C1	5.03	119.44	109.15
5	A	475(G)	MAN	O2-C2-C1	5.02	119.43	109.15
5	A	475(G)	MAN	C2-C3-C4	4.53	118.74	110.89
5	N	475(G)	MAN	C2-C3-C4	4.52	118.72	110.89
5	N	475(G)	MAN	O3-C3-C4	-4.13	100.80	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	477(A)	NAG	O5-C5-C6-O6
6	A	477(A)	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	476(A)	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	388/388 (100%)	-0.55	7 (1%)	68	71	3, 12, 43, 78	0
1	N	388/388 (100%)	-0.63	1 (0%)	94	94	3, 12, 43, 78	0
2	B	122/122 (100%)	-0.24	2 (1%)	72	74	13, 27, 50, 80	0
2	H	122/122 (100%)	-0.30	2 (1%)	72	74	13, 27, 50, 80	0
3	C	109/109 (100%)	0.75	21 (19%)	1	1	13, 38, 72, 102	0
3	L	109/109 (100%)	0.84	23 (21%)	1	0	13, 38, 72, 102	0
All	All	1238/1238 (100%)	-0.28	56 (4%)	33	36	3, 18, 64, 102	0

The worst 5 of 56 RSRZ outliers are listed below:

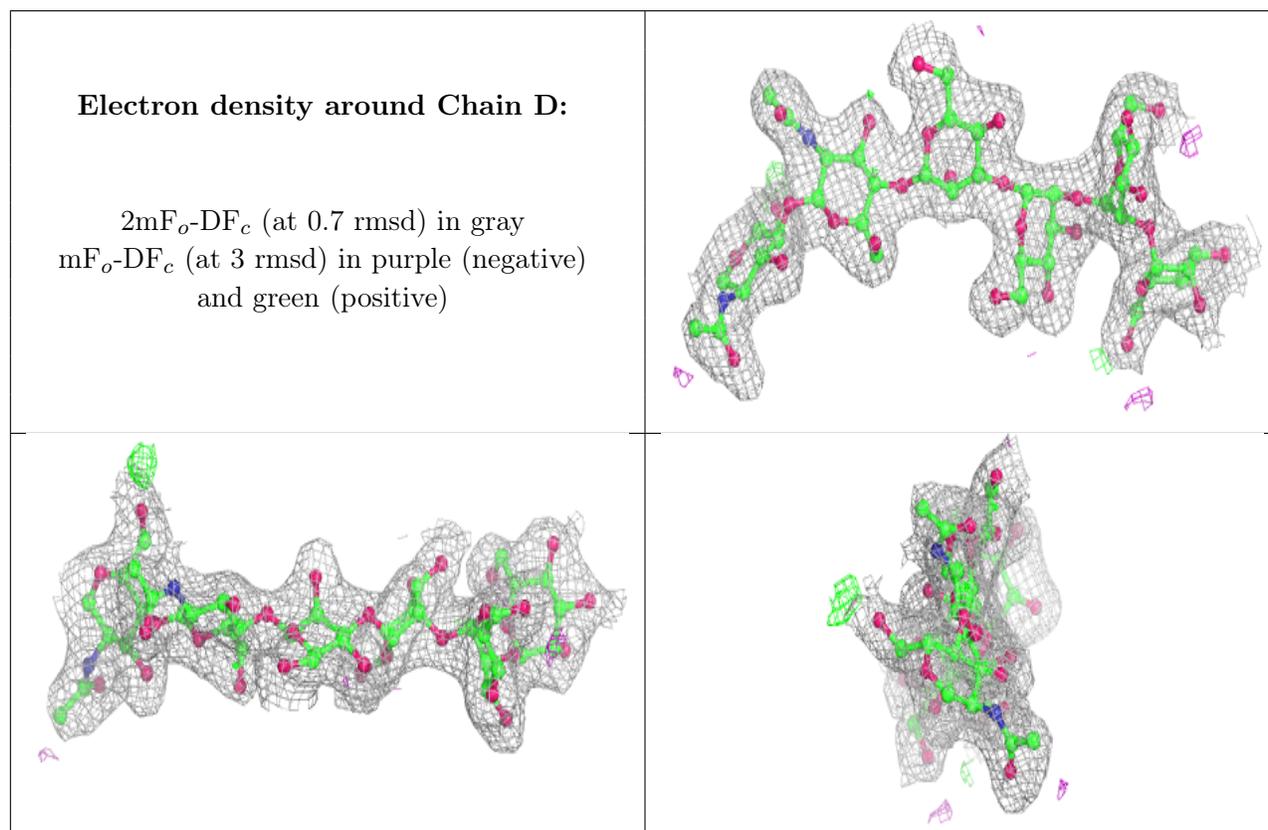| Mol	Chain	Res	Type	RSRZ
3	L	109	TYR	10.2
3	C	108	ASP	8.8
3	C	109	TYR	8.5
3	L	106	ILE	7.4
2	B	113	SER	6.6

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

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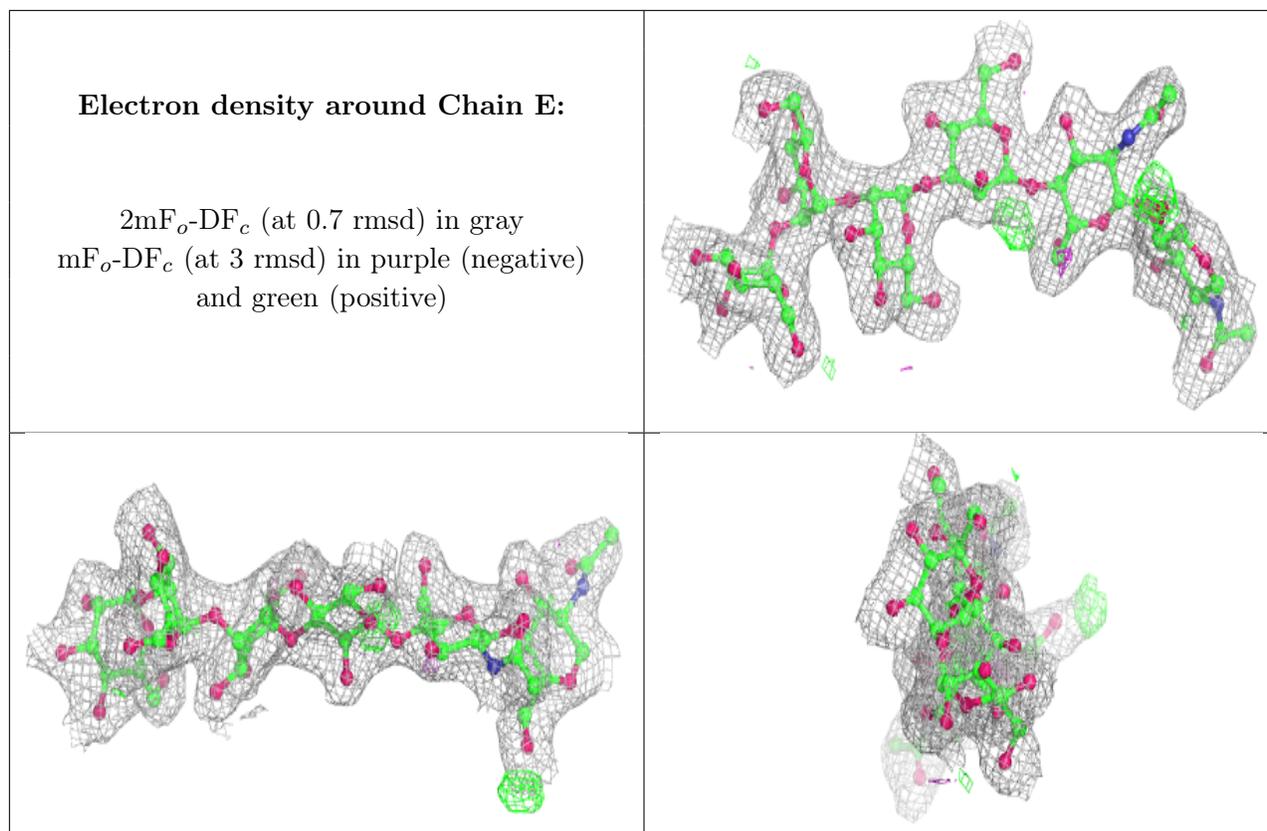
6.3 Carbohydrates ⓘ

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	MAN	D	5	11/12	0.95	0.10	9,16,20,27	0
4	NAG	E	1	14/15	0.95	0.10	5,15,25,29	0
4	NAG	D	1	14/15	0.96	0.10	5,15,25,29	0
4	MAN	D	6	11/12	0.96	0.11	10,12,15,17	0
4	MAN	D	4	11/12	0.96	0.09	12,14,17,24	0
4	NAG	E	2	14/15	0.96	0.09	7,12,19,28	0
4	BMA	E	3	11/12	0.96	0.10	11,13,17,23	0
4	MAN	E	5	11/12	0.96	0.11	9,16,20,27	0
4	BMA	D	3	11/12	0.97	0.09	11,13,17,23	0
4	MAN	E	4	11/12	0.97	0.11	12,14,17,24	0
4	NAG	D	2	14/15	0.97	0.12	7,12,19,28	0
4	MAN	E	6	11/12	0.97	0.10	10,12,15,17	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 D:

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

Electron density around Chain E:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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
7	CA	N	478	1/1	0.72	0.17	65,65,65,65	0
6	NAG	N	477(A)	14/15	0.84	0.17	44,48,51,56	0
7	CA	A	478	1/1	0.85	0.09	65,65,65,65	0
6	NAG	A	477(A)	14/15	0.86	0.19	44,48,51,56	0
5	MAN	A	475(G)	11/12	0.86	0.16	34,36,40,42	0
6	NAG	A	476(A)	14/15	0.86	0.20	40,53,58,64	0
6	NAG	N	476(A)	14/15	0.88	0.14	40,53,58,64	0
5	MAN	N	475(G)	11/12	0.91	0.14	34,36,40,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.