



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:54 PM UTC

PDB ID : 7A9D / pdb_00007a9d
Title : Crystal structure of H12 Haemagglutinin
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Deposited on : 2020-09-01
Resolution : 2.70 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

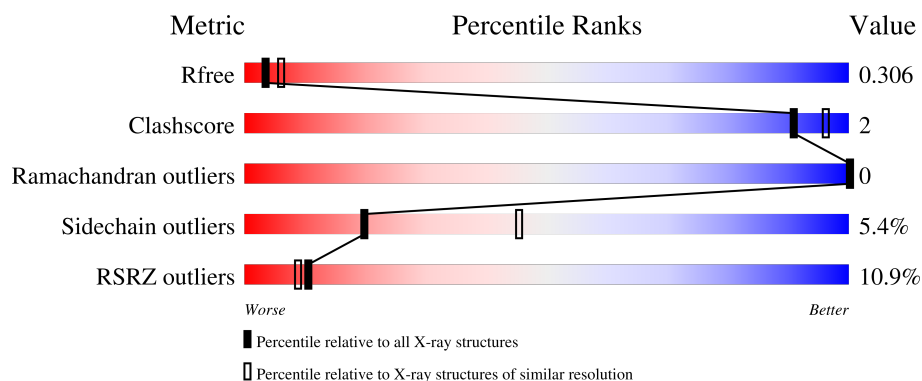
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	323	11% 93% 6%
1	C	323	11% 91% 7%
2	B	167	19% 86% 7% 7%
2	D	167	3% 92% 7%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7816 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2544	1600	439	490	15			
1	C	322	Total	C	N	O	S	0	0	0
			2544	1600	439	490	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP C6KJK3
A	0	PRO	-	expression tag	UNP C6KJK3
C	-1	ASP	-	expression tag	UNP C6KJK3
C	0	PRO	-	expression tag	UNP C6KJK3

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	0	0
			1249	771	226	246	6			
2	D	167	Total	C	N	O	S	0	0	0
			1339	824	242	266	7			

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



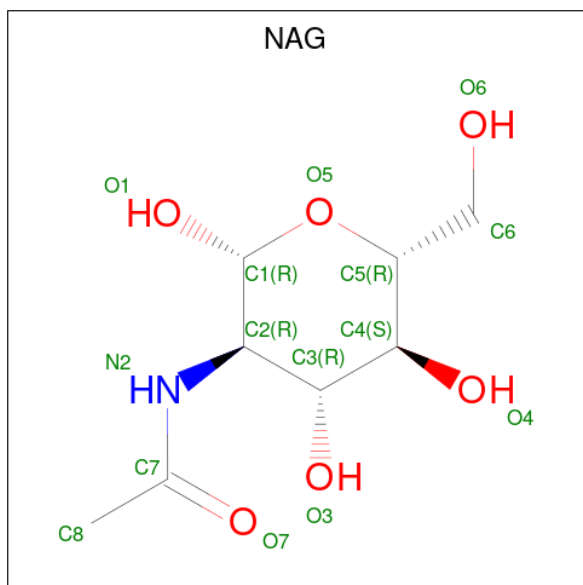
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

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

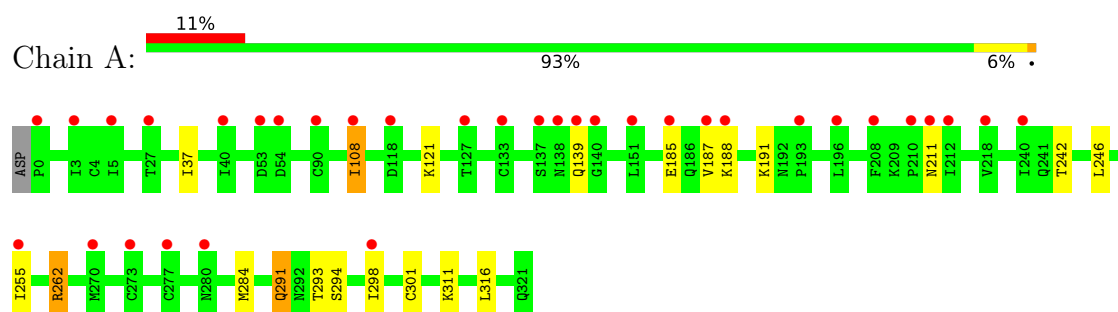


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

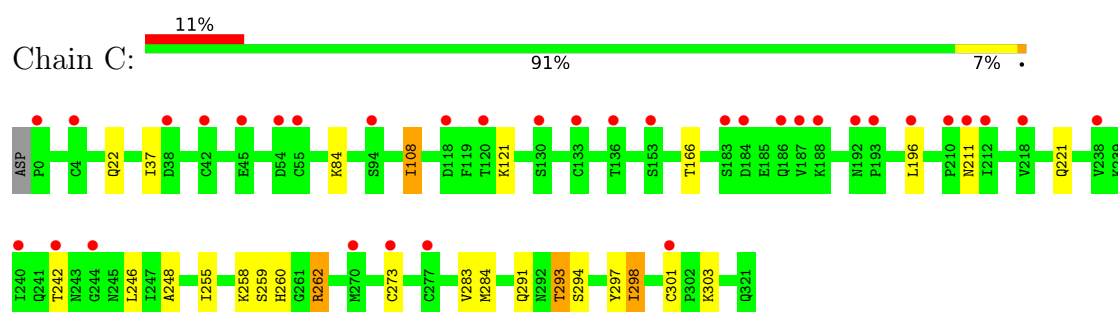
3 Residue-property plots [i](#)

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.

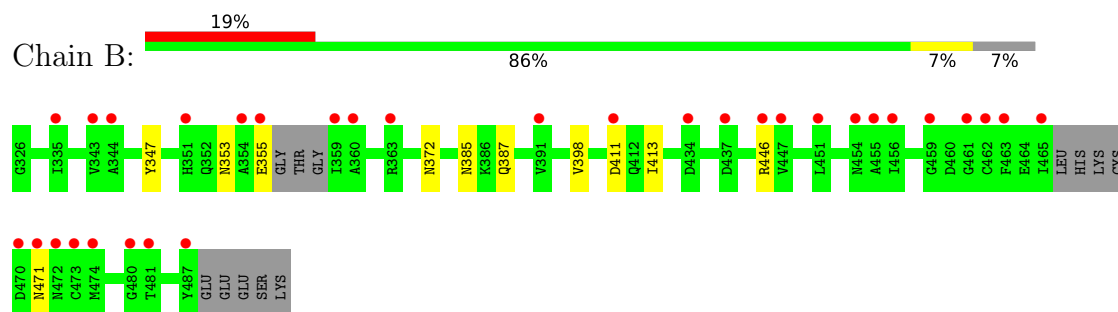
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	104.51Å 104.51Å 694.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	89.75 – 2.70 89.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (89.75-2.70) 96.7 (89.75-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.268 , 0.303 0.272 , 0.306	Depositor DCC
R_{free} test set	1989 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7816	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: 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	1.06	0/2602	1.30	0/3530
1	C	1.02	0/2602	1.28	0/3530
2	B	1.02	0/1268	1.55	0/1710
2	D	0.99	0/1361	1.49	0/1836
All	All	1.03	0/7833	1.37	0/10606

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	2544	0	2503	6	0
1	C	2544	0	2502	10	0
2	B	1249	0	1175	4	0
2	D	1339	0	1259	6	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	28	0	26	0	0
4	C	42	0	39	0	0
4	D	14	0	13	0	0
All	All	7816	0	7567	26	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 2.

All (26) 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:C:242:THR:HG21	1:C:246:LEU:HD22	1.74	0.70
2:B:353:ASN:HD21	2:B:471:ASN:ND2	1.94	0.65
1:C:291:GLN:HE21	1:C:293:THR:H	1.48	0.59
2:B:353:ASN:HD21	2:B:471:ASN:HD21	1.51	0.57
1:A:284:MET:HE1	1:A:291:GLN:HG3	1.90	0.52
2:D:353:ASN:HD21	2:D:471:ASN:HD22	1.58	0.52
1:C:262:ARG:NH2	1:C:297:TYR:O	2.45	0.49
1:C:246:LEU:HD23	1:C:248:ALA:HB2	1.95	0.48
2:D:353:ASN:HD21	2:D:471:ASN:ND2	2.11	0.48
2:D:456:ILE:HG23	2:D:464:GLU:HB2	1.97	0.47
1:C:108:ILE:HG12	1:C:255:ILE:HB	1.96	0.46
1:C:284:MET:HE1	1:C:291:GLN:HG3	1.97	0.46
1:A:108:ILE:HG12	1:A:255:ILE:HB	1.96	0.46
2:D:398:VAL:HG12	2:D:398:VAL:O	2.17	0.45
1:C:242:THR:CG2	1:C:246:LEU:HD22	2.43	0.44
2:B:398:VAL:HG12	2:B:398:VAL:O	2.18	0.44
1:A:262:ARG:CZ	1:A:298:ILE:HG22	2.47	0.43
1:C:259:SER:OG	1:C:260:HIS:N	2.52	0.43
1:C:262:ARG:CZ	1:C:298:ILE:HG22	2.48	0.43
1:C:291:GLN:NE2	1:C:294:SER:H	2.17	0.43
1:A:187:VAL:O	1:A:191:LYS:HA	2.18	0.43
2:D:385:ASN:C	2:D:385:ASN:ND2	2.77	0.42
1:A:291:GLN:NE2	1:A:294:SER:O	2.51	0.41
2:B:372:ASN:HD22	2:B:372:ASN:N	2.18	0.41
2:D:411:ASP:O	2:D:414:THR:HG22	2.20	0.41
1:A:242:THR:HG21	1:A:246:LEU:HD22	2.03	0.41

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	320/323 (99%)	308 (96%)	12 (4%)	0	100	100
1	C	320/323 (99%)	307 (96%)	13 (4%)	0	100	100
2	B	149/167 (89%)	143 (96%)	6 (4%)	0	100	100
2	D	165/167 (99%)	159 (96%)	6 (4%)	0	100	100
All	All	954/980 (97%)	917 (96%)	37 (4%)	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	291/292 (100%)	278 (96%)	13 (4%)	24	52
1	C	291/292 (100%)	274 (94%)	17 (6%)	18	42
2	B	133/143 (93%)	126 (95%)	7 (5%)	20	46
2	D	143/143 (100%)	134 (94%)	9 (6%)	16	39
All	All	858/870 (99%)	812 (95%)	46 (5%)	20	45

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	108	ILE
1	A	121	LYS
1	A	139	GLN
1	A	185	GLU
1	A	188	LYS
1	A	211	ASN
1	A	262	ARG
1	A	291	GLN
1	A	293	THR

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Mol	Chain	Res	Type
1	A	301	CYS
1	A	311	LYS
1	A	316	LEU
1	C	22	GLN
1	C	37	ILE
1	C	84	LYS
1	C	108	ILE
1	C	121	LYS
1	C	166	THR
1	C	196	LEU
1	C	211	ASN
1	C	221	GLN
1	C	258	LYS
1	C	262	ARG
1	C	273	CYS
1	C	283	VAL
1	C	293	THR
1	C	298	ILE
1	C	301	CYS
1	C	303	LYS
2	B	347	TYR
2	B	355	GLU
2	B	385	ASN
2	B	387	GLN
2	B	411	ASP
2	B	413	ILE
2	B	446	ARG
2	D	384	MET
2	D	385	ASN
2	D	386	LYS
2	D	411	ASP
2	D	413	ILE
2	D	423	LEU
2	D	446	ARG
2	D	456	ILE
2	D	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	98	GLN

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	245	ASN
1	A	272	GLN
1	A	321	GLN
1	C	139	GLN
1	C	178	HIS
1	C	186	GLN
1	C	192	ASN
1	C	245	ASN
1	C	291	GLN
1	C	321	GLN
2	B	351	HIS
2	B	372	ASN
2	B	375	ASN
2	B	385	ASN
2	B	403	ASN
2	B	454	ASN
2	B	471	ASN
2	D	372	ASN
2	D	375	ASN
2	D	385	ASN
2	D	403	ASN
2	D	444	HIS
2	D	454	ASN
2	D	471	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](#)

4 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	E	1	1,3	14,14,15	0.49	0	17,19,21	1.57	3 (17%)
3	NAG	E	2	3	14,14,15	0.37	0	17,19,21	0.52	0
3	NAG	F	1	1,3	14,14,15	0.32	0	17,19,21	1.28	3 (17%)
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.63	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C4-C3-C2	4.84	118.11	111.02
3	F	1	NAG	O5-C1-C2	-2.92	106.77	111.29
3	E	1	NAG	C3-C4-C5	2.77	115.25	110.23
3	F	1	NAG	C4-C3-C2	2.58	114.80	111.02
3	E	1	NAG	O4-C4-C3	-2.28	105.00	110.38
3	F	1	NAG	C3-C4-C5	2.27	114.34	110.23

There are no chirality outliers.

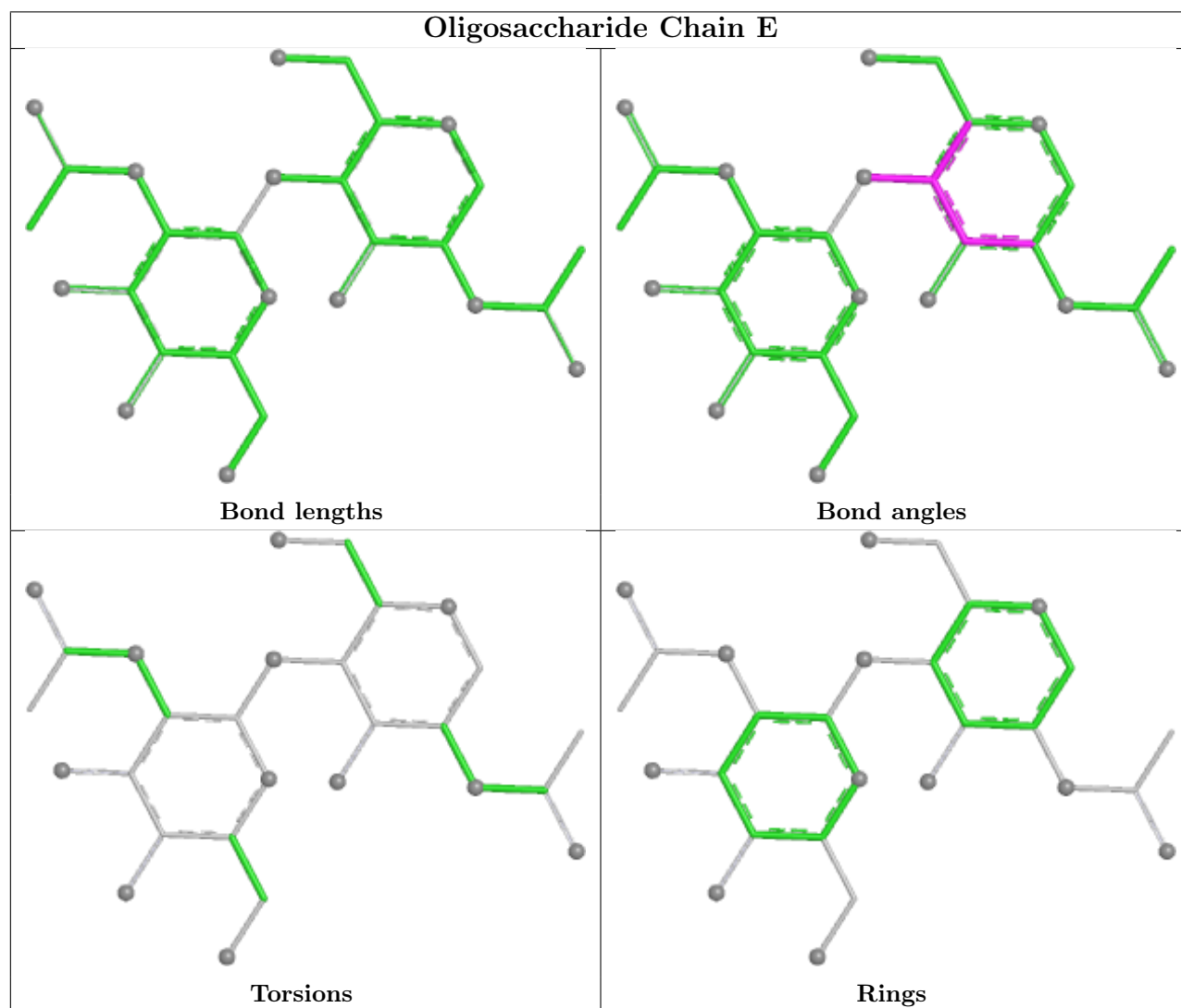
All (1) torsion outliers are listed below:

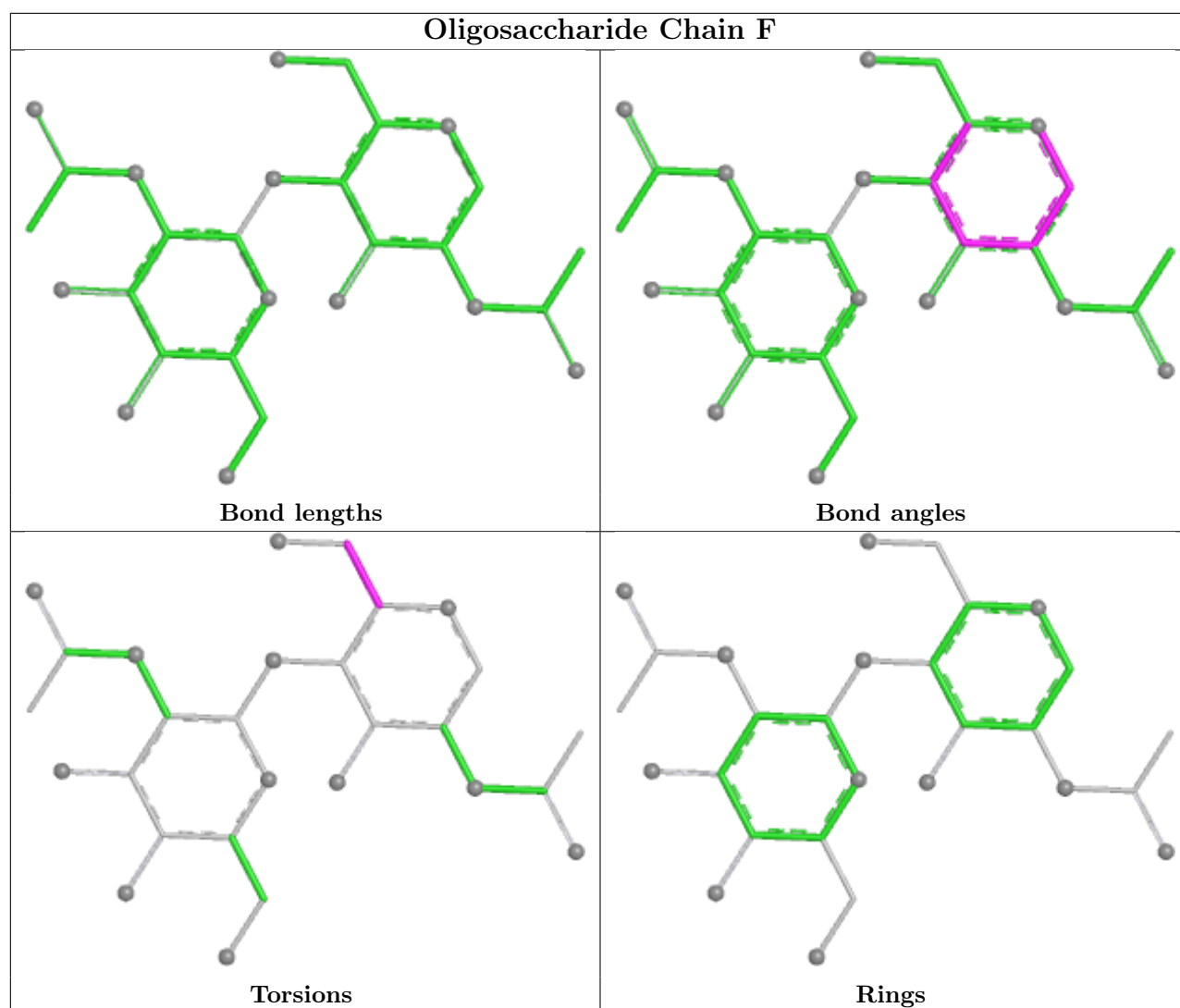
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	NAG	C	403	1	14,14,15	0.34	0	17,19,21	0.97	1 (5%)
4	NAG	A	402	1	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	C	401	1	14,14,15	0.34	0	17,19,21	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	402	1	14,14,15	0.31	0	17,19,21	0.90	0
4	NAG	A	401	1	14,14,15	0.25	0	17,19,21	0.74	1 (5%)
4	NAG	D	501	2	14,14,15	0.42	0	17,19,21	0.78	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
4	NAG	C	403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	1/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	401	1	-	1/6/23/26	0/1/1/1
4	NAG	D	501	2	-	4/6/23/26	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(°)	Ideal(°)
4	C	401	NAG	O5-C1-C2	-2.64	107.21	111.29
4	C	403	NAG	C1-C2-N2	-2.47	106.54	110.43
4	C	401	NAG	C2-N2-C7	2.38	126.09	122.90
4	A	401	NAG	O5-C1-C2	-2.10	108.04	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	NAG	C3-C2-N2-C7
4	C	402	NAG	O5-C5-C6-O6
4	D	501	NAG	O5-C5-C6-O6
4	D	501	NAG	C4-C5-C6-O6
4	C	402	NAG	C4-C5-C6-O6
4	C	403	NAG	C4-C5-C6-O6
4	A	401	NAG	O5-C5-C6-O6
4	C	403	NAG	O5-C5-C6-O6
4	D	501	NAG	C3-C2-N2-C7
4	D	501	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	322/323 (99%)	0.99	34 (10%)	11	9	60, 81, 101, 139	0
1	C	322/323 (99%)	0.86	34 (10%)	11	9	34, 65, 98, 107	0
2	B	155/167 (92%)	1.29	32 (20%)	2	2	51, 88, 135, 147	0
2	D	167/167 (100%)	0.42	5 (2%)	52	49	34, 49, 66, 94	0
All	All	966/980 (98%)	0.90	105 (10%)	10	9	34, 71, 107, 147	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	PRO	5.9
2	B	465	ILE	5.1
2	B	355	GLU	4.2
1	C	196	LEU	4.1
2	B	473	CYS	3.9
2	B	487	TYR	3.7
2	B	470	ASP	3.5
1	A	240	ILE	3.5
2	B	456	ILE	3.5
1	C	193	PRO	3.5
1	C	187	VAL	3.5
2	B	344	ALA	3.4
1	A	196	LEU	3.4
1	C	218	VAL	3.2
1	A	138	ASN	3.2
1	A	53	ASP	3.2
2	B	451	LEU	3.1
1	C	242	THR	3.1
2	B	343	VAL	3.1
1	A	193	PRO	3.1
2	B	359	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	463	PHE	3.0
1	A	118	ASP	3.0
2	D	363	ARG	3.0
1	A	90	CYS	3.0
1	A	54	ASP	3.0
1	A	212	ILE	3.0
1	A	127	THR	3.0
2	B	455	ALA	3.0
2	D	364	ASP	2.9
1	A	273	CYS	2.9
1	C	133	CYS	2.9
2	B	481	THR	2.9
1	C	240	ILE	2.9
1	C	55	CYS	2.8
1	C	136	THR	2.8
2	B	462	CYS	2.7
1	A	211	ASN	2.7
1	C	54	ASP	2.7
1	A	3	ILE	2.7
1	A	139	GLN	2.7
1	A	185	GLU	2.7
1	A	187	VAL	2.7
1	A	210	PRO	2.7
2	B	335	ILE	2.6
1	C	4	CYS	2.6
1	C	192	ASN	2.6
1	C	118	ASP	2.6
1	A	40	ILE	2.6
2	B	363	ARG	2.5
1	C	277	CYS	2.5
1	A	188	LYS	2.5
1	A	277	CYS	2.5
2	D	462	CYS	2.5
2	B	459	GLY	2.5
1	A	218	VAL	2.5
2	B	454	ASN	2.4
1	C	153	SER	2.4
2	B	437	ASP	2.4
1	C	188	LYS	2.4
1	A	151	LEU	2.4
2	B	446	ARG	2.4
1	A	255	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	2.3
2	B	411	ASP	2.3
1	A	27	THR	2.3
1	A	270	MET	2.3
1	C	130	SER	2.3
1	C	0	PRO	2.3
1	C	273	CYS	2.3
2	B	471	ASN	2.3
2	B	354	ALA	2.3
1	C	45	GLU	2.3
2	B	472	ASN	2.3
1	A	137	SER	2.3
1	C	183	SER	2.3
2	B	434	ASP	2.3
2	B	360	ALA	2.2
2	B	351	HIS	2.2
1	C	184	ASP	2.2
2	D	411	ASP	2.2
2	B	480	GLY	2.2
1	C	42	CYS	2.2
1	C	210	PRO	2.2
2	B	447	VAL	2.2
1	C	212	ILE	2.2
1	A	133	CYS	2.2
2	D	492	LYS	2.1
2	B	474	MET	2.1
1	A	108	ILE	2.1
1	C	94	SER	2.1
2	B	391	VAL	2.1
1	C	270	MET	2.1
1	A	5	ILE	2.1
1	A	280	ASN	2.1
1	C	120	THR	2.1
1	C	211	ASN	2.1
1	C	301	CYS	2.1
2	B	461	GLY	2.1
1	A	208	PHE	2.1
1	C	38	ASP	2.0
1	C	186	GLN	2.0
1	A	140	GLY	2.0
1	C	244	GLY	2.0
1	C	238	VAL	2.0

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

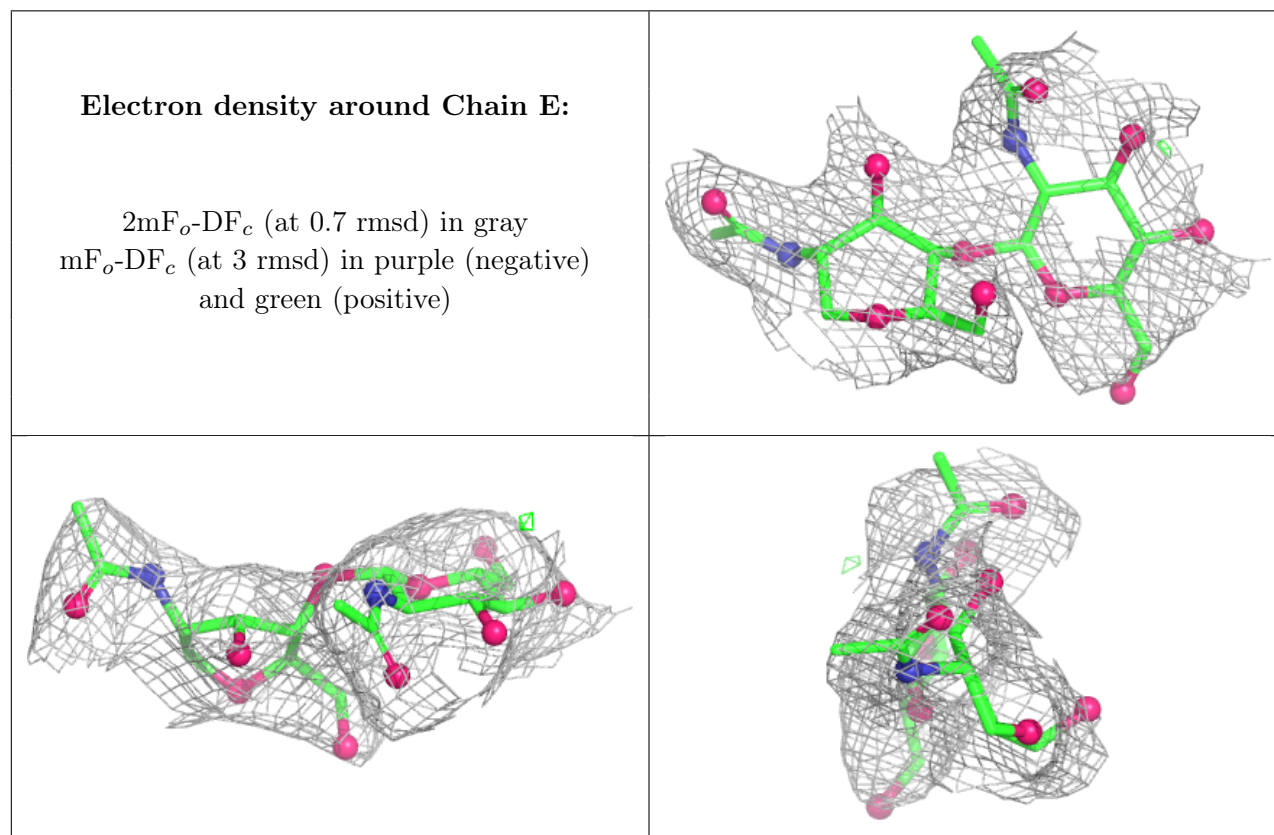
There are no non-standard protein/DNA/RNA residues in this entry.

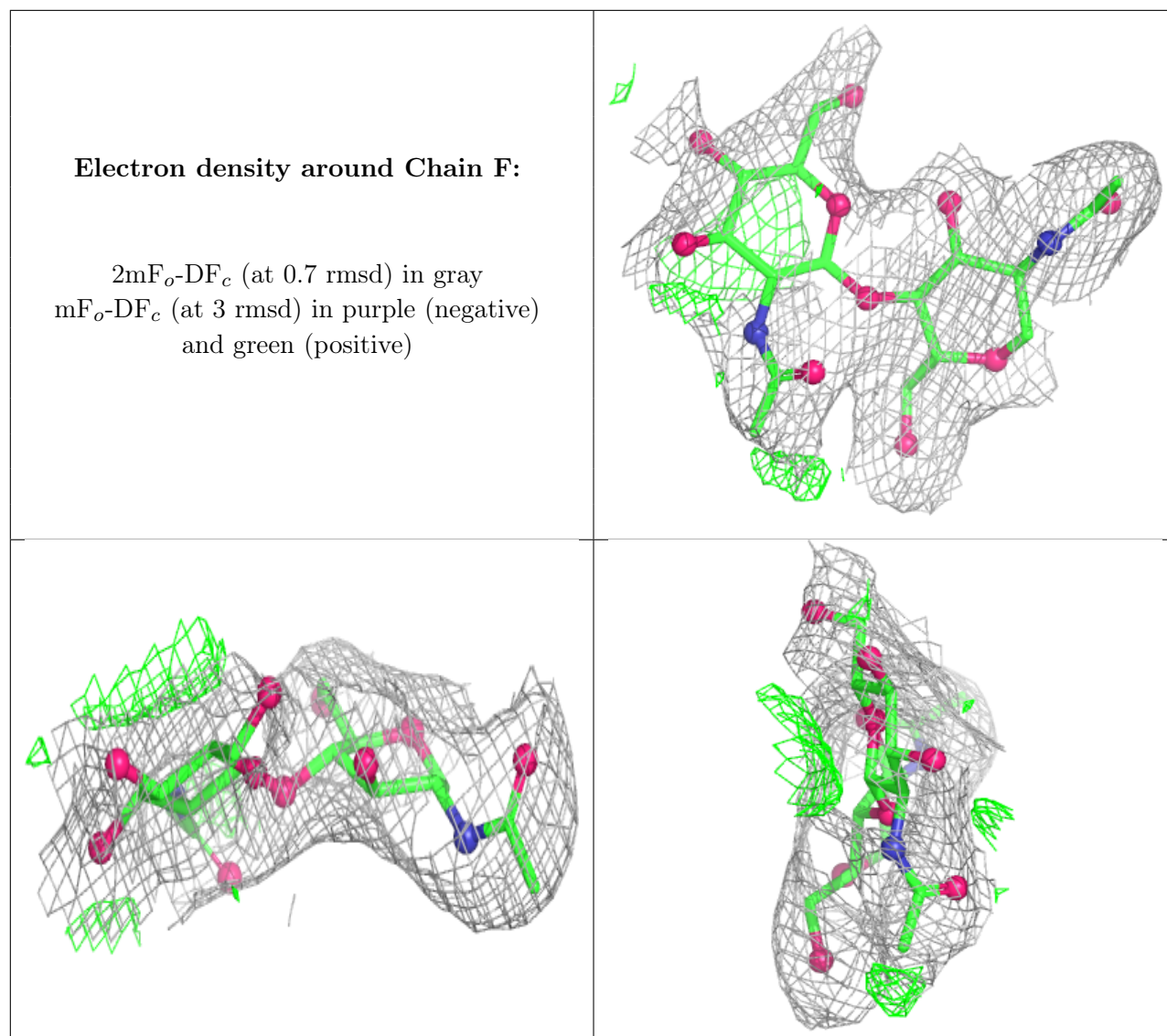
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.59	0.17	80,87,89,90	0
3	NAG	E	2	14/15	0.75	0.11	99,103,104,106	0
3	NAG	E	1	14/15	0.78	0.16	78,81,86,94	0
3	NAG	F	1	14/15	0.91	0.09	56,58,64,72	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	402	14/15	0.52	0.19	109,111,116,118	0
4	NAG	C	401	14/15	0.64	0.16	84,89,92,93	0
4	NAG	D	501	14/15	0.64	0.16	80,87,89,90	0
4	NAG	A	401	14/15	0.69	0.14	94,97,98,99	0
4	NAG	C	403	14/15	0.75	0.15	100,102,104,105	0
4	NAG	C	402	14/15	0.83	0.12	78,79,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.