



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 05:34 PM BST

PDB ID : 4FZH
Title : Structure of the Ulster Strain Newcastle Disease Virus Hemagglutinin-Neuraminidase Reveals Auto-Inhibitory Interactions Associated with Low Virulence
Authors : Yuan, P.; Paterson, R.G.; Leser, G.P.; Lamb, R.A.; Jardetzky, T.S.
Deposited on : 2012-07-06
Resolution : 3.50 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 ⓘ symbol.

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	:	2.13.1
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)	:	2.13.1

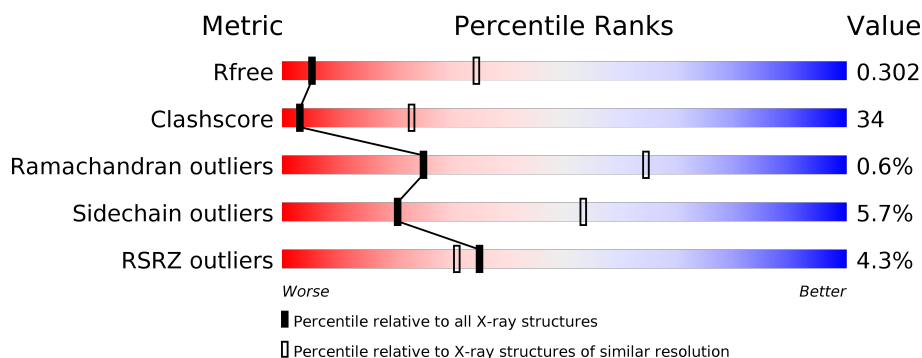
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



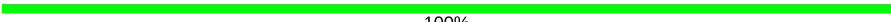
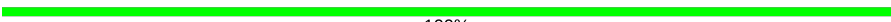
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	536	<div> <div>10%</div> <div>44%</div> <div>42%</div> <div>5%</div> <div>9%</div> </div>
1	B	536	<div> <div>45%</div> <div>42%</div> <div>•</div> <div>9%</div> </div>
1	C	536	<div> <div>4%</div> <div>40%</div> <div>47%</div> <div>•</div> <div>9%</div> </div>
1	D	536	<div> <div>10%</div> <div>42%</div> <div>46%</div> <div>•</div> <div>9%</div> </div>
2	E	2	<div>100%</div>
2	F	2	<div>100%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%

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
2	NAG	F	2	-	-	-	X
2	NAG	H	2	-	-	-	X
3	NAG	A	702	-	-	-	X
3	NAG	B	702	-	-	-	X
3	NAG	D	701	-	-	-	X
3	NAG	D	702	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15242 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-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3758	2368	638	732	20			
1	B	486	Total	C	N	O	S	0	0	0
			3758	2368	638	732	20			
1	C	486	Total	C	N	O	S	0	0	0
			3758	2368	638	732	20			
1	D	486	Total	C	N	O	S	0	0	0
			3758	2368	638	732	20			

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	expression tag	UNP P12558
A	82	GLY	-	expression tag	UNP P12558
A	83	ILE	-	expression tag	UNP P12558
A	84	LEU	-	expression tag	UNP P12558
A	85	PRO	-	expression tag	UNP P12558
A	86	SER	-	expression tag	UNP P12558
A	87	PRO	-	expression tag	UNP P12558
A	88	GLY	-	expression tag	UNP P12558
A	89	MET	-	expression tag	UNP P12558
A	90	PRO	-	expression tag	UNP P12558
A	91	ALA	-	expression tag	UNP P12558
A	92	LEU	-	expression tag	UNP P12558
A	93	LEU	-	expression tag	UNP P12558
A	94	SER	-	expression tag	UNP P12558
A	95	LEU	-	expression tag	UNP P12558
A	96	VAL	-	expression tag	UNP P12558
A	97	SER	-	expression tag	UNP P12558
A	98	LEU	-	expression tag	UNP P12558
A	99	LEU	-	expression tag	UNP P12558
A	100	SER	-	expression tag	UNP P12558
A	101	VAL	-	expression tag	UNP P12558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	LEU	-	expression tag	UNP P12558
A	103	LEU	-	expression tag	UNP P12558
A	104	MET	-	expression tag	UNP P12558
A	105	GLY	-	expression tag	UNP P12558
A	106	CYS	-	expression tag	UNP P12558
A	107	VAL	-	expression tag	UNP P12558
A	108	ALA	-	expression tag	UNP P12558
A	109	GLU	-	expression tag	UNP P12558
A	110	THR	-	expression tag	UNP P12558
A	111	GLY	-	expression tag	UNP P12558
A	112	HIS	-	expression tag	UNP P12558
A	113	HIS	-	expression tag	UNP P12558
A	114	HIS	-	expression tag	UNP P12558
A	115	HIS	-	expression tag	UNP P12558
A	116	HIS	-	expression tag	UNP P12558
A	117	HIS	-	expression tag	UNP P12558
A	118	LEU	-	expression tag	UNP P12558
A	119	VAL	-	expression tag	UNP P12558
A	120	PRO	-	expression tag	UNP P12558
A	121	ARG	-	expression tag	UNP P12558
A	122	GLY	-	expression tag	UNP P12558
A	123	SER	-	expression tag	UNP P12558
B	81	MET	-	expression tag	UNP P12558
B	82	GLY	-	expression tag	UNP P12558
B	83	ILE	-	expression tag	UNP P12558
B	84	LEU	-	expression tag	UNP P12558
B	85	PRO	-	expression tag	UNP P12558
B	86	SER	-	expression tag	UNP P12558
B	87	PRO	-	expression tag	UNP P12558
B	88	GLY	-	expression tag	UNP P12558
B	89	MET	-	expression tag	UNP P12558
B	90	PRO	-	expression tag	UNP P12558
B	91	ALA	-	expression tag	UNP P12558
B	92	LEU	-	expression tag	UNP P12558
B	93	LEU	-	expression tag	UNP P12558
B	94	SER	-	expression tag	UNP P12558
B	95	LEU	-	expression tag	UNP P12558
B	96	VAL	-	expression tag	UNP P12558
B	97	SER	-	expression tag	UNP P12558
B	98	LEU	-	expression tag	UNP P12558
B	99	LEU	-	expression tag	UNP P12558
B	100	SER	-	expression tag	UNP P12558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	101	VAL	-	expression tag	UNP P12558
B	102	LEU	-	expression tag	UNP P12558
B	103	LEU	-	expression tag	UNP P12558
B	104	MET	-	expression tag	UNP P12558
B	105	GLY	-	expression tag	UNP P12558
B	106	CYS	-	expression tag	UNP P12558
B	107	VAL	-	expression tag	UNP P12558
B	108	ALA	-	expression tag	UNP P12558
B	109	GLU	-	expression tag	UNP P12558
B	110	THR	-	expression tag	UNP P12558
B	111	GLY	-	expression tag	UNP P12558
B	112	HIS	-	expression tag	UNP P12558
B	113	HIS	-	expression tag	UNP P12558
B	114	HIS	-	expression tag	UNP P12558
B	115	HIS	-	expression tag	UNP P12558
B	116	HIS	-	expression tag	UNP P12558
B	117	HIS	-	expression tag	UNP P12558
B	118	LEU	-	expression tag	UNP P12558
B	119	VAL	-	expression tag	UNP P12558
B	120	PRO	-	expression tag	UNP P12558
B	121	ARG	-	expression tag	UNP P12558
B	122	GLY	-	expression tag	UNP P12558
B	123	SER	-	expression tag	UNP P12558
C	81	MET	-	expression tag	UNP P12558
C	82	GLY	-	expression tag	UNP P12558
C	83	ILE	-	expression tag	UNP P12558
C	84	LEU	-	expression tag	UNP P12558
C	85	PRO	-	expression tag	UNP P12558
C	86	SER	-	expression tag	UNP P12558
C	87	PRO	-	expression tag	UNP P12558
C	88	GLY	-	expression tag	UNP P12558
C	89	MET	-	expression tag	UNP P12558
C	90	PRO	-	expression tag	UNP P12558
C	91	ALA	-	expression tag	UNP P12558
C	92	LEU	-	expression tag	UNP P12558
C	93	LEU	-	expression tag	UNP P12558
C	94	SER	-	expression tag	UNP P12558
C	95	LEU	-	expression tag	UNP P12558
C	96	VAL	-	expression tag	UNP P12558
C	97	SER	-	expression tag	UNP P12558
C	98	LEU	-	expression tag	UNP P12558
C	99	LEU	-	expression tag	UNP P12558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	SER	-	expression tag	UNP P12558
C	101	VAL	-	expression tag	UNP P12558
C	102	LEU	-	expression tag	UNP P12558
C	103	LEU	-	expression tag	UNP P12558
C	104	MET	-	expression tag	UNP P12558
C	105	GLY	-	expression tag	UNP P12558
C	106	CYS	-	expression tag	UNP P12558
C	107	VAL	-	expression tag	UNP P12558
C	108	ALA	-	expression tag	UNP P12558
C	109	GLU	-	expression tag	UNP P12558
C	110	THR	-	expression tag	UNP P12558
C	111	GLY	-	expression tag	UNP P12558
C	112	HIS	-	expression tag	UNP P12558
C	113	HIS	-	expression tag	UNP P12558
C	114	HIS	-	expression tag	UNP P12558
C	115	HIS	-	expression tag	UNP P12558
C	116	HIS	-	expression tag	UNP P12558
C	117	HIS	-	expression tag	UNP P12558
C	118	LEU	-	expression tag	UNP P12558
C	119	VAL	-	expression tag	UNP P12558
C	120	PRO	-	expression tag	UNP P12558
C	121	ARG	-	expression tag	UNP P12558
C	122	GLY	-	expression tag	UNP P12558
C	123	SER	-	expression tag	UNP P12558
D	81	MET	-	expression tag	UNP P12558
D	82	GLY	-	expression tag	UNP P12558
D	83	ILE	-	expression tag	UNP P12558
D	84	LEU	-	expression tag	UNP P12558
D	85	PRO	-	expression tag	UNP P12558
D	86	SER	-	expression tag	UNP P12558
D	87	PRO	-	expression tag	UNP P12558
D	88	GLY	-	expression tag	UNP P12558
D	89	MET	-	expression tag	UNP P12558
D	90	PRO	-	expression tag	UNP P12558
D	91	ALA	-	expression tag	UNP P12558
D	92	LEU	-	expression tag	UNP P12558
D	93	LEU	-	expression tag	UNP P12558
D	94	SER	-	expression tag	UNP P12558
D	95	LEU	-	expression tag	UNP P12558
D	96	VAL	-	expression tag	UNP P12558
D	97	SER	-	expression tag	UNP P12558
D	98	LEU	-	expression tag	UNP P12558

Continued on next page...

Continued from previous page...

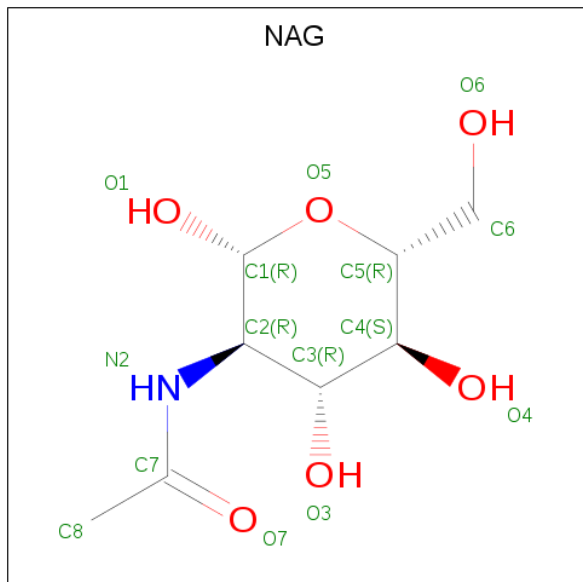
Chain	Residue	Modelled	Actual	Comment	Reference
D	99	LEU	-	expression tag	UNP P12558
D	100	SER	-	expression tag	UNP P12558
D	101	VAL	-	expression tag	UNP P12558
D	102	LEU	-	expression tag	UNP P12558
D	103	LEU	-	expression tag	UNP P12558
D	104	MET	-	expression tag	UNP P12558
D	105	GLY	-	expression tag	UNP P12558
D	106	CYS	-	expression tag	UNP P12558
D	107	VAL	-	expression tag	UNP P12558
D	108	ALA	-	expression tag	UNP P12558
D	109	GLU	-	expression tag	UNP P12558
D	110	THR	-	expression tag	UNP P12558
D	111	GLY	-	expression tag	UNP P12558
D	112	HIS	-	expression tag	UNP P12558
D	113	HIS	-	expression tag	UNP P12558
D	114	HIS	-	expression tag	UNP P12558
D	115	HIS	-	expression tag	UNP P12558
D	116	HIS	-	expression tag	UNP P12558
D	117	HIS	-	expression tag	UNP P12558
D	118	LEU	-	expression tag	UNP P12558
D	119	VAL	-	expression tag	UNP P12558
D	120	PRO	-	expression tag	UNP P12558
D	121	ARG	-	expression tag	UNP P12558
D	122	GLY	-	expression tag	UNP P12558
D	123	SER	-	expression tag	UNP P12558

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

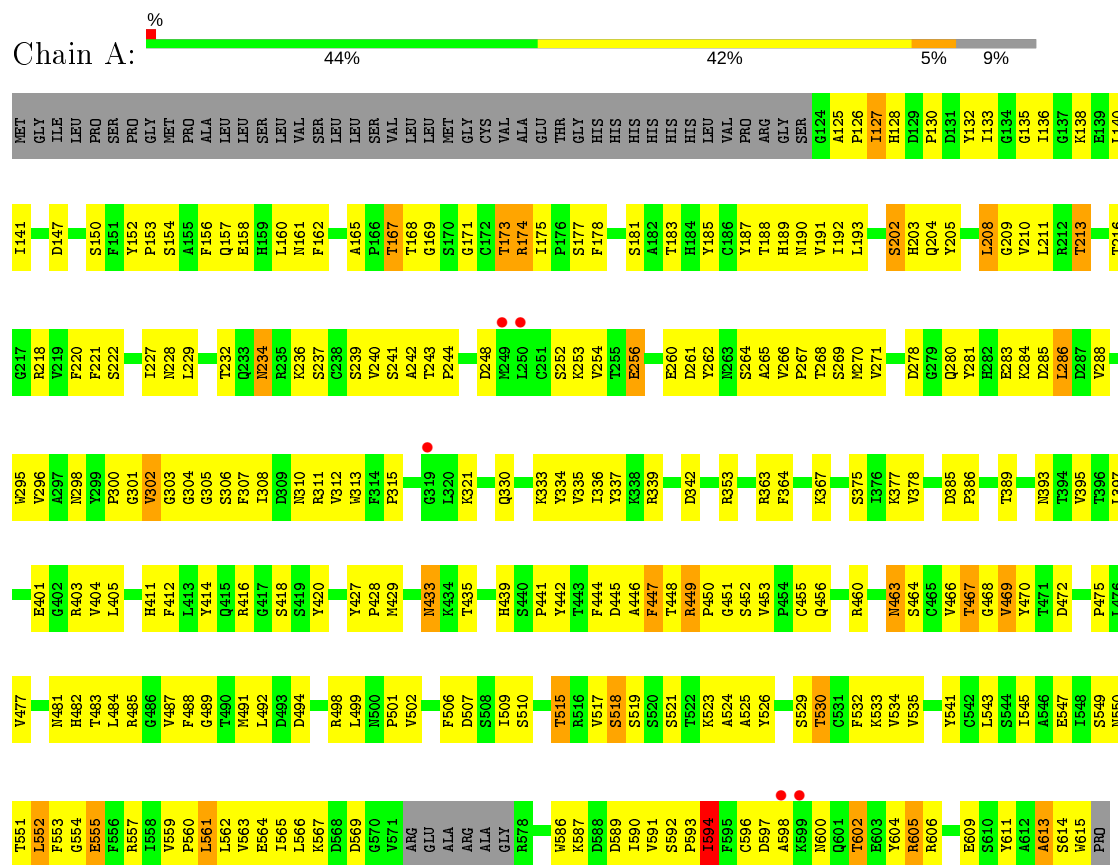


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

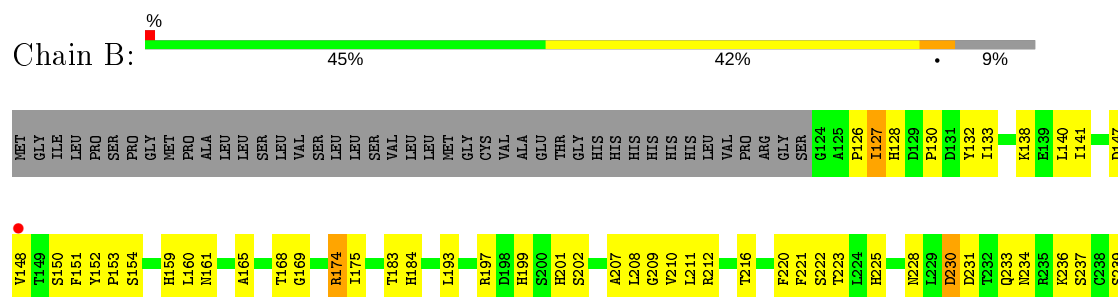
3 Residue-property plots

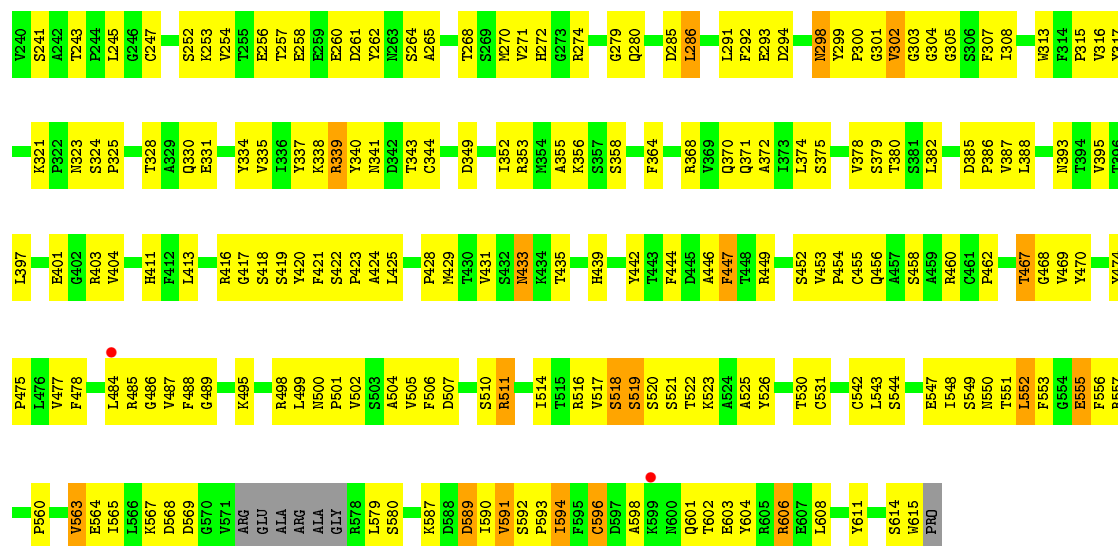
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hemagglutinin-neuraminidase

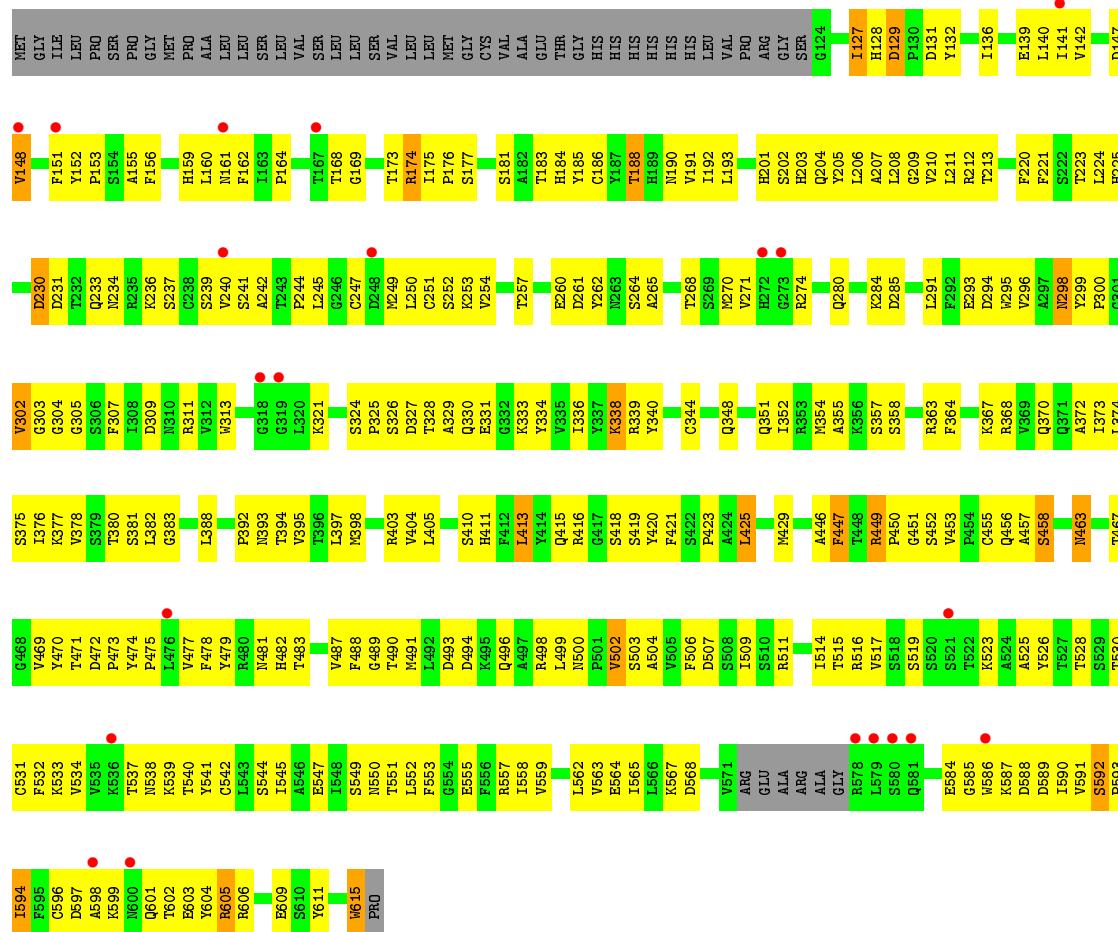


• Molecule 1: Hemagglutinin-neuraminidase

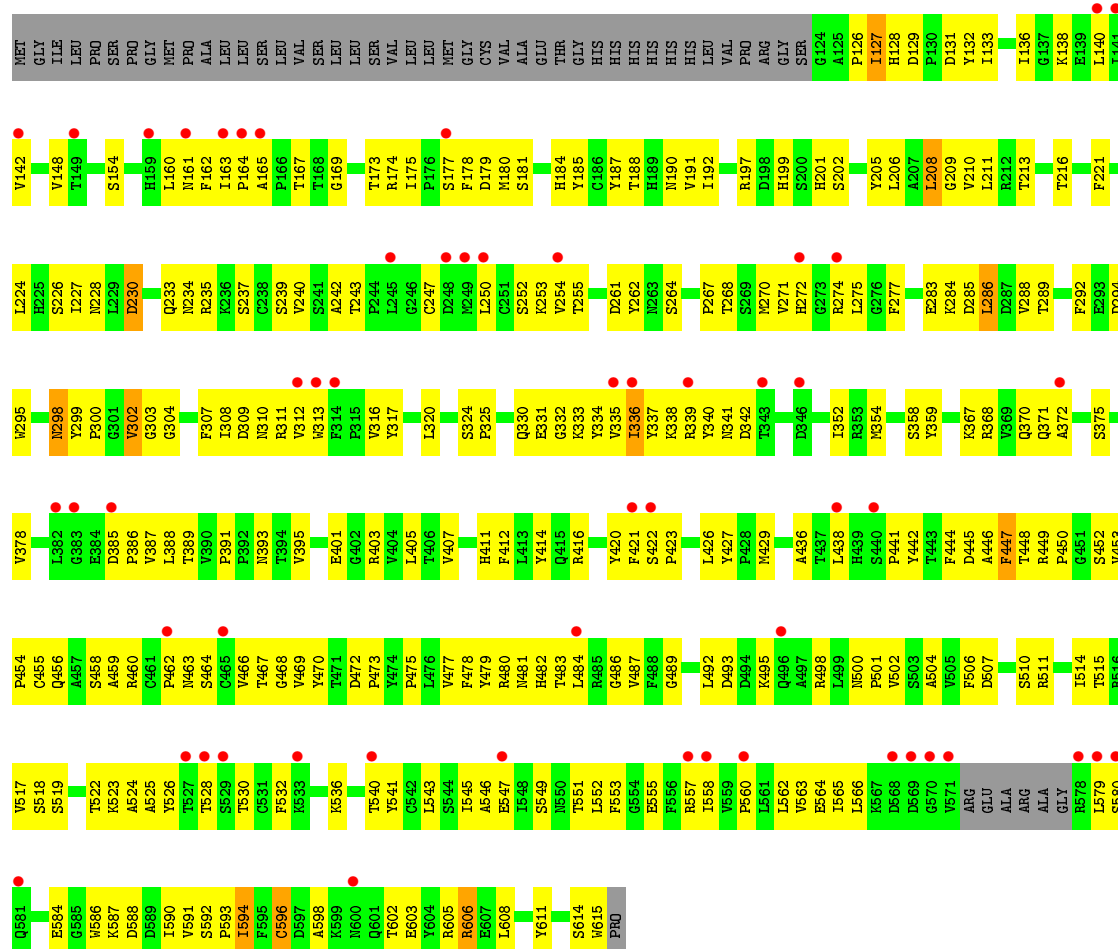
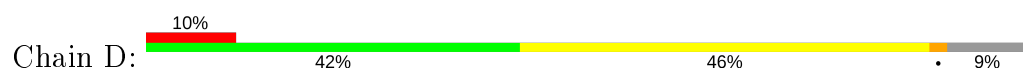




• Molecule 1: Hemagglutinin-neuraminidase



• Molecule 1: Hemagglutinin-neuraminidase



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



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



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



Mol
1962

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

Chain H:

100%

Mol
1962

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.61Å 124.61Å 284.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.91 – 3.50 47.49 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.91-3.50) 98.5 (47.49-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.236 , 0.304 0.230 , 0.302	Depositor DCC
R_{free} test set	1663 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	117.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 89.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15242	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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	0.39	0/3852	0.58	1/5243 (0.0%)
1	B	0.36	0/3852	0.56	0/5243
1	C	0.32	0/3852	0.52	0/5243
1	D	0.27	0/3852	0.49	0/5243
All	All	0.34	0/15408	0.54	1/20972 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	594	ILE	N-CA-C	5.34	125.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	613	ALA	Peptide

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	3758	0	3594	255	1
1	B	3758	0	3594	245	1
1	C	3758	0	3595	288	1
1	D	3758	0	3594	256	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	28	0	26	0	0
All	All	15242	0	14568	1000	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 34.

The worst 5 of 1000 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:587:LYS:HD3	1:B:169:GLY:HA3	1.23	1.19
1:B:525:ALA:HB3	1:B:547:GLU:HB2	1.30	1.11
1:C:174:ARG:HH11	1:C:174:ARG:HB3	1.18	1.07
1:A:598:ALA:HA	1:B:596:CYS:HB3	1.33	1.07
1:A:190:ASN:HD21	1:A:202:SER:HB2	1.12	1.07

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:B:353:ARG:NH2	1:C:609:GLU:OE2[4_455]	2.14	0.06
1:A:353:ARG:NH2	1:A:609:GLU:OE2[4_555]	2.18	0.02

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	482/536 (90%)	437 (91%)	42 (9%)	3 (1%)	25	64
1	B	482/536 (90%)	439 (91%)	40 (8%)	3 (1%)	25	64
1	C	482/536 (90%)	438 (91%)	41 (8%)	3 (1%)	25	64
1	D	482/536 (90%)	441 (92%)	38 (8%)	3 (1%)	25	64
All	All	1928/2144 (90%)	1755 (91%)	161 (8%)	12 (1%)	25	64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	594	ILE
1	B	594	ILE
1	C	594	ILE
1	D	302	VAL
1	D	594	ILE

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	418/464 (90%)	387 (93%)	31 (7%)	13	44
1	B	418/464 (90%)	394 (94%)	24 (6%)	20	53
1	C	418/464 (90%)	394 (94%)	24 (6%)	20	53
1	D	418/464 (90%)	402 (96%)	16 (4%)	33	65
All	All	1672/1856 (90%)	1577 (94%)	95 (6%)	20	53

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	511	ARG
1	B	596	CYS
1	D	336	ILE
1	B	519	SER
1	B	552	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	463	ASN
1	B	500	ASN
1	D	128	HIS
1	B	234	ASN
1	B	393	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 ⓘ

8 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	0.58	0	17,19,21	0.68	0
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.68	0
2	NAG	F	1	1,2	14,14,15	0.54	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	F	2	2	14,14,15	0.53	0	17,19,21	0.69	0
2	NAG	G	1	1,2	14,14,15	0.54	0	17,19,21	0.71	0
2	NAG	G	2	2	14,14,15	0.52	0	17,19,21	0.63	0
2	NAG	H	1	1,2	14,14,15	0.56	0	17,19,21	0.61	0
2	NAG	H	2	2	14,14,15	0.54	0	17,19,21	0.64	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	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	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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

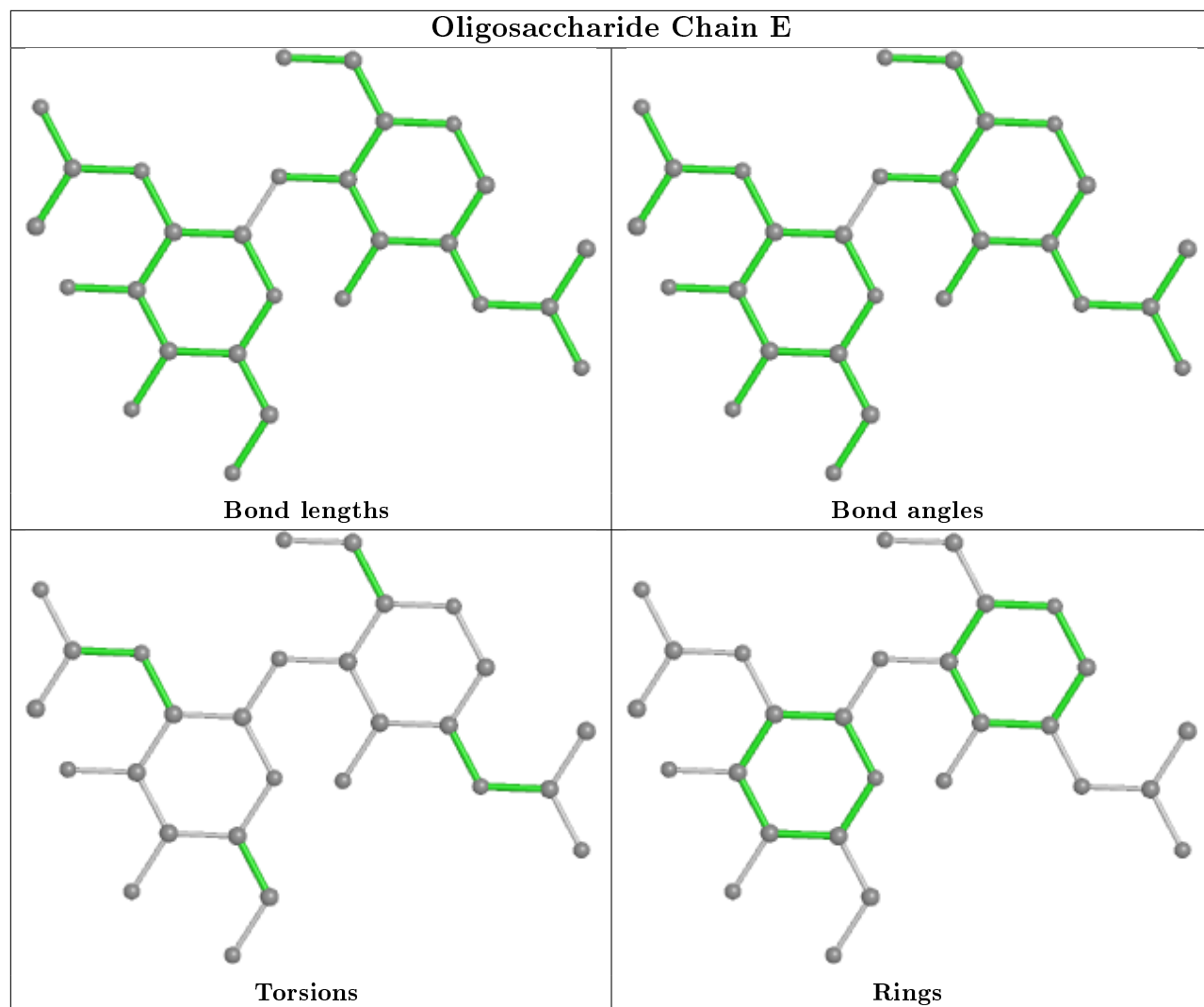
All (2) torsion outliers are listed below:

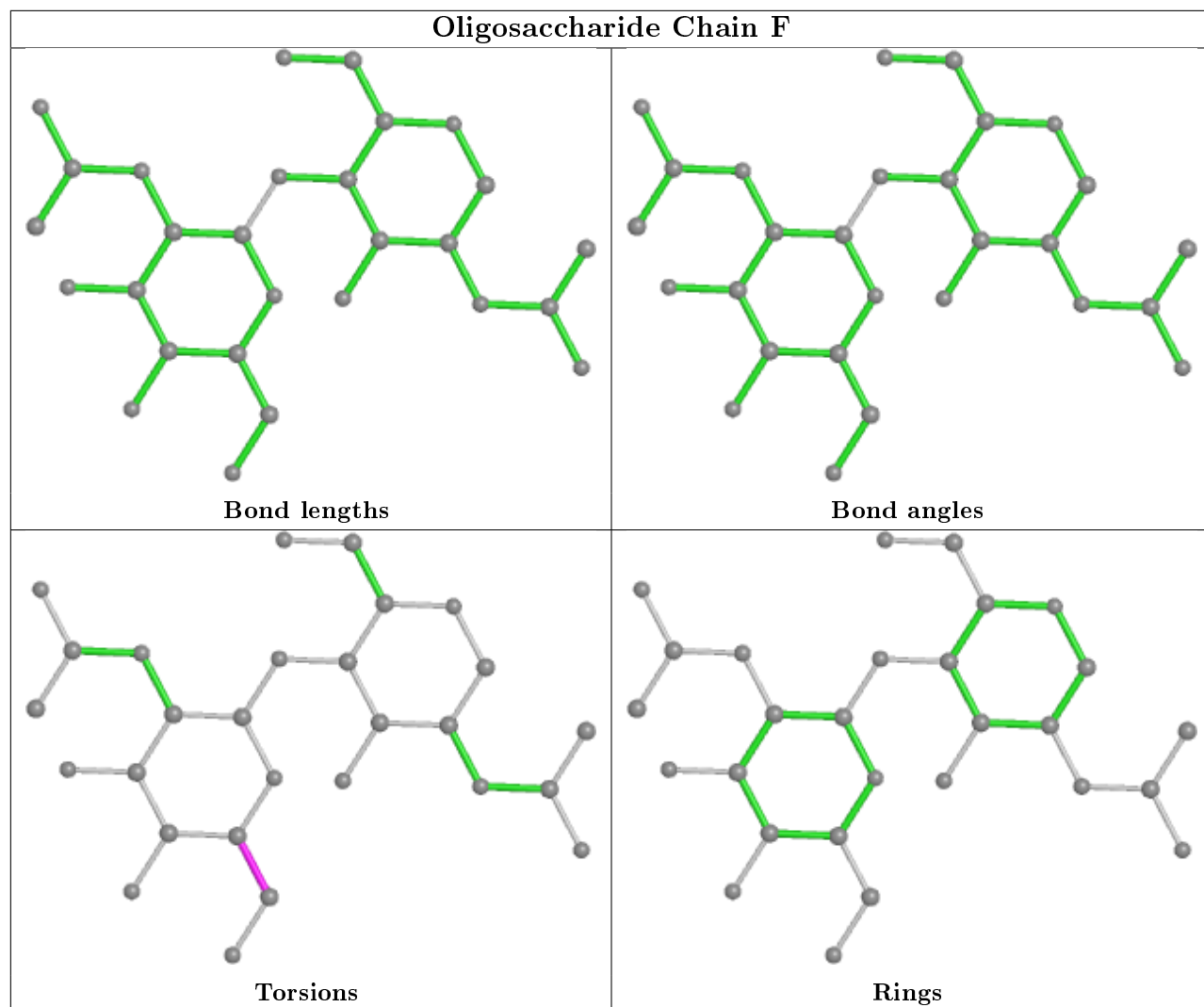
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

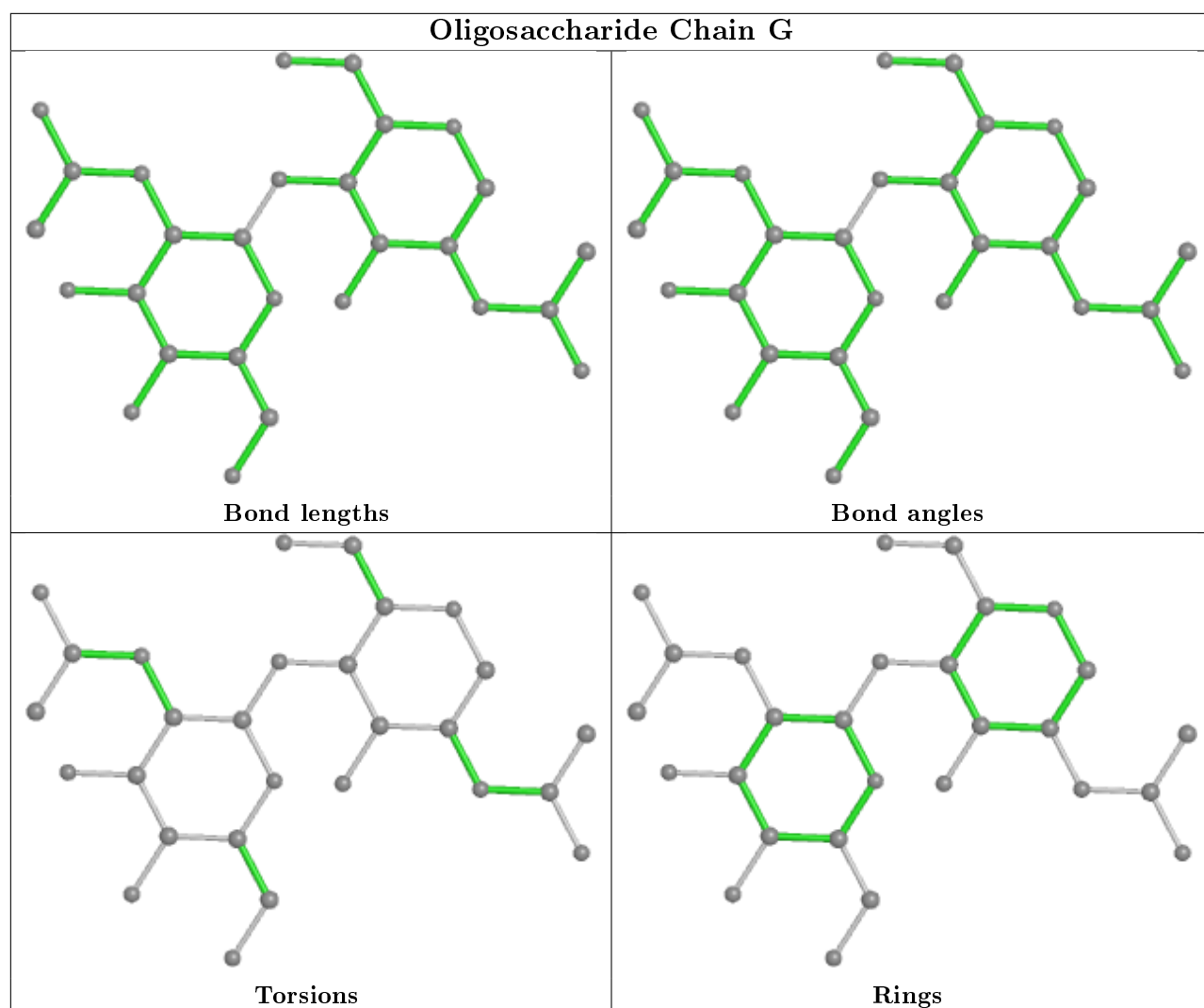
There are no ring outliers.

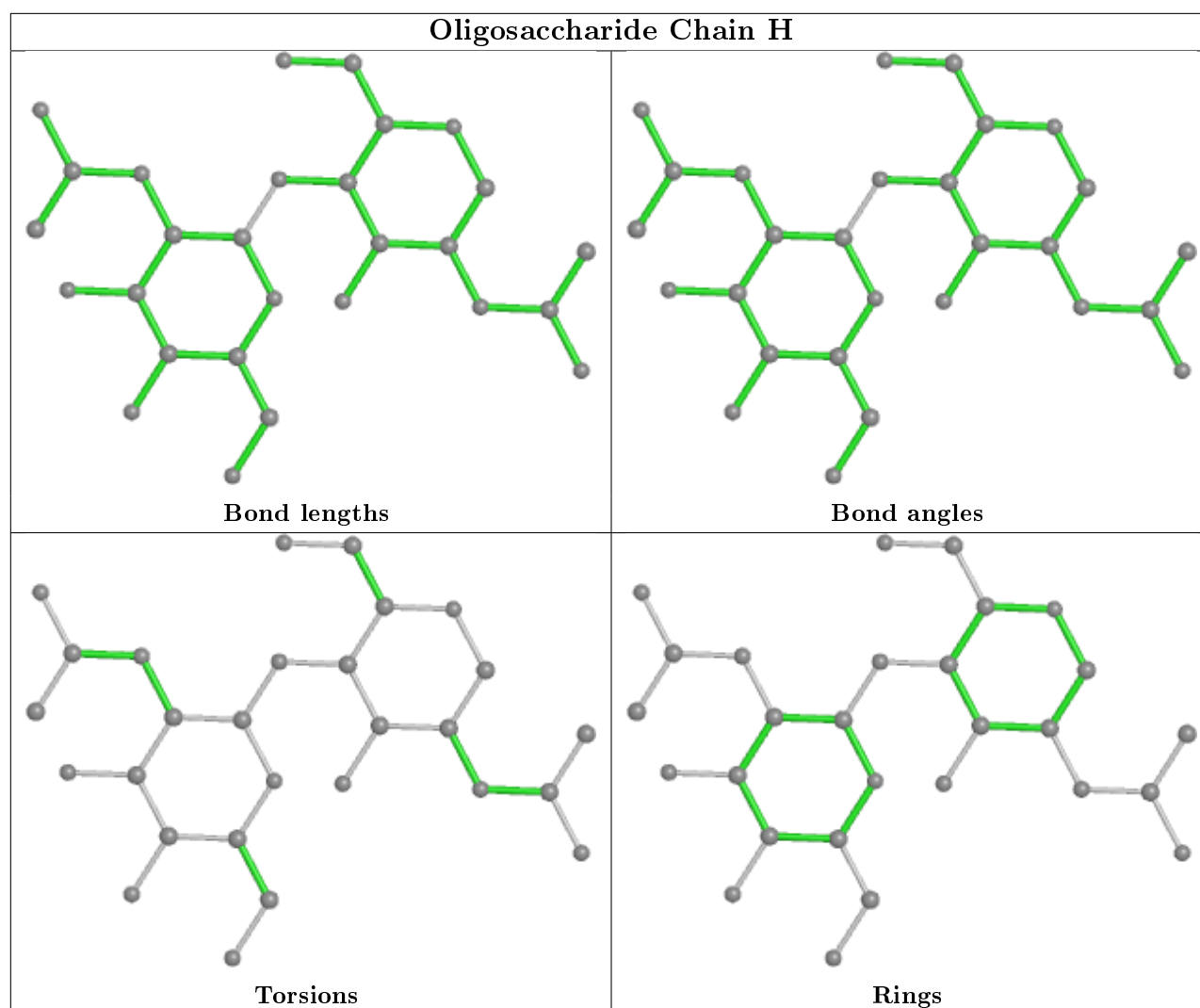
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
3	NAG	C	701	1	14,14,15	0.52	0	17,19,21	0.68	0
3	NAG	A	702	1	14,14,15	0.56	0	17,19,21	0.60	0
3	NAG	D	701	1	14,14,15	0.57	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	702	1	14,14,15	0.60	0	17,19,21	0.57	0
3	NAG	B	701	1	14,14,15	0.51	0	17,19,21	0.75	0
3	NAG	D	702	1	14,14,15	0.54	0	17,19,21	0.55	0
3	NAG	A	701	1	14,14,15	0.53	0	17,19,21	0.68	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	C	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
3	NAG	D	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1	-	2/6/23/26	0/1/1/1
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	701	NAG	C1-O5-C5	2.45	115.51	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	702	NAG	O5-C5-C6-O6
3	D	702	NAG	C4-C5-C6-O6

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	486/536 (90%)	-0.20	5 (1%) 82 77	80, 118, 161, 215	0
1	B	486/536 (90%)	-0.21	3 (0%) 89 86	85, 131, 178, 249	0
1	C	486/536 (90%)	0.01	21 (4%) 35 31	118, 155, 220, 274	0
1	D	486/536 (90%)	0.54	55 (11%) 5 6	144, 208, 259, 360	0
All	All	1944/2144 (90%)	0.04	84 (4%) 35 31	80, 146, 237, 360	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	571	VAL	13.5
1	D	570	GLY	8.5
1	D	336	ILE	5.8
1	D	421	PHE	5.2
1	D	528	THR	5.1

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

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

6.3 Carbohydrates [i](#)

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

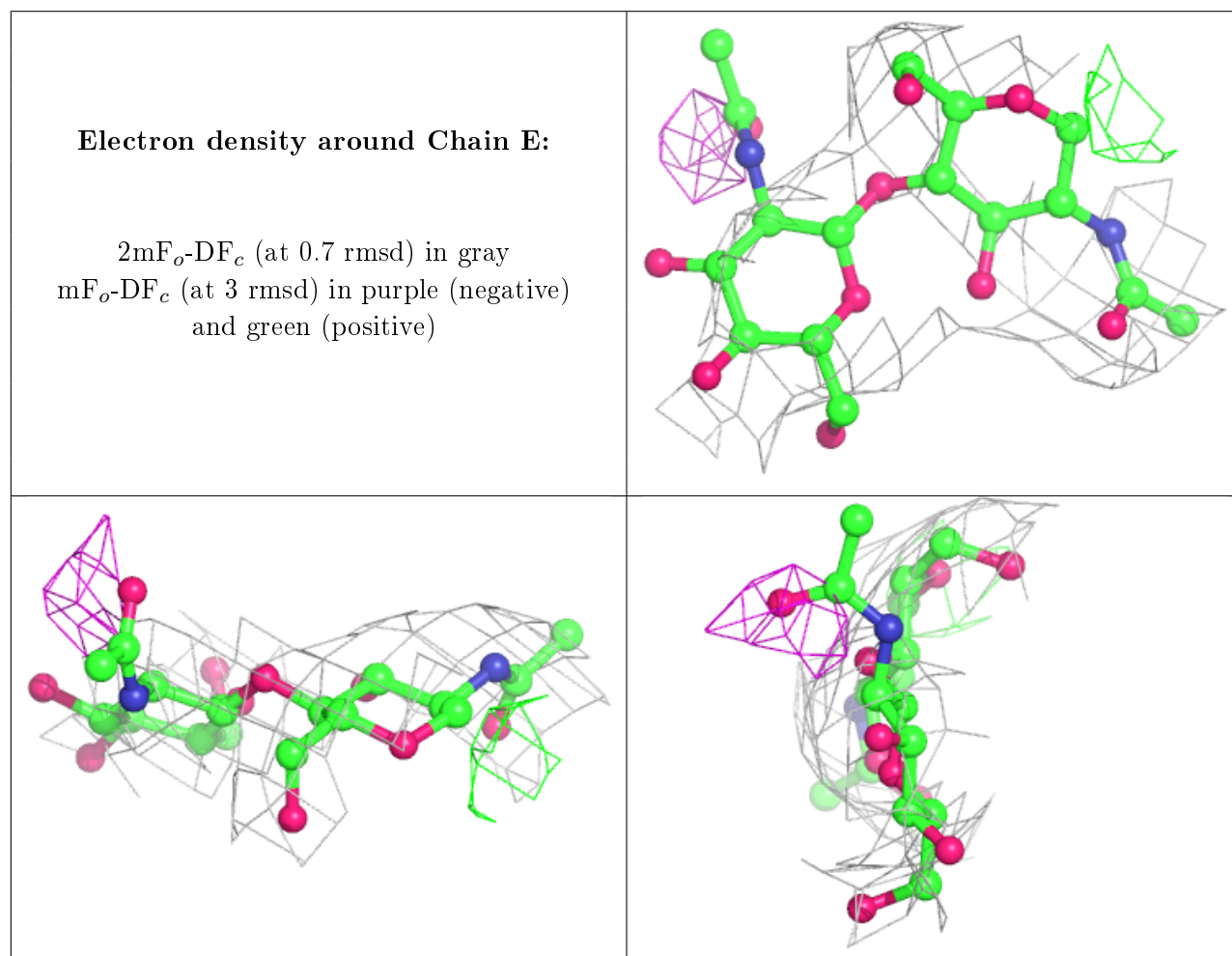
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.56	0.61	197,207,217,218	0
2	NAG	E	1	14/15	0.69	0.24	144,163,172,183	0

Continued on next page...

Continued from previous page...

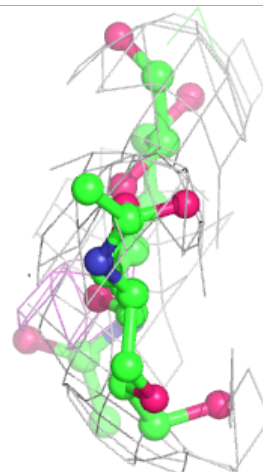
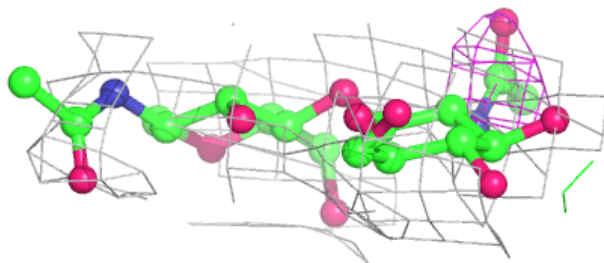
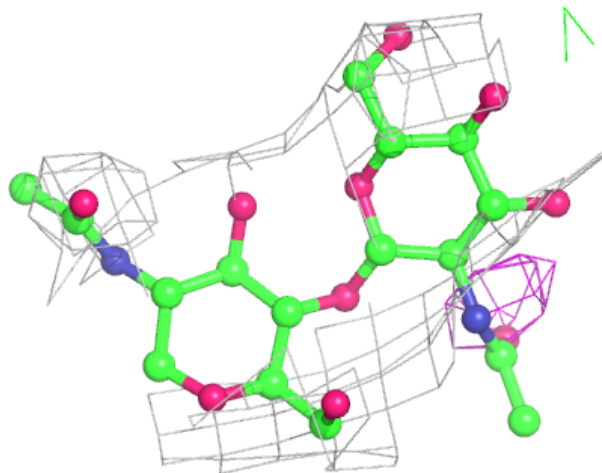
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	F	2	14/15	0.69	0.42	173,181,190,192	0
2	NAG	G	2	14/15	0.72	0.38	196,203,205,205	0
2	NAG	E	2	14/15	0.78	0.59	195,205,213,214	0
2	NAG	G	1	14/15	0.80	0.33	158,168,178,187	0
2	NAG	H	1	14/15	0.81	0.21	149,165,171,183	0
2	NAG	F	1	14/15	0.86	0.27	138,148,153,163	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.



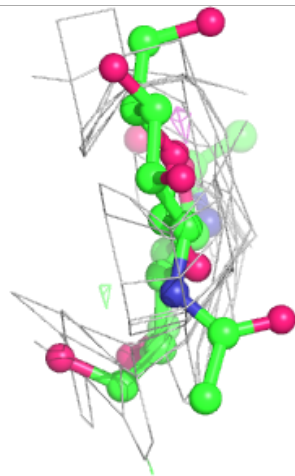
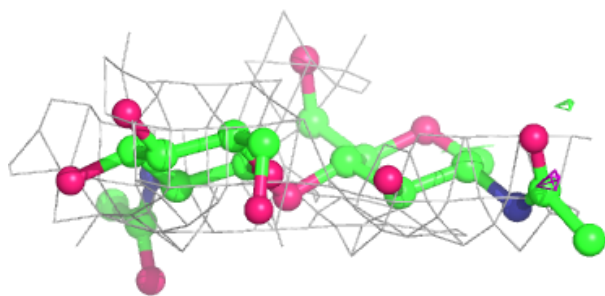
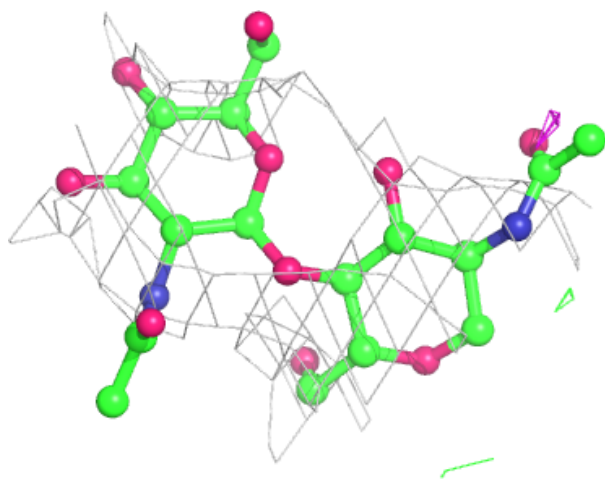
Electron density around Chain F:

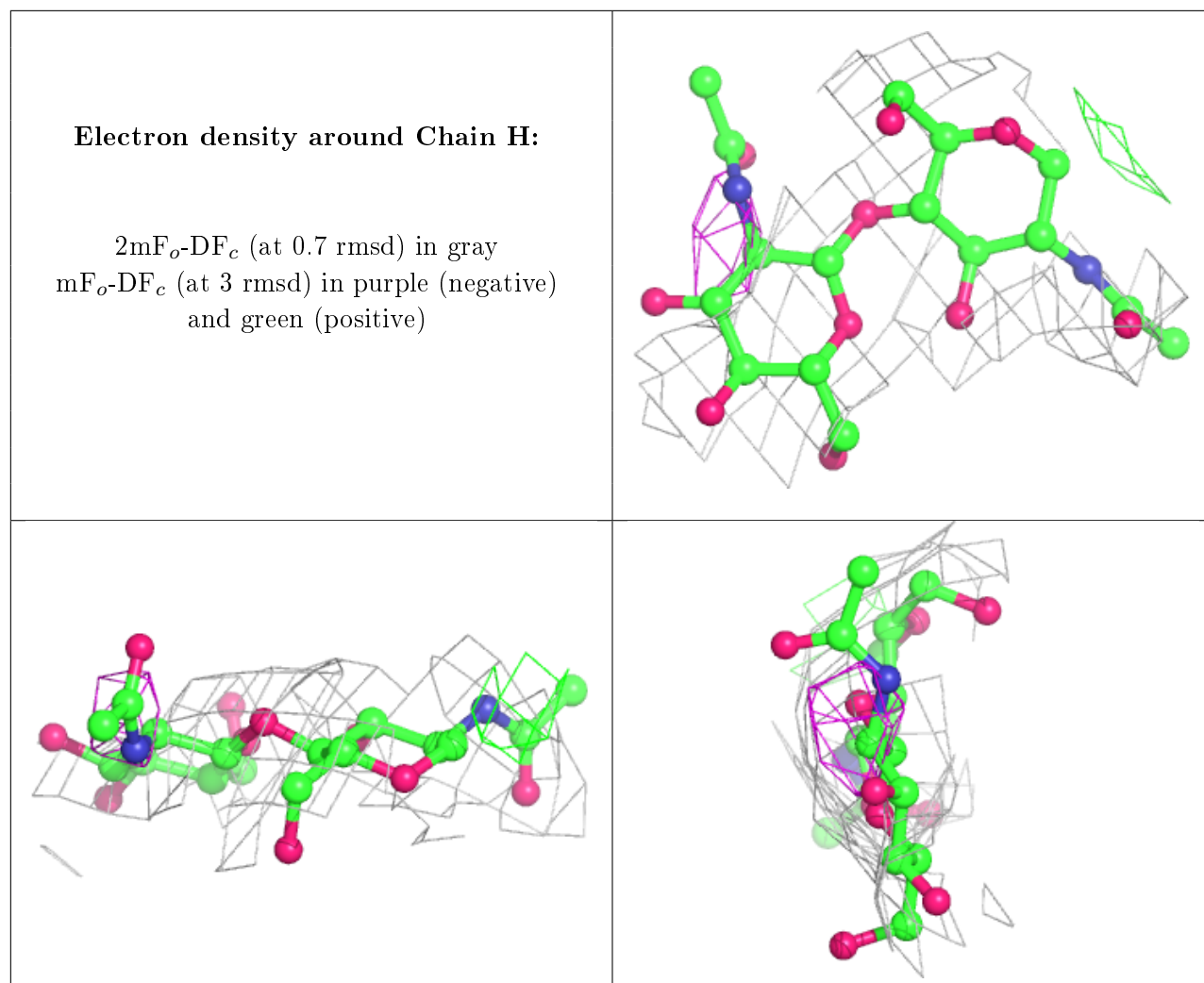
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
3	NAG	D	701	14/15	0.31	0.50	198,215,218,219	0
3	NAG	D	702	14/15	0.47	0.42	173,180,182,183	0
3	NAG	B	702	14/15	0.62	0.48	168,177,181,182	0
3	NAG	A	702	14/15	0.75	0.45	157,170,174,176	0
3	NAG	C	701	14/15	0.78	0.19	140,152,163,164	0
3	NAG	A	701	14/15	0.82	0.30	148,159,161,163	0
3	NAG	B	701	14/15	0.87	0.17	137,143,151,151	0

6.5 Other polymers ⓘ

There are no such residues in this entry.