



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 10:35 PM UTC

PDB ID : 9OWF / pdb_00009owf
Title : X-ray crystal structure of Zika virus envelope glycoprotein in complex with Fab of F25.S02
Authors : Hurlburt, N.K.; Pancera, M.
Deposited on : 2025-06-02
Resolution : 2.30 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 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

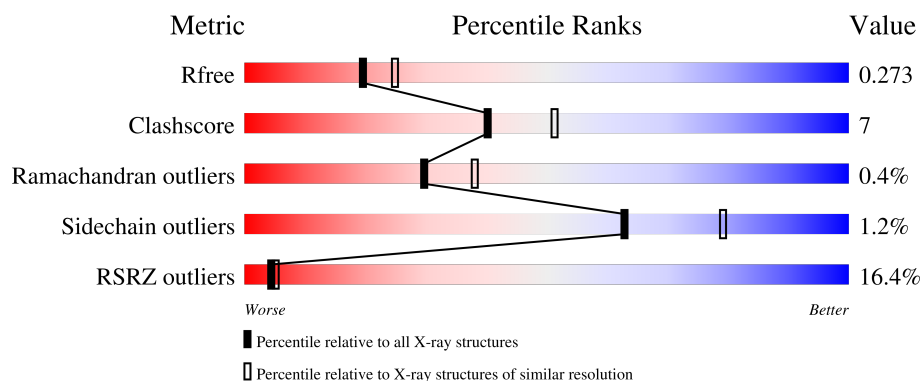
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	404	<div> <div>9%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	B	404	<div> <div>12%</div> <div>89%</div> <div>10%</div> </div>
2	C	238	<div> <div>27%</div> <div>73%</div> <div>18%</div> <div>.</div> <div>8%</div> </div>
2	H	238	<div> <div>16%</div> <div>70%</div> <div>18%</div> <div>.</div> <div>11%</div> </div>
3	D	217	<div> <div>22%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	217	
4	E	6	
5	F	5	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26033 atoms, of which 12882 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 Genome polyprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	C	H	N	O	S	0	0	0
			6097	1924	3013	539	595	26			
1	B	404	Total	C	H	N	O	S	0	0	0
			6063	1924	2979	539	595	26			

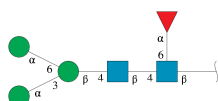
- Molecule 2 is a protein called F25.S02 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	220	Total	C	H	N	O	S	0	0	0
			3273	1049	1619	279	319	7			
2	H	212	Total	C	H	N	O	S	0	0	0
			3181	1021	1573	271	309	7			

- Molecule 3 is a protein called F25.S02 light chain.

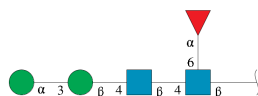
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	211	Total	C	H	N	O	S	0	0	0
			3097	985	1524	263	319	6			
3	L	212	Total	C	H	N	O	S	0	0	0
			3109	988	1530	264	321	6			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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
4	E	6	Total	C	H	N	O		0	0	0
			138	40	67	2	29				

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-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
5	F	5	Total	C	H	N	O	0	0	0
			117	34	57	2	24			

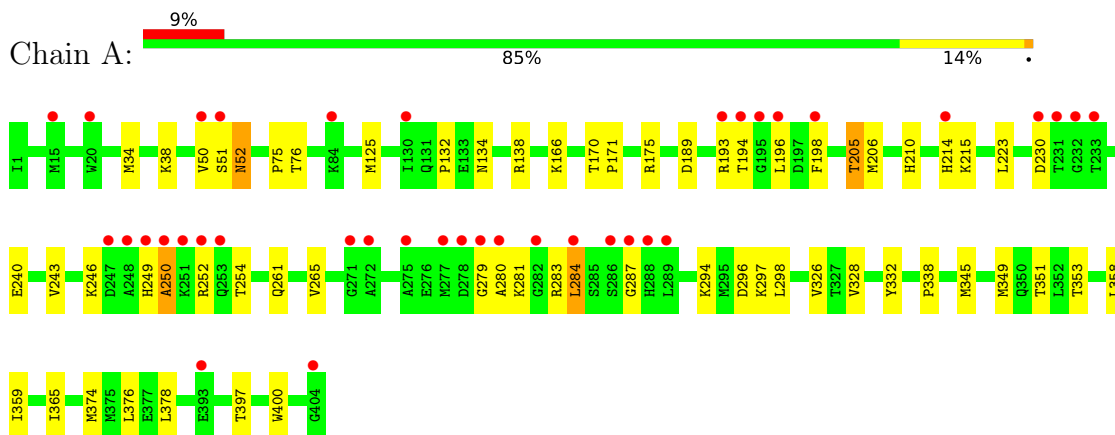
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	122	Total	H	O	0	0
			262	140	122		
6	B	104	Total	H	O	0	0
			236	132	104		
6	C	31	Total	H	O	0	0
			63	32	31		
6	D	58	Total	H	O	0	0
			118	60	58		
6	H	43	Total	H	O	0	0
			101	58	43		
6	L	80	Total	H	O	0	0
			178	98	80		

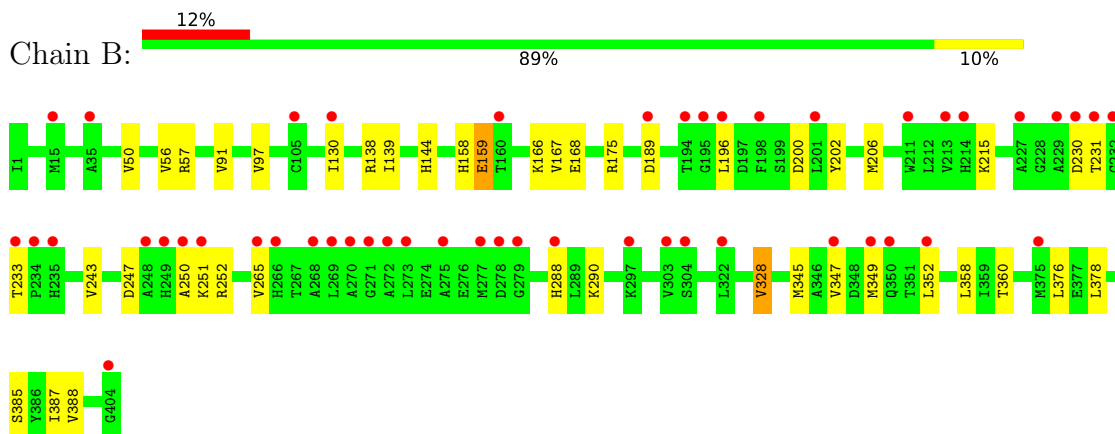
3 Residue-property plots [i](#)

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.

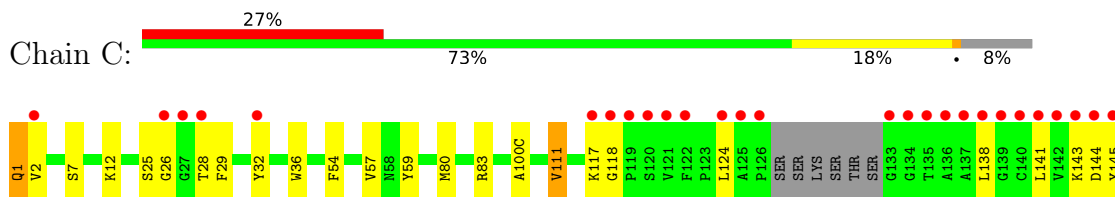
- Molecule 1: Genome polypeptide

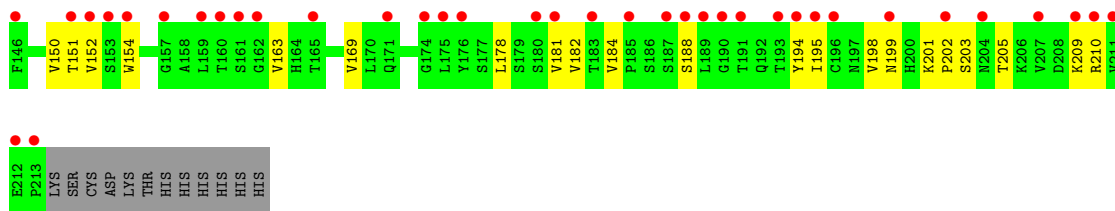


- Molecule 1: Genome polypeptide

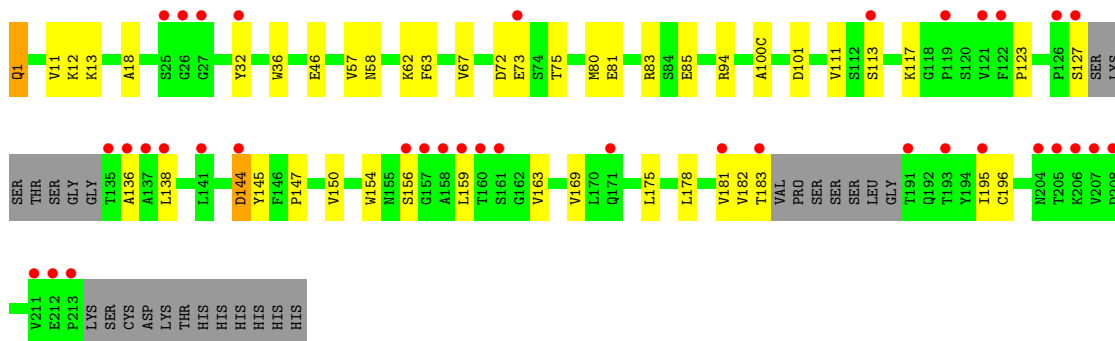


- Molecule 2: F25.S02 heavy chain

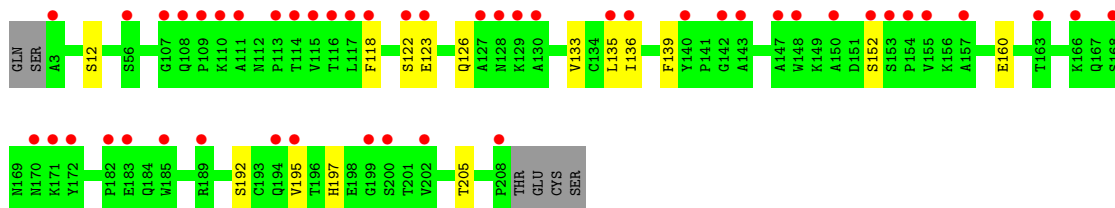
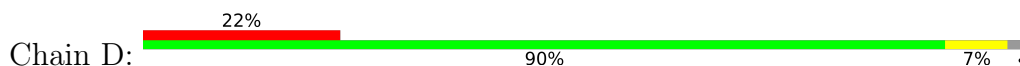




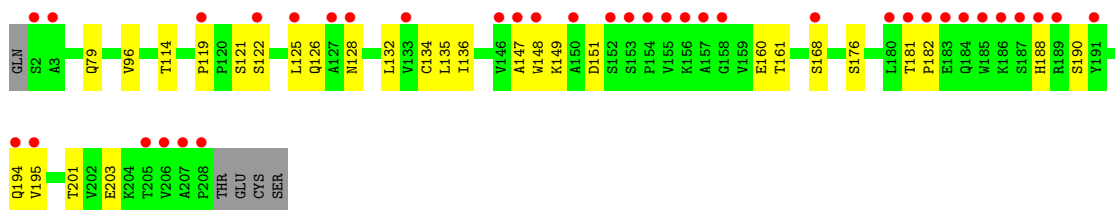
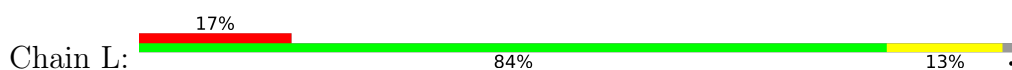
• Molecule 2: F25.S02 heavy chain



• Molecule 3: F25.S02 light chain



• Molecule 3: F25.S02 light chain



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



MAG1
MAG2
BMA3
MAN4
FUC5

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.86Å 117.86Å 346.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.30 48.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.70-2.30) 99.2 (48.70-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.274 0.226 , 0.273	Depositor DCC
R_{free} test set	5420 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26033	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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

5.1 Standard geometry

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

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	0.19	0/3149	0.41	0/4266
1	B	0.20	0/3149	0.41	0/4266
2	C	0.18	0/1688	0.39	0/2300
2	H	0.18	0/1640	0.40	1/2233 (0.0%)
3	D	0.18	0/1613	0.40	0/2201
3	L	0.20	0/1619	0.46	0/2209
All	All	0.19	0/12858	0.41	1/17475 (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	B	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	O-C-N	-6.33	112.86	123.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	ARG	Sidechain
1	B	252	ARG	Sidechain
2	H	1	PCA	Mainchain

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	3084	3013	3012	45	0
1	B	3084	2979	3012	32	0
2	C	1654	1619	1618	40	0
2	H	1608	1573	1571	30	0
3	D	1573	1524	1523	13	0
3	L	1579	1530	1528	16	0
4	E	71	67	61	2	0
5	F	60	57	52	1	0
6	A	122	140	0	0	0
6	B	104	132	0	0	0
6	C	31	32	0	1	0
6	D	58	60	0	0	0
6	H	43	58	0	0	0
6	L	80	98	0	0	0
All	All	13151	12882	12377	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 7.

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)
3:D:123:GLU:OE1	3:D:123:GLU:N	2.11	0.84
2:H:145:TYR:CE2	2:H:150:VAL:HG23	2.15	0.82
2:C:141:LEU:HD11	2:C:143:LYS:HD2	1.62	0.81
1:A:194:THR:HG23	1:A:287:GLY:HA3	1.64	0.79
1:B:56:VAL:HG21	1:B:202:TYR:HE1	1.48	0.78

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	402/404 (100%)	391 (97%)	9 (2%)	2 (0%)	24	31
1	B	402/404 (100%)	386 (96%)	15 (4%)	1 (0%)	43	55
2	C	216/238 (91%)	209 (97%)	5 (2%)	2 (1%)	14	17
2	H	206/238 (87%)	198 (96%)	6 (3%)	2 (1%)	12	15
3	D	209/217 (96%)	205 (98%)	4 (2%)	0	100	100
3	L	210/217 (97%)	201 (96%)	9 (4%)	0	100	100
All	All	1645/1718 (96%)	1590 (97%)	48 (3%)	7 (0%)	30	38

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	250	ALA
1	B	159	GLU
2	C	144	ASP
2	C	100(C)	ALA

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	337/337 (100%)	334 (99%)	3 (1%)	70	84
1	B	337/337 (100%)	333 (99%)	4 (1%)	63	79
2	C	181/199 (91%)	180 (99%)	1 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	176/199 (88%)	174 (99%)	2 (1%)	65	81
3	D	177/183 (97%)	175 (99%)	2 (1%)	65	81
3	L	178/183 (97%)	173 (97%)	5 (3%)	38	56
All	All	1386/1438 (96%)	1369 (99%)	17 (1%)	63	79

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	114	THR
3	L	190	SER
2	C	111	VAL
3	D	12	SER
3	D	152	SER

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

Mol	Chain	Res	Type
2	C	39	GLN
3	D	37	GLN
3	L	126	GLN
2	H	192	GLN
3	L	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PCA	C	1	2	7,8,9	1.92	1 (14%)	9,10,12	2.15	5 (55%)
2	PCA	H	1	2	7,8,9	1.91	1 (14%)	9,10,12	2.00	4 (44%)

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	PCA	C	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	PCA	CD-N	4.97	1.46	1.34
2	H	1	PCA	CD-N	4.93	1.46	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	PCA	CB-CA-N	2.99	111.47	103.24
2	H	1	PCA	CB-CA-N	2.97	111.42	103.24
2	C	1	PCA	CA-N-CD	-2.84	103.86	113.58
2	C	1	PCA	OE-CD-CG	-2.81	121.71	126.72
2	H	1	PCA	CA-N-CD	-2.80	103.97	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	PCA	1	0

5.5 Carbohydrates [i](#)

11 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	E	1	1,4	14,14,15	0.48	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.32	0	17,19,21	0.50	0
4	BMA	E	3	4	11,11,12	0.61	0	15,15,17	0.76	0
4	MAN	E	4	4	11,11,12	0.73	0	15,15,17	1.11	1 (6%)
4	MAN	E	5	4	11,11,12	0.72	0	15,15,17	0.94	1 (6%)
4	FUC	E	6	4	10,10,11	0.74	0	14,14,16	0.61	0
5	NAG	F	1	1,5	14,14,15	0.41	0	17,19,21	0.51	0
5	NAG	F	2	5	14,14,15	0.31	0	17,19,21	0.48	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.68	0
5	MAN	F	4	5	11,11,12	0.80	0	15,15,17	0.76	0
5	FUC	F	5	5	10,10,11	0.69	0	14,14,16	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
4	NAG	E	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	2/2/19/22	0/1/1/1
4	FUC	E	6	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	FUC	F	5	5	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	C1-O5-C5	3.39	116.73	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	MAN	C1-O5-C5	2.57	115.63	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

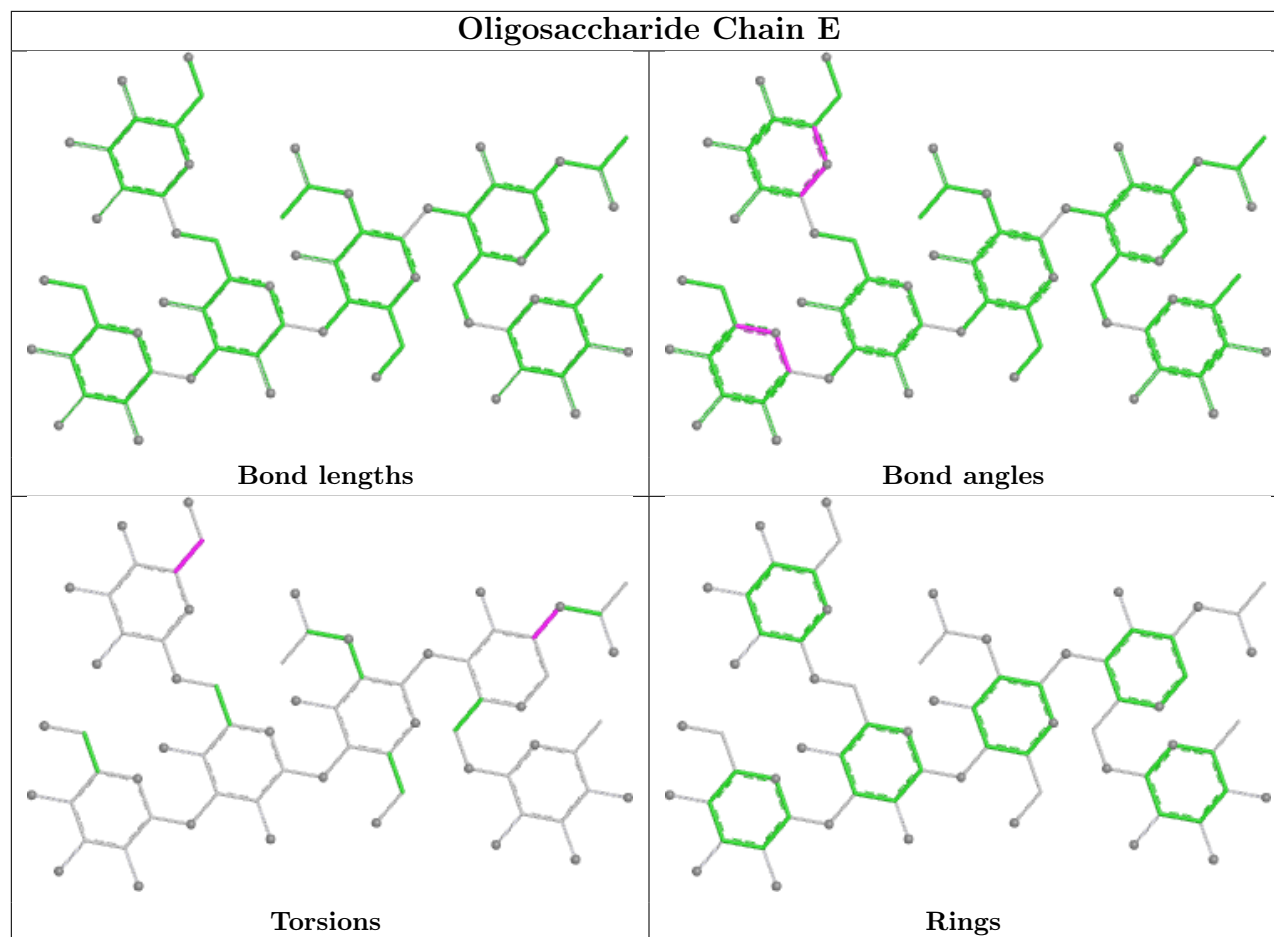
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
5	F	1	NAG	C1-C2-N2-C7
4	E	5	MAN	C4-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6

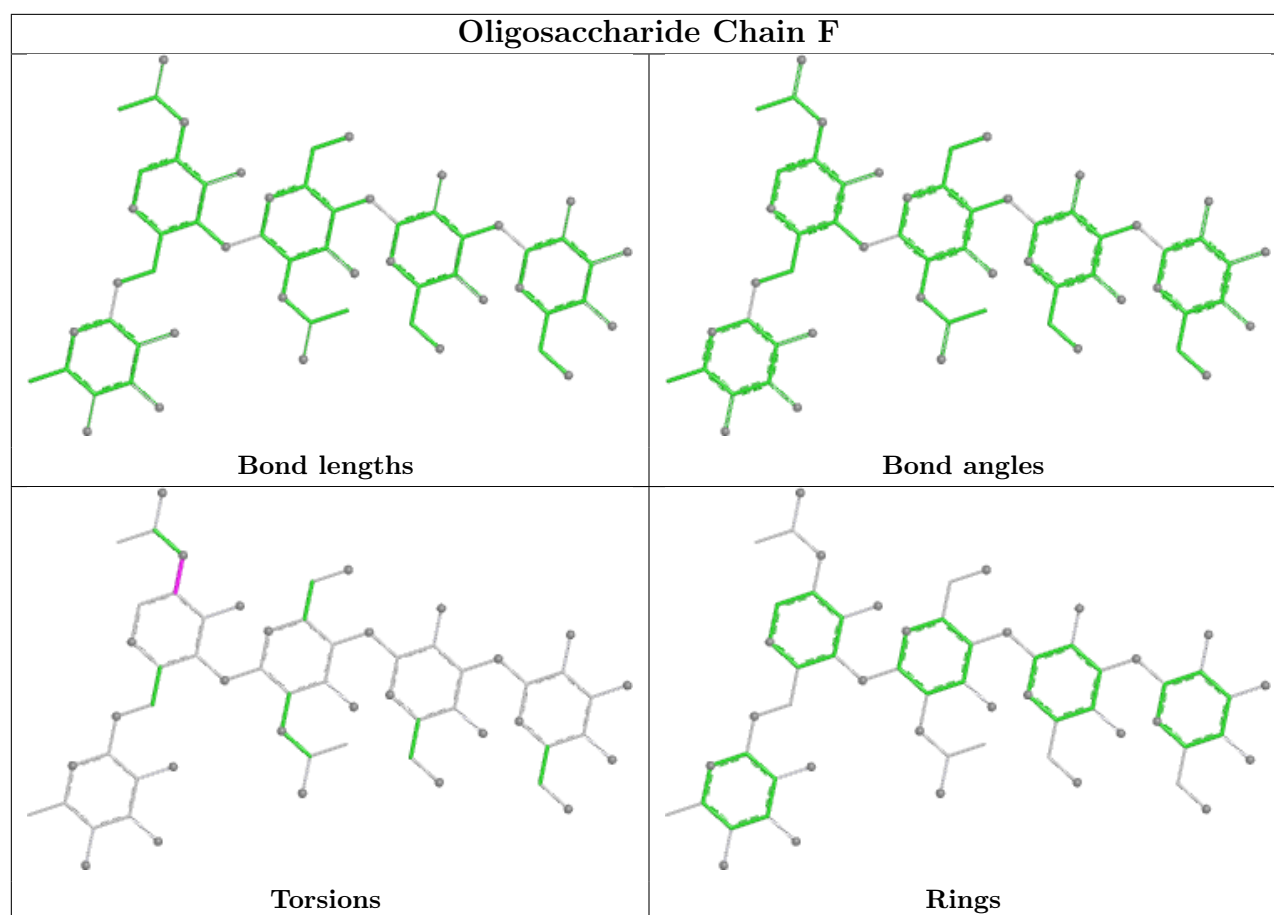
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	1	0
4	E	1	NAG	2	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.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	404/404 (100%)	0.75	38 (9%) 14 15	40, 66, 111, 150	0
1	B	404/404 (100%)	0.88	49 (12%) 8 9	41, 65, 111, 158	0
2	C	219/238 (92%)	1.34	64 (29%) 1 1	42, 80, 134, 211	0
2	H	211/238 (88%)	1.04	37 (17%) 4 4	37, 78, 123, 135	0
3	D	211/217 (97%)	1.13	48 (22%) 2 2	42, 86, 126, 154	0
3	L	212/217 (97%)	0.78	37 (17%) 4 4	37, 59, 132, 168	0
All	All	1661/1718 (96%)	0.95	273 (16%) 4 5	37, 69, 125, 211	0

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	195	ILE	9.3
1	B	234	PRO	9.1
3	L	2	SER	7.8
3	L	208	PRO	6.9
1	B	404	GLY	6.5

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

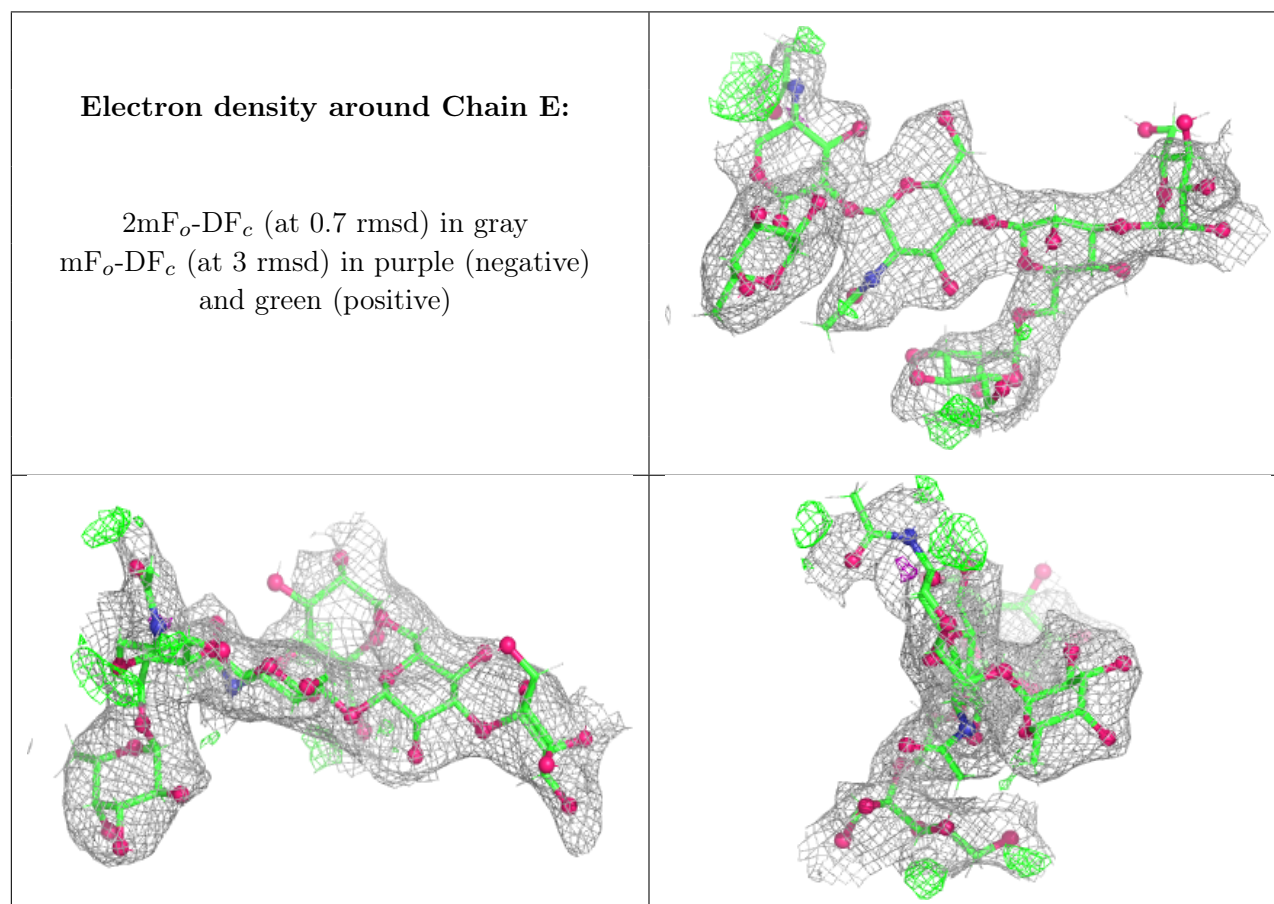
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PCA	C	1	8/9	0.90	0.20	68,80,96,99	0
2	PCA	H	1	8/9	0.91	0.22	63,70,81,85	0

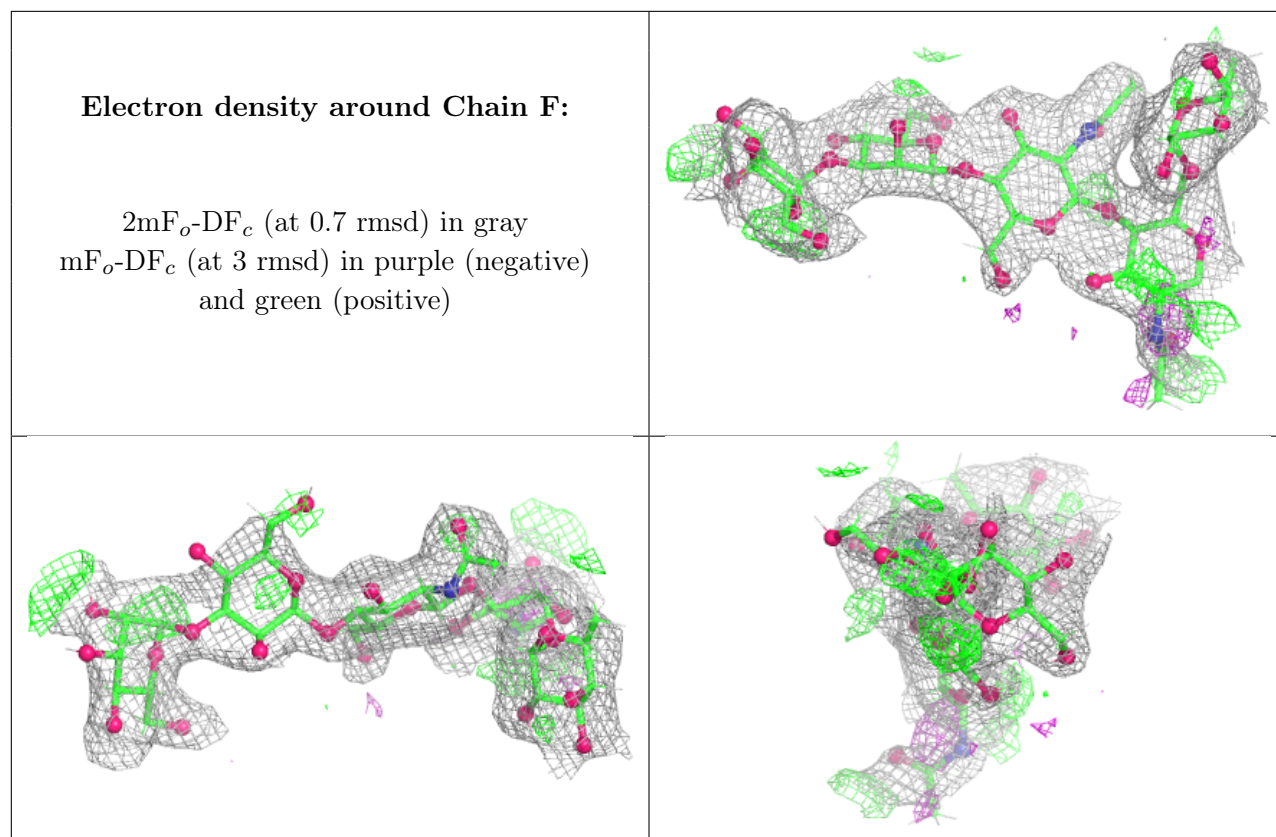
6.3 Carbohydrates [i](#)

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
4	NAG	E	1	14/15	-	-	72,89,107,110	0
4	NAG	E	2	14/15	-	-	77,85,102,103	0
4	BMA	E	3	11/12	-	-	88,101,118,119	0
4	MAN	E	4	11/12	-	-	94,105,122,126	0
4	MAN	E	5	11/12	-	-	97,114,133,134	0
4	FUC	E	6	10/11	-	-	69,83,95,102	0
5	NAG	F	1	14/15	-	-	61,81,97,98	0
5	NAG	F	2	14/15	-	-	59,71,85,89	0
5	BMA	F	3	11/12	-	-	77,91,108,119	0
5	MAN	F	4	11/12	-	-	71,95,117,122	0
5	FUC	F	5	10/11	-	-	59,71,83,97	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.