



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:06 AM UTC

PDB ID : 5K8D / pdb_00005k8d
Title : Crystal structure of rFVIIIFc
Authors : Leksa, N.; Quan, C.
Deposited on : 2016-05-29
Resolution : 4.19 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

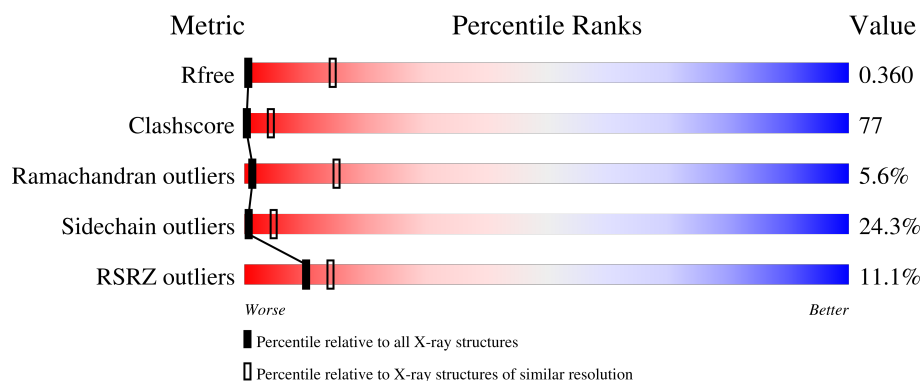
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	740	9% 19% 45% 16% • 17%
2	B	865	8% 18% 37% 15% • 28%
3	C	4	75% 25%
4	D	2	100%
5	E	7	14% 43% 43%

2 Entry composition [i](#)

There are 7 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 Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4937	3190	824	898	25			

- Molecule 2 is a protein called Coagulation factor VIII,Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			5035	3234	862	908	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2332	TYR	-	linker	UNP P00451

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



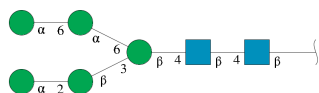
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O		0	0	0
			50	28	2	20				

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranos e-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



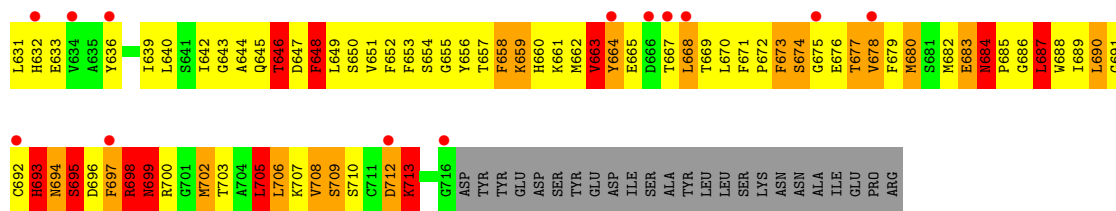
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

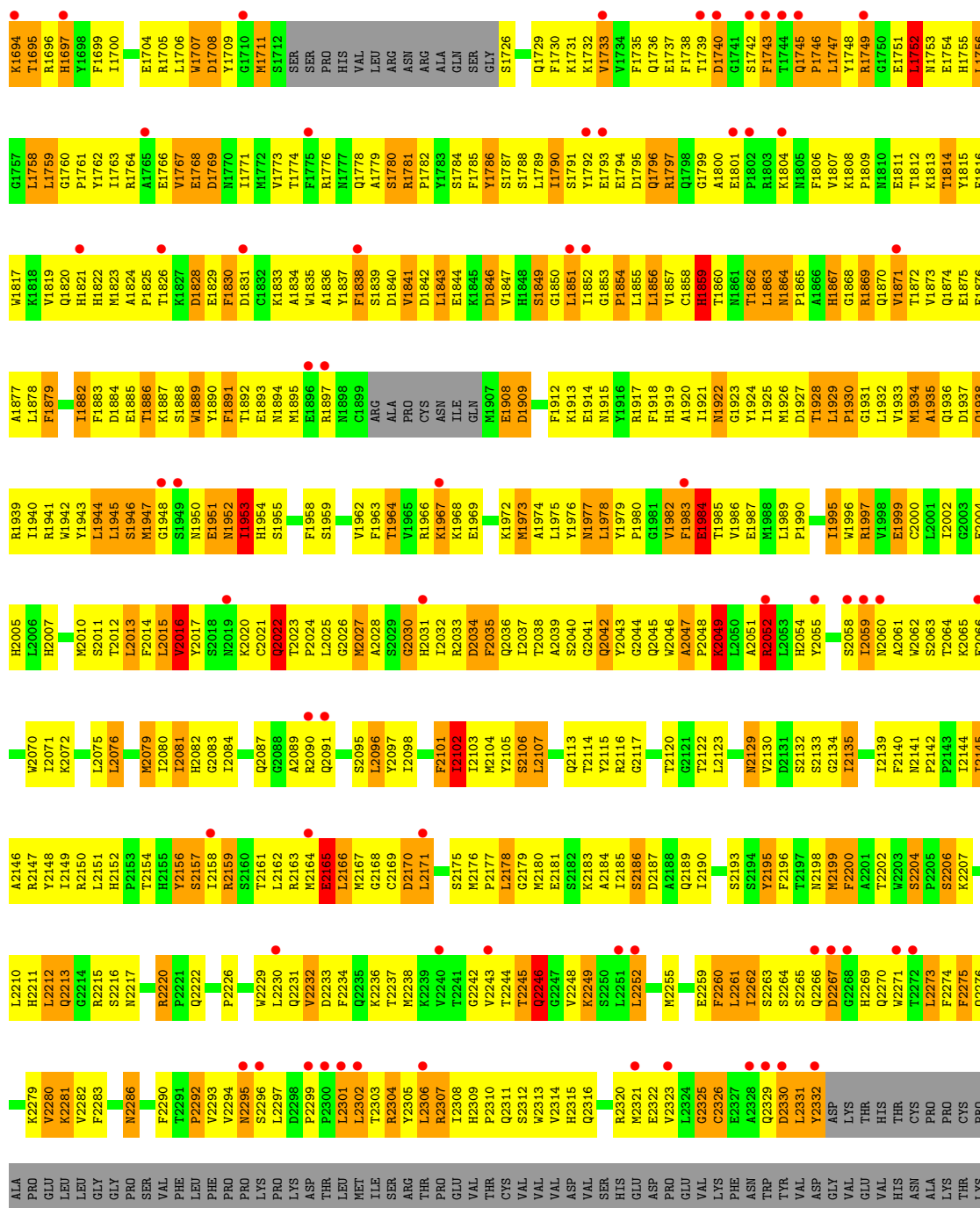
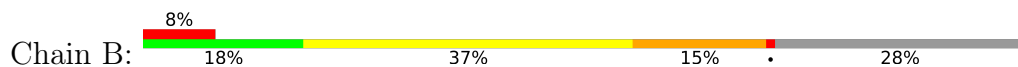
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cu	0	0
			1	1		
7	B	1	Total	Cu	0	0
			1	1		



● Molecule 2: Coagulation factor VIII,Ig gamma-1 chain C region



PRO ARG
LEU PRO
GLU SER
GLN ARG
TYR ASN
SER SER
TYR TYR
ARG ASN
VAL VAL
VAL SER
SER VAL
THR THR
THR CYS
VAL VAL
LEU VAL
HIS HIS
GLN GLN
PHE ASP
TYR TYR
PRO LEU
SER ASN
GLY ASP
GLY ILE
LYS GLU
TYR VAL
CYS TRP
LYS CYS
LYS VAL
SER VAL
ASN ASN
GLN GLN
LYS LYS
LEU PRO
PRO ASN
ALA TYR
PRO TYR
LYS ILE
THR THR
LYS THR
THR THR
PRO THR
PRO ILE
SER VAL
LEU LYS
ASP ASP
SER SER
GLY ASP
GLN GLN
PRO PHE
SER PHE
PHE LEU
PRO TYR
GLN VAL
TYR VAL
LYS TYR
LEU THR

LEU PRO
PRO PRO
SER SER
ARG ARG
ASP ASP
GLU GLU
LEU THR
THR THR
LYS LYS
ASN ASN
GLN VAL
VAL VAL
SER SER
LEU LEU
THR THR
CYS VAL
LEU VAL
HIS HIS
GLN GLN
PHE ASP
TYR TYR
PRO LEU
SER ASN
GLY ASP
GLY ILE
LYS GLU
TYR VAL
CYS TRP
LYS CYS
LYS VAL
SER VAL
ASN ASN
GLN GLN
LYS LYS
LEU PRO
PRO ASN
ALA TYR
PRO TYR
LYS ILE
THR THR
LYS THR
THR THR
PRO THR
PRO ILE
SER VAL
LEU LYS
ASP ASP
SER SER
GLY ASP
GLN GLN
PRO PHE
SER PHE
PHE LEU
PRO TYR
GLN VAL
TYR VAL
LYS TYR
LEU THR

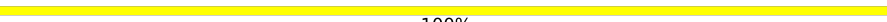
THR VAL
ASP ASP
LYS SER
SER SER
TRP TRP
GLN GLN
GLY GLY
VAL VAL
PHE PHE
SER SER
CYS CYS
SER SER
VAL VAL
MET MET
HIS HIS
GLU GLU
ALA ALA
LEU LEU
HIS HIS
ASN ASN
HIS HIS
TYR TYR
THR THR
GLN GLN
LYS LYS
SER SER
LEU LEU
SER SER
LEU LEU
SER SER
PRO PRO
GLY GLY

- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  75% 25%

MAG1
MAG2
BMA3
MAN4

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

Chain D:  100%

MAG1
MAG2

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

Chain E:  14% 43% 43%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.29Å 136.29Å 365.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.60 – 4.19 37.60 – 4.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.60-4.19) 98.8 (37.60-4.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.298 , 0.362 0.298 , 0.360	Depositor DCC
R_{free} test set	1309 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	126.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 293.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, NAG, CA, CU, BMA

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	0.94	14/5077 (0.3%)	1.23	34/6890 (0.5%)
2	B	0.89	14/5178 (0.3%)	1.19	29/7011 (0.4%)
All	All	0.91	28/10255 (0.3%)	1.21	63/13901 (0.5%)

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	2
2	B	0	2
All	All	0	4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	PHE	CG-CD2	9.64	1.59	1.38
2	B	1897	ARG	NE-CZ	9.64	1.43	1.33
1	A	712	ASP	CG-OD2	9.18	1.42	1.25
1	A	712	ASP	CG-OD1	8.84	1.42	1.25
1	A	434	GLU	CD-OE1	8.79	1.42	1.25

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2325	GLY	N-CA-C	9.91	123.96	110.58
1	A	149	SER	N-CA-C	-9.33	101.91	113.38
1	A	228	TRP	CA-C-N	8.37	130.30	119.84
1	A	228	TRP	C-N-CA	8.37	130.30	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	ASN	N-CA-C	-8.36	102.52	112.89

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	ALA	Peptide
1	A	693	HIS	Peptide
2	B	1790	ILE	Peptide
2	B	1828	ASP	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	4937	0	4820	828	1
2	B	5035	0	4902	803	0
3	C	50	0	43	1	0
4	D	28	0	25	0	0
5	E	83	0	70	4	0
6	A	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	10138	0	9860	1540	1

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 77.

The worst 5 of 1540 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:2046:TRP:CZ3	2:B:2059:ILE:HA	1.37	1.59
1:A:287:GLU:HB3	1:A:673:PHE:CE2	1.51	1.42
2:B:1934:MET:CE	2:B:1940:ILE:HD13	1.46	1.41
2:B:1934:MET:HE3	2:B:1940:ILE:CD1	1.55	1.37
2:B:1738:PHE:CD2	2:B:1747:LEU:HD12	1.57	1.36

All (1) 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:A:250:ARG:NH1	1:A:496:LYS:NZ[7_555]	1.94	0.26

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	599/740 (81%)	448 (75%)	111 (18%)	40 (7%)	1	12
2	B	613/865 (71%)	498 (81%)	87 (14%)	28 (5%)	2	17
All	All	1212/1605 (76%)	946 (78%)	198 (16%)	68 (6%)	1	15

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	TRP
1	A	127	LYS
1	A	229	PRO
1	A	243	PRO
1	A	312	ILE

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	542/660 (82%)	413 (76%)	129 (24%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	550/776 (71%)	414 (75%)	136 (25%)	1	4
All	All	1092/1436 (76%)	827 (76%)	265 (24%)	1	5

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2175	SER
2	B	2212	LEU
2	B	2307	ARG
1	A	588	THR
1	A	573	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1770	ASN
2	B	2222	GLN
2	B	1820	GLN
2	B	2287	GLN
2	B	2005	HIS

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](#)

13 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	C	1	1,3	14,14,15	0.45	0	17,19,21	0.72	0
3	NAG	C	2	3	14,14,15	0.39	0	17,19,21	1.11	1 (5%)
3	BMA	C	3	3	11,11,12	0.33	0	15,15,17	1.53	3 (20%)
3	MAN	C	4	3	11,11,12	0.29	0	15,15,17	0.82	1 (6%)
4	NAG	D	1	2,4	14,14,15	0.67	0	17,19,21	1.44	2 (11%)
4	NAG	D	2	4	14,14,15	0.43	0	17,19,21	1.71	5 (29%)
5	NAG	E	1	2,5	14,14,15	0.53	0	17,19,21	2.39	5 (29%)
5	NAG	E	2	5	14,14,15	0.55	0	17,19,21	1.43	3 (17%)
5	BMA	E	3	5	11,11,12	0.57	0	15,15,17	0.98	1 (6%)
5	BMA	E	4	5	11,11,12	0.28	0	15,15,17	0.69	0
5	MAN	E	5	5	11,11,12	0.26	0	15,15,17	0.51	0
5	MAN	E	6	5	11,11,12	0.61	0	15,15,17	1.29	2 (13%)
5	MAN	E	7	5	11,11,12	0.48	0	15,15,17	0.66	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	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	BMA	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	1	NAG	C2-N2-C7	5.84	130.73	122.90
3	C	3	BMA	C1-C2-C3	4.40	116.05	109.64
5	E	1	NAG	O5-C5-C6	4.34	116.11	107.66
4	D	2	NAG	C4-C3-C2	3.78	116.56	111.02
4	D	2	NAG	C3-C4-C5	3.48	116.54	110.23

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

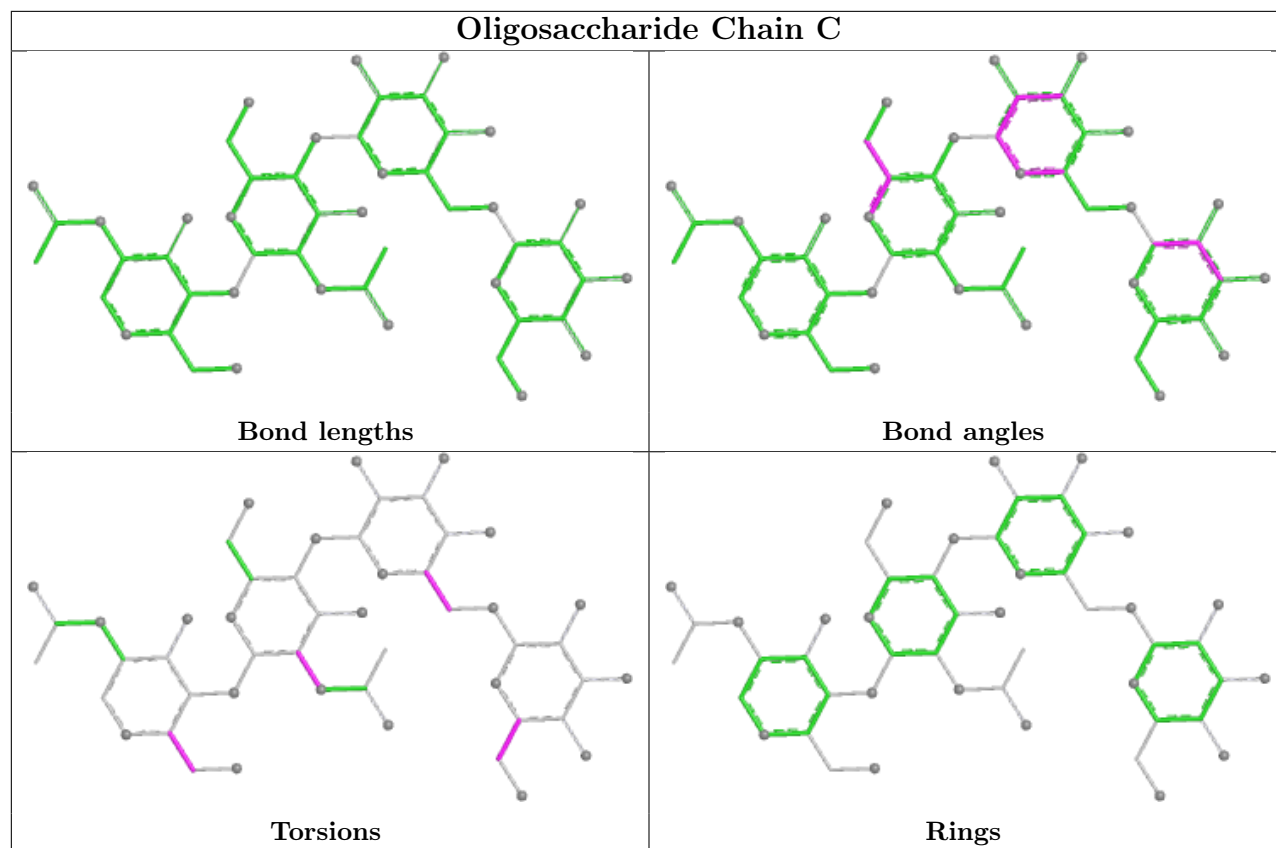
Mol	Chain	Res	Type	Atoms
5	E	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6

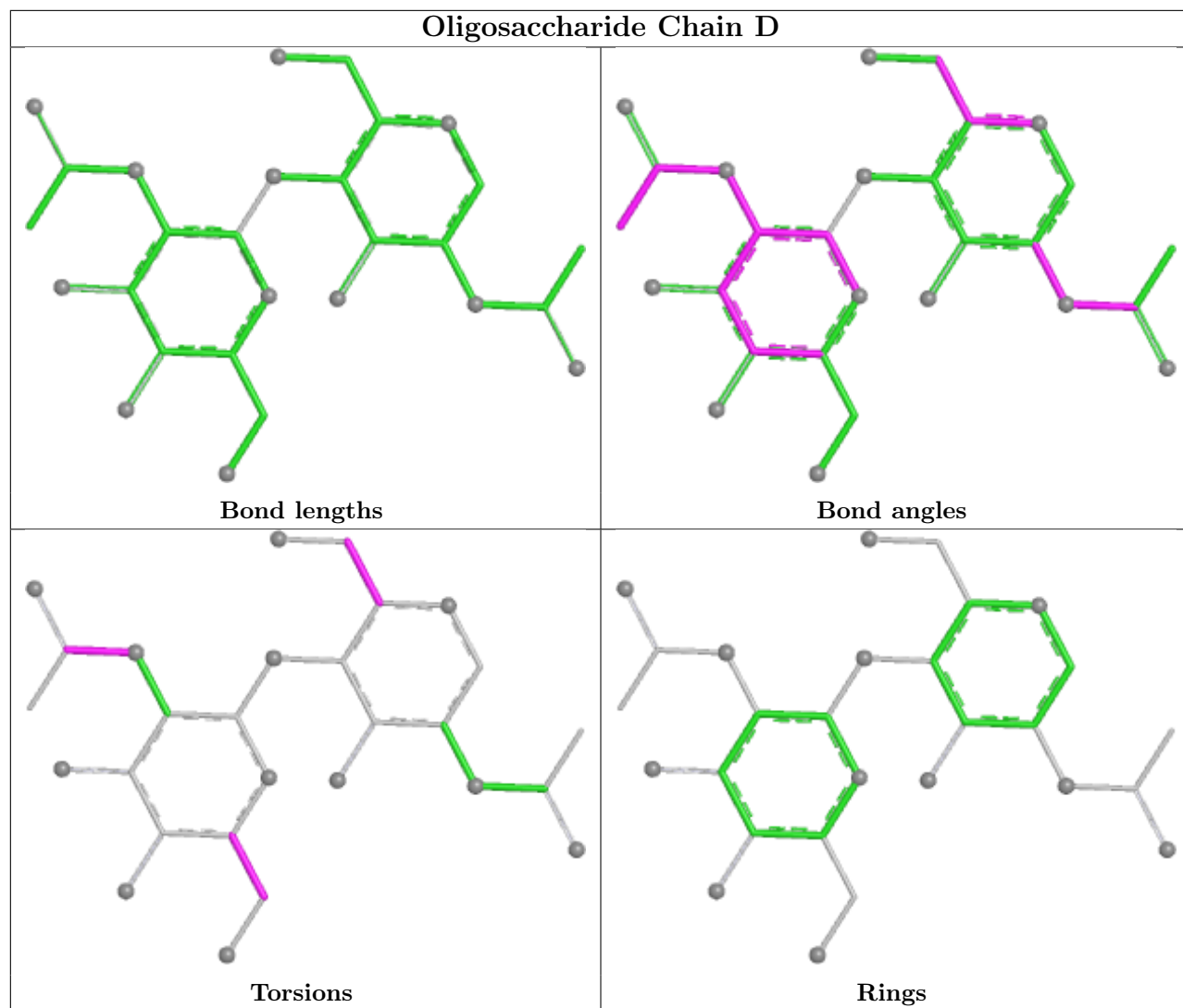
There are no ring outliers.

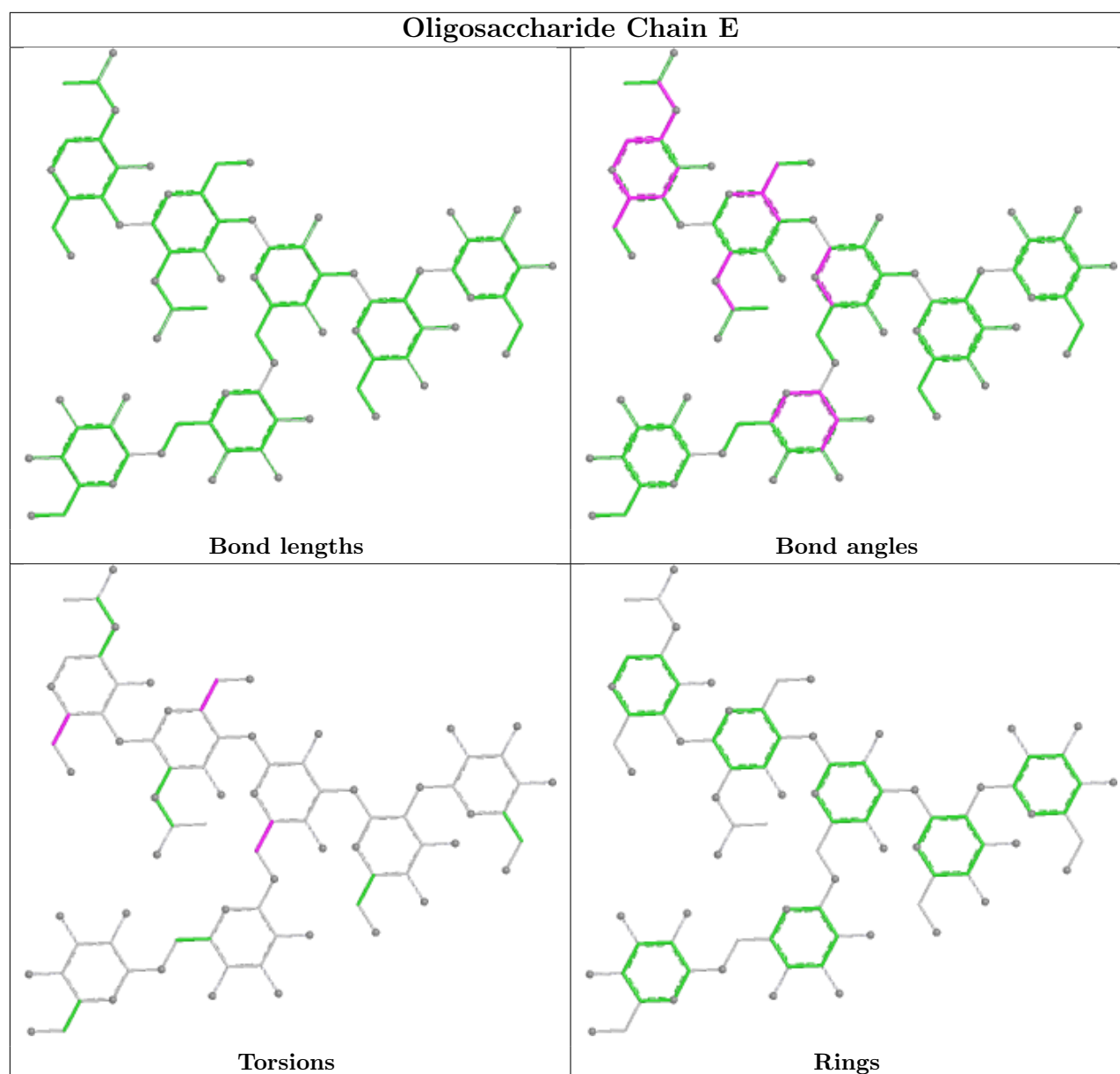
7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	1	0
5	E	2	NAG	1	0
5	E	3	BMA	3	0
5	E	5	MAN	1	0
5	E	7	MAN	1	0
5	E	6	MAN	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	611/740 (82%)	0.75	70 (11%) 9 13	99, 186, 319, 397	0
2	B	619/865 (71%)	0.77	67 (10%) 11 14	106, 195, 319, 424	0
All	All	1230/1605 (76%)	0.76	137 (11%) 10 14	99, 191, 319, 424	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1838	PHE	7.1
2	B	2058	SER	6.1
1	A	190	GLN	5.7
1	A	528	CYS	4.7
1	A	491	LEU	4.4

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.

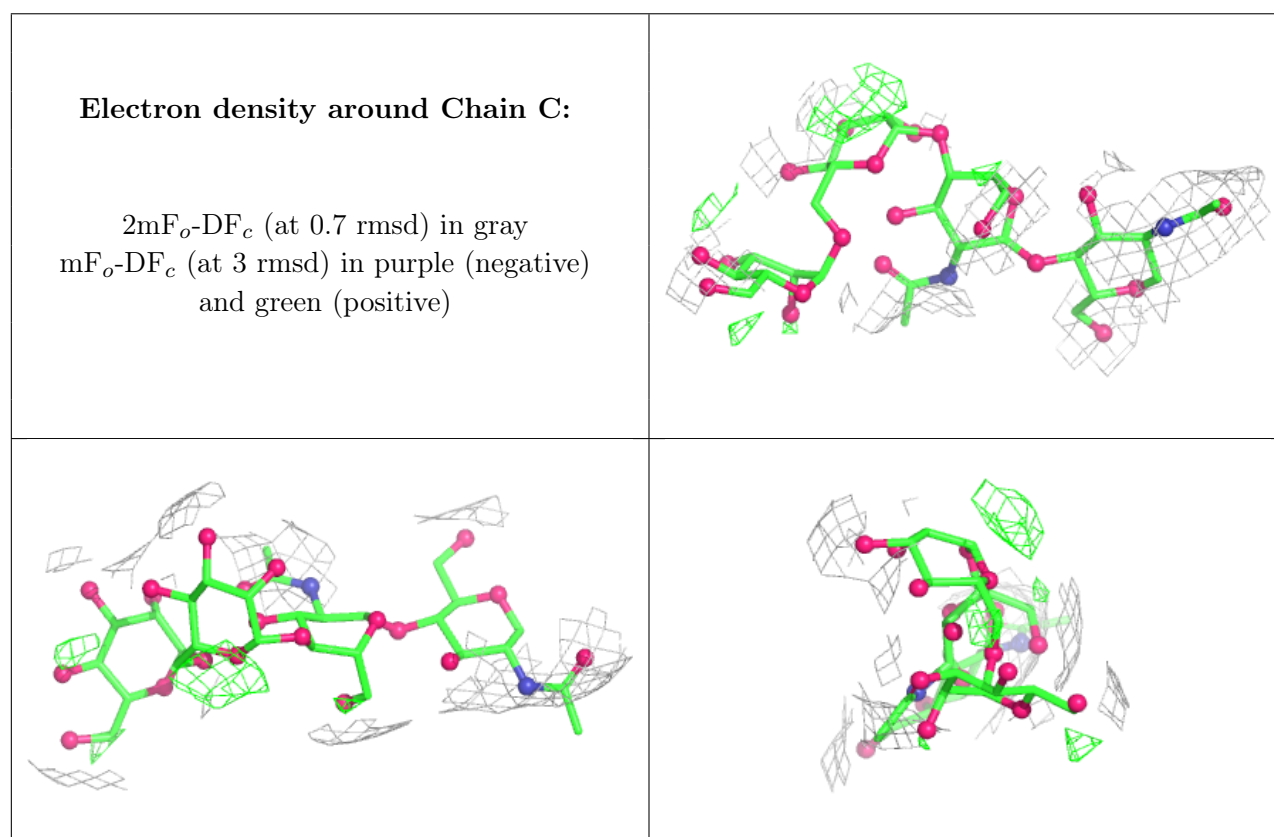
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	E	5	11/12	0.25	0.18	192,215,228,233	11
4	NAG	D	2	14/15	0.27	0.14	307,363,404,410	0
3	BMA	C	3	11/12	0.39	0.12	181,207,223,224	11
3	MAN	C	4	11/12	0.41	0.15	193,218,224,226	11
5	BMA	E	4	11/12	0.61	0.24	222,241,252,258	11

Continued on next page...

Continued from previous page...

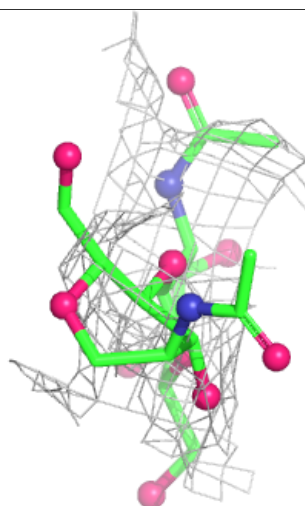
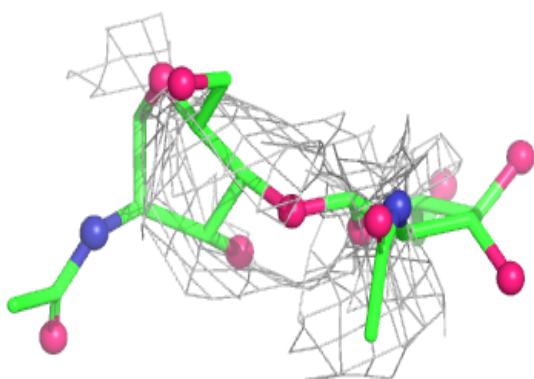
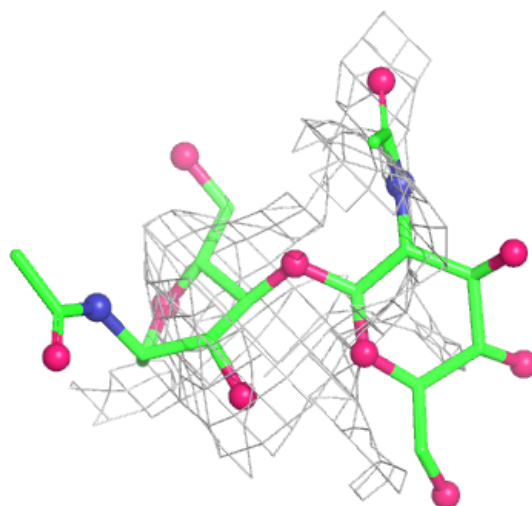
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	E	6	11/12	0.65	0.14	348,364,380,392	0
4	NAG	D	1	14/15	0.66	0.16	275,361,420,429	0
5	BMA	E	3	11/12	0.67	0.13	278,295,314,335	0
5	MAN	E	7	11/12	0.79	0.16	303,330,373,383	0
3	NAG	C	1	14/15	0.87	0.22	199,244,264,269	0
3	NAG	C	2	14/15	0.88	0.11	169,231,241,258	14
5	NAG	E	2	14/15	0.91	0.18	228,247,271,273	0
5	NAG	E	1	14/15	0.95	0.16	151,202,230,232	0

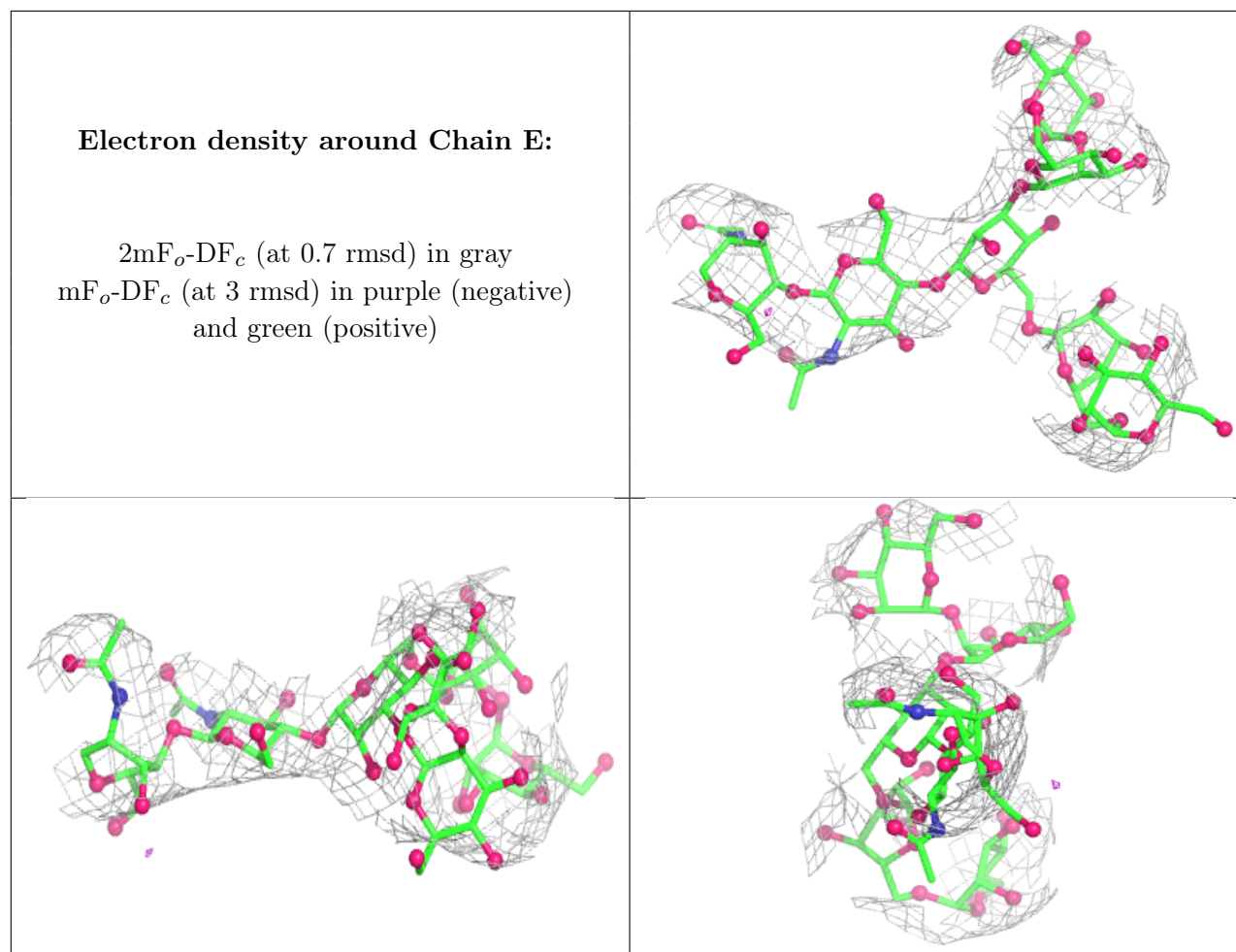
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





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($\text{\AA}^2$)	Q<0.9
6	CA	A	806	1/1	0.91	0.10	236,236,236,236	0
6	CA	A	807	1/1	0.97	0.12	165,165,165,165	0
6	CA	A	805	1/1	0.99	0.09	215,215,215,215	0
7	CU	A	808	1/1	0.99	0.06	167,167,167,167	0
7	CU	B	2610	1/1	0.99	0.09	150,150,150,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.