



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 10:46 AM BST

PDB ID : 4W4O
Title : High-resolution crystal structure of Fc bound to its human receptor Fc-gamma-RI
Authors : Caaveiro, J.M.M.; Kiyoshi, M.; Tsumoto, K.
Deposited on : 2014-08-15
Resolution : 1.80 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

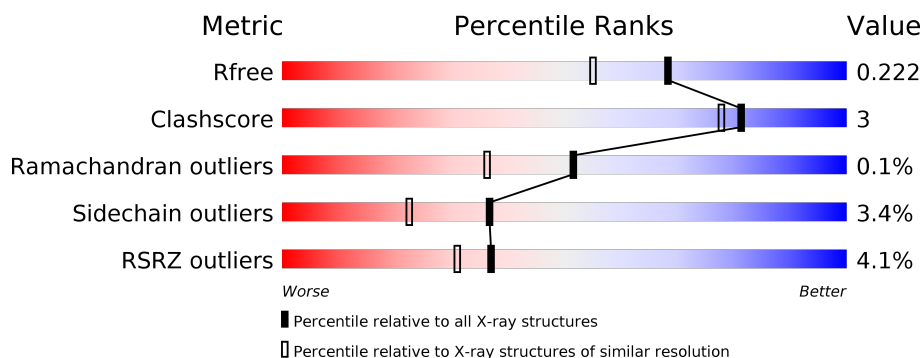
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



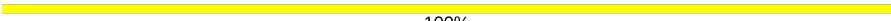
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	224	<div> <div style="width: 89%;"></div> <div style="width: 6%;"></div> <div style="width: 5%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
1	B	224	<div> <div style="width: 86%;"></div> <div style="width: 6%;"></div> <div style="width: 7%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
2	C	280	<div> <div style="width: 9%;"></div> <div style="width: 77%;"></div> <div style="width: 13%;"></div> <div style="width: 8%;"></div> <div style="width: 0%;"></div> </div>
3	D	9	<div> <div style="width: 100%;"></div> </div>
3	E	9	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> </div>
4	F	2	<div> <div style="width: 100%;"></div> </div>

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Mol	Chain	Length	Quality of chain
5	G	6	 100%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6420 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	3	0
			1728	1103	291	328	6			
1	B	209	Total	C	N	O	S	0	3	0
			1682	1073	282	321	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ALA	SER	conflict	UNP P01857
B	444	ALA	SER	conflict	UNP P01857

- Molecule 2 is a protein called High affinity immunoglobulin gamma Fc receptor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	259	Total	C	N	O	S	0	4	0
			2064	1310	356	387	11			

There are 25 discrepancies between the modelled and reference sequences:

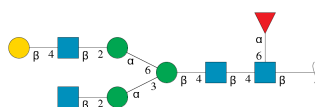
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	PRO	THR	engineered mutation	UNP P12314
C	25	LYS	THR	engineered mutation	UNP P12314
C	38	SER	THR	engineered mutation	UNP P12314
C	46	PRO	LEU	engineered mutation	UNP P12314
C	63	ILE	THR	engineered mutation	UNP P12314
C	69	THR	SER	engineered mutation	UNP P12314
C	71	HIS	ARG	engineered mutation	UNP P12314
C	77	GLU	VAL	engineered mutation	UNP P12314
C	78	ASP	ASN	engineered mutation	UNP P12314
C	100	VAL	ILE	engineered mutation	UNP P12314
C	114	LEU	PHE	engineered mutation	UNP P12314
C	160	MET	ILE	engineered mutation	UNP P12314

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Chain	Residue	Modelled	Actual	Comment	Reference
C	163	SER	ASN	engineered mutation	UNP P12314
C	195	THR	ASN	engineered mutation	UNP P12314
C	206	THR	ASN	engineered mutation	UNP P12314
C	207	PRO	LEU	engineered mutation	UNP P12314
C	240	ASP	ASN	engineered mutation	UNP P12314
C	283	HIS	LEU	engineered mutation	UNP P12314
C	285	GLN	LEU	engineered mutation	UNP P12314
C	290	HIS	-	expression tag	UNP P12314
C	291	HIS	-	expression tag	UNP P12314
C	292	HIS	-	expression tag	UNP P12314
C	293	HIS	-	expression tag	UNP P12314
C	294	HIS	-	expression tag	UNP P12314
C	295	HIS	-	expression tag	UNP P12314

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
3	D	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	E	9	Total	C	N	O	0	0	0
			110	62	4	44			

- 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	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

ose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

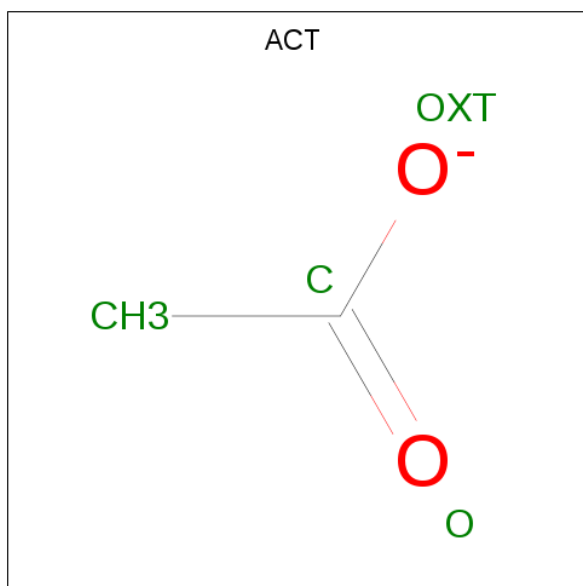


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	G	6	Total	C	N	O	0	0
			72	40	2	30		0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Zn	0	0
			2	2		
6	A	3	Total	Zn	0	0
			3	3		
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

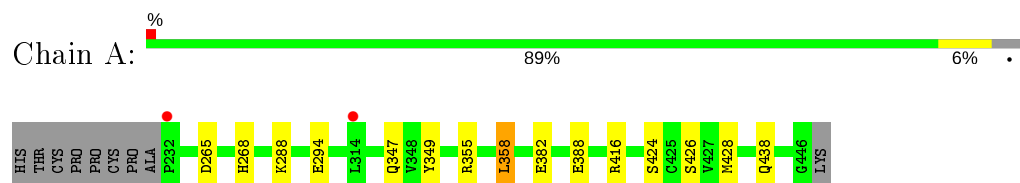
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	219	Total 222	O 222	0	3
9	B	178	Total 180	O 180	0	2
9	C	169	Total 170	O 170	0	1

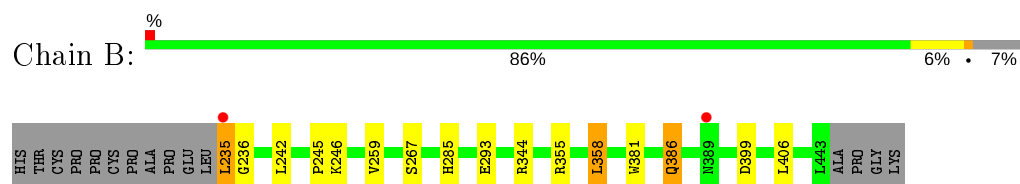
3 Residue-property plots [i](#)

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.

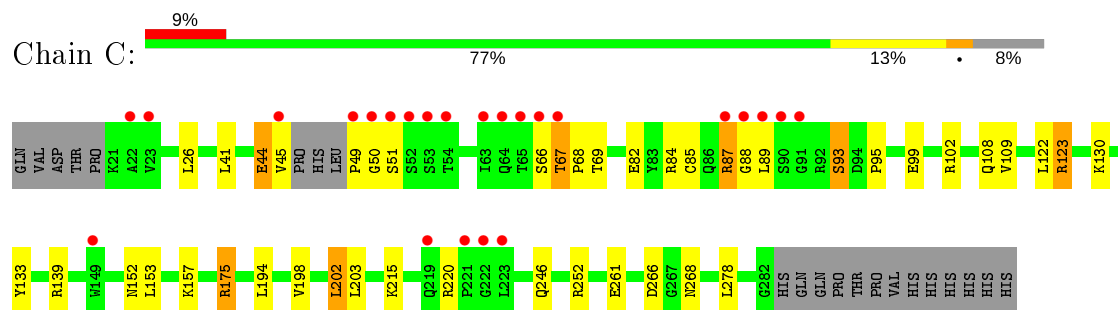
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: High affinity immunoglobulin gamma Fc receptor I

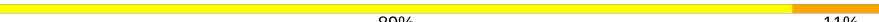


- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

anose-(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 E:  89% 11%

NAG1
NAG2
BMA3
MAN4
NAG5
GAL6
MAN7
NAG8
FUC9

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

Chain F:  100%

NAG1
NAG2

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

Chain G:  100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.98 Å 126.50 Å 71.61 Å 90.00° 118.95° 90.00°	Depositor
Resolution (Å)	39.70 – 1.80 37.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.70-1.80) 98.5 (37.59-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.173 , 0.215 0.184 , 0.222	Depositor DCC
R_{free} test set	4800 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6420	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: GOL, ZN, BMA, NAG, GAL, FUC, ACT, MAN

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	1.07	1/1785 (0.1%)	1.02	6/2432 (0.2%)
1	B	0.99	3/1737 (0.2%)	0.89	0/2367
2	C	0.97	1/2125 (0.0%)	1.05	10/2881 (0.3%)
All	All	1.01	5/5647 (0.1%)	1.00	16/7680 (0.2%)

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	B	0	1
2	C	0	6
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	SER	CB-OG	-8.10	1.31	1.42
2	C	99	GLU	CD-OE1	6.65	1.32	1.25
1	B	293	GLU	CD-OE1	5.85	1.32	1.25
1	B	381	TRP	CZ3-CH2	5.11	1.48	1.40
1	B	267	SER	CB-OG	-5.09	1.35	1.42

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	175	ARG	NE-CZ-NH2	10.18	125.39	120.30
2	C	266	ASP	CB-CG-OD1	8.02	125.52	118.30
2	C	175	ARG	NE-CZ-NH1	-7.28	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	139	ARG	NE-CZ-NH1	7.25	123.93	120.30
2	C	261	GLU	OE1-CD-OE2	6.99	131.69	123.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	235	LEU	Peptide
2	C	44	GLU	Peptide
2	C	49	PRO	Peptide
2	C	50	GLY	Peptide
2	C	66	SER	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	1728	0	1709	4	0
1	B	1682	0	1659	9	0
2	C	2064	0	2046	18	0
3	D	110	0	93	0	0
3	E	110	0	94	1	0
4	F	28	0	25	0	0
5	G	72	0	61	0	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	24	0	18	1	0
7	B	4	0	3	0	0
7	C	8	0	6	0	0
8	A	6	0	8	0	0
8	B	6	0	8	1	0
9	A	222	0	0	0	0
9	B	180	0	0	1	1
9	C	170	0	0	2	1
All	All	6420	0	5730	30	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 3.

The worst 5 of 30 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:C:67:THR:HG22	2:C:68:PRO:HD2	1.60	0.81
1:B:246:LYS:HG3	3:E:6:GAL:O4	1.97	0.65
1:A:355:ARG:HA	1:A:358:LEU:HD22	1.83	0.60
2:C:109:VAL:HG12	2:C:122:LEU:HD23	1.84	0.59
1:B:285:HIS:ND1	9:B:602:HOH:O	2.33	0.56

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)
9:B:725:HOH:O	9:C:549:HOH:O[4_546]	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	216/224 (96%)	214 (99%)	2 (1%)	0	100	100
1	B	210/224 (94%)	206 (98%)	4 (2%)	0	100	100
2	C	259/280 (92%)	250 (96%)	8 (3%)	1 (0%)	34	21
All	All	685/728 (94%)	670 (98%)	14 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	88	GLY

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	201/206 (98%)	198 (98%)	3 (2%)	65	56
1	B	197/206 (96%)	192 (98%)	5 (2%)	47	34
2	C	232/249 (93%)	219 (94%)	13 (6%)	21	8
All	All	630/661 (95%)	609 (97%)	21 (3%)	37	23

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	45	VAL
2	C	69	THR
2	C	203	LEU
2	C	44	GLU
2	C	246	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	42	HIS
2	C	101	HIS
2	C	71	HIS
1	B	315	ASN
2	C	55	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

23 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
3	FUC	D	9	3	10,10,11	1.15	1 (10%)	14,14,16	2.16	5 (35%)
3	NAG	E	5	3	14,14,15	0.91	0	17,19,21	1.38	4 (23%)
3	NAG	D	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	2.56	7 (41%)
4	NAG	F	1	2,4	14,14,15	0.79	0	17,19,21	1.42	3 (17%)
3	MAN	E	7	3	11,11,12	1.12	0	15,15,17	1.66	5 (33%)
3	NAG	E	2	3	14,14,15	0.96	0	17,19,21	1.63	5 (29%)
3	NAG	D	8	3	14,14,15	0.77	0	17,19,21	1.47	4 (23%)
3	MAN	E	4	3	11,11,12	1.10	0	15,15,17	2.03	5 (33%)
3	NAG	E	1	1,3	14,14,15	1.38	4 (28%)	17,19,21	1.24	1 (5%)
3	GAL	E	6	3	11,11,12	1.29	1 (9%)	15,15,17	2.45	5 (33%)
3	MAN	D	4	3	11,11,12	0.89	1 (9%)	15,15,17	1.70	3 (20%)
5	MAN	G	4	5	11,11,12	1.17	1 (9%)	15,15,17	1.54	4 (26%)
3	NAG	E	8	3	14,14,15	0.68	0	17,19,21	1.69	5 (29%)
5	MAN	G	5	5	11,11,12	1.45	2 (18%)	15,15,17	3.48	8 (53%)
3	NAG	D	2	3	14,14,15	1.39	2 (14%)	17,19,21	1.46	4 (23%)
5	MAN	G	6	5	11,11,12	1.01	0	15,15,17	3.40	6 (40%)
3	GAL	D	6	3	11,11,12	2.31	5 (45%)	15,15,17	2.92	7 (46%)
5	NAG	G	2	5	14,14,15	0.61	0	17,19,21	1.31	3 (17%)
3	MAN	D	7	3	11,11,12	0.90	0	15,15,17	2.11	5 (33%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	2.60	7 (41%)
3	NAG	D	5	3	14,14,15	0.92	1 (7%)	17,19,21	1.20	2 (11%)
5	NAG	G	1	2,5	14,14,15	0.89	1 (7%)	17,19,21	1.37	1 (5%)
3	FUC	E	9	3	10,10,11	1.02	1 (10%)	14,14,16	2.35	3 (21%)

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	FUC	D	9	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	5	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	GAL	E	6	3	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
3	NAG	E	8	3	-	4/6/23/26	0/1/1/1
3	NAG	D	8	3	-	2/6/23/26	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
3	NAG	D	5	3	-	0/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	1/6/23/26	0/1/1/1
3	FUC	E	9	3	-	-	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	GAL	O2-C2	4.61	1.53	1.43
3	D	2	NAG	O5-C1	-4.29	1.36	1.43
3	D	6	GAL	O3-C3	-4.08	1.33	1.43
5	G	5	MAN	O5-C1	-3.34	1.38	1.43
5	G	1	NAG	C1-C2	2.75	1.56	1.52

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	6	MAN	C1-C2-C3	-8.17	99.62	109.67
4	F	2	NAG	C1-O5-C5	7.43	122.26	112.19
3	E	6	GAL	C1-O5-C5	7.42	122.25	112.19
5	G	5	MAN	O5-C1-C2	6.72	121.15	110.77
5	G	5	MAN	C1-O5-C5	-6.53	103.34	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	8	NAG	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	D	8	NAG	C4-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
3	E	7	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	6	GAL	1	0

5.5 Carbohydrates [i](#)

26 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	D	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	2.56	7 (41%)
3	NAG	D	2	3	14,14,15	1.39	2 (14%)	17,19,21	1.46	4 (23%)
3	BMA	D	3	3	11,11,12	0.86	0	15,15,17	2.21	8 (53%)
3	MAN	D	4	3	11,11,12	0.89	1 (9%)	15,15,17	1.70	3 (20%)
3	NAG	D	5	3	14,14,15	0.92	1 (7%)	17,19,21	1.20	2 (11%)
3	GAL	D	6	3	11,11,12	2.31	5 (45%)	15,15,17	2.92	7 (46%)
3	MAN	D	7	3	11,11,12	0.90	0	15,15,17	2.11	5 (33%)
3	NAG	D	8	3	14,14,15	0.77	0	17,19,21	1.47	4 (23%)
3	FUC	D	9	3	10,10,11	1.15	1 (10%)	14,14,16	2.16	5 (35%)
3	NAG	E	1	1,3	14,14,15	1.38	4 (28%)	17,19,21	1.24	1 (5%)
3	NAG	E	2	3	14,14,15	0.96	0	17,19,21	1.63	5 (29%)
3	BMA	E	3	3	11,11,12	0.79	0	15,15,17	1.50	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	4	3	11,11,12	1.10	0	15,15,17	2.03	5 (33%)
3	NAG	E	5	3	14,14,15	0.91	0	17,19,21	1.38	4 (23%)
3	GAL	E	6	3	11,11,12	1.29	1 (9%)	15,15,17	2.45	5 (33%)
3	MAN	E	7	3	11,11,12	1.12	0	15,15,17	1.66	5 (33%)
3	NAG	E	8	3	14,14,15	0.68	0	17,19,21	1.69	5 (29%)
3	FUC	E	9	3	10,10,11	1.02	1 (10%)	14,14,16	2.35	3 (21%)
4	NAG	F	1	2,4	14,14,15	0.79	0	17,19,21	1.42	3 (17%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	2.60	7 (41%)
5	NAG	G	1	2,5	14,14,15	0.89	1 (7%)	17,19,21	1.37	1 (5%)
5	NAG	G	2	5	14,14,15	0.61	0	17,19,21	1.31	3 (17%)
5	BMA	G	3	5	11,11,12	1.13	1 (9%)	15,15,17	1.99	4 (26%)
5	MAN	G	4	5	11,11,12	1.17	1 (9%)	15,15,17	1.54	4 (26%)
5	MAN	G	5	5	11,11,12	1.45	2 (18%)	15,15,17	3.48	8 (53%)
5	MAN	G	6	5	11,11,12	1.01	0	15,15,17	3.40	6 (40%)

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	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	0/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	2/6/23/26	0/1/1/1
3	FUC	D	9	3	-	-	0/1/1/1
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	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	0/6/23/26	0/1/1/1
3	GAL	E	6	3	-	1/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	NAG	E	8	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	E	9	3	-	-	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	GAL	O2-C2	4.61	1.53	1.43
3	D	2	NAG	O5-C1	-4.29	1.36	1.43
3	D	6	GAL	O3-C3	-4.08	1.33	1.43
5	G	5	MAN	O5-C1	-3.34	1.38	1.43
5	G	1	NAG	C1-C2	2.75	1.56	1.52

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	6	MAN	C1-C2-C3	-8.17	99.62	109.67
4	F	2	NAG	C1-O5-C5	7.43	122.26	112.19
3	E	6	GAL	C1-O5-C5	7.42	122.25	112.19
5	G	5	MAN	O5-C1-C2	6.72	121.15	110.77
5	G	5	MAN	C1-O5-C5	-6.53	103.34	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

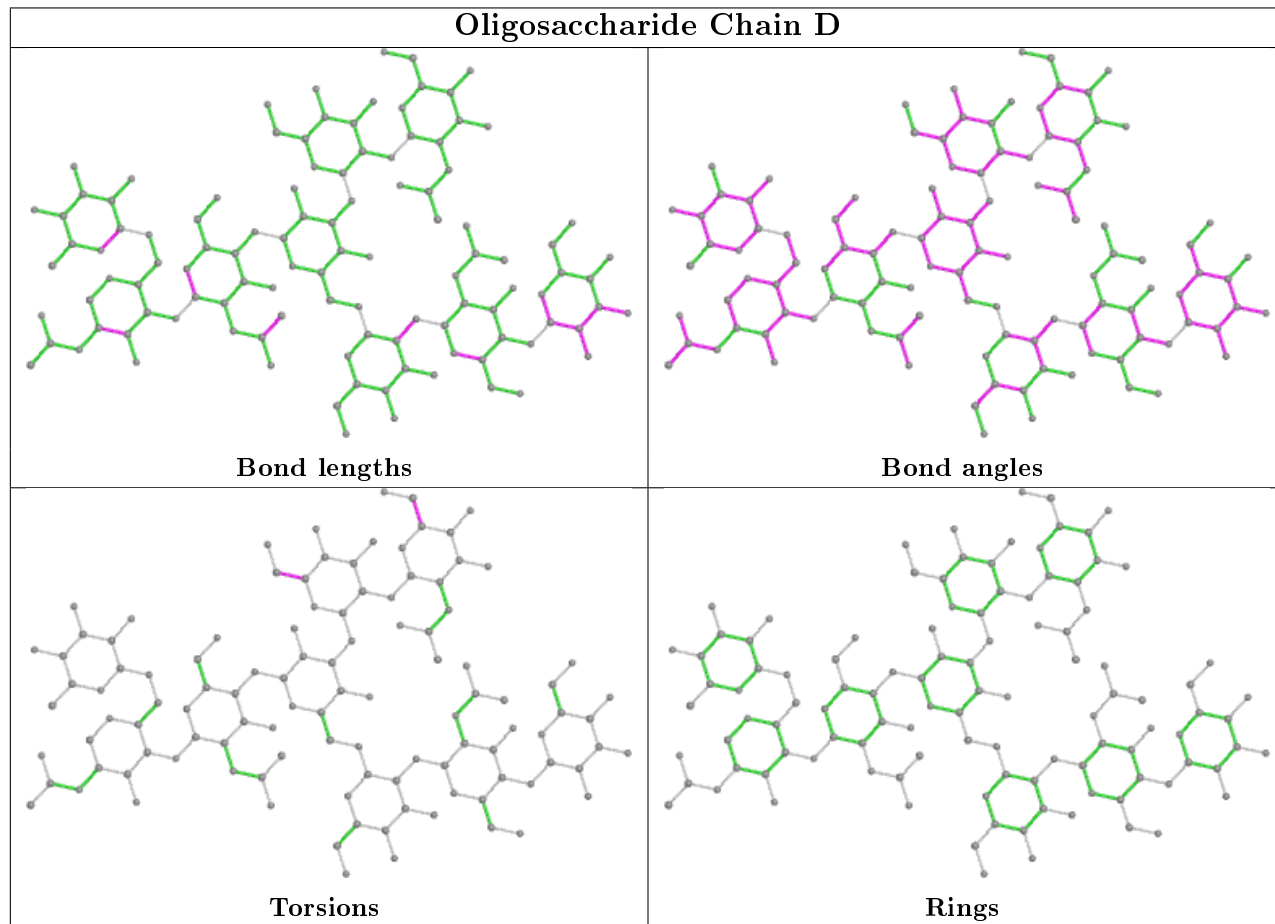
Mol	Chain	Res	Type	Atoms
3	D	8	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
3	D	8	NAG	C4-C5-C6-O6

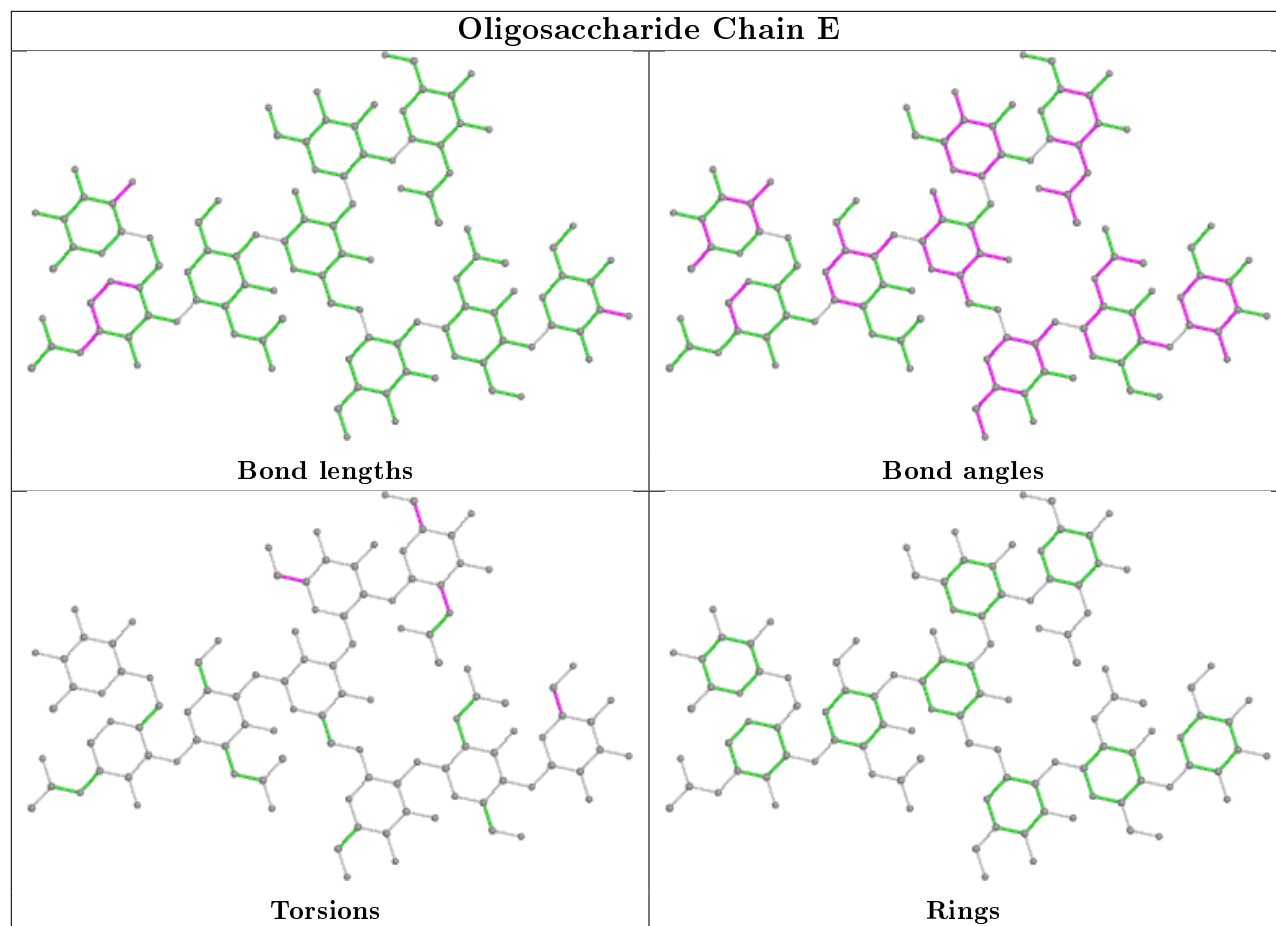
There are no ring outliers.

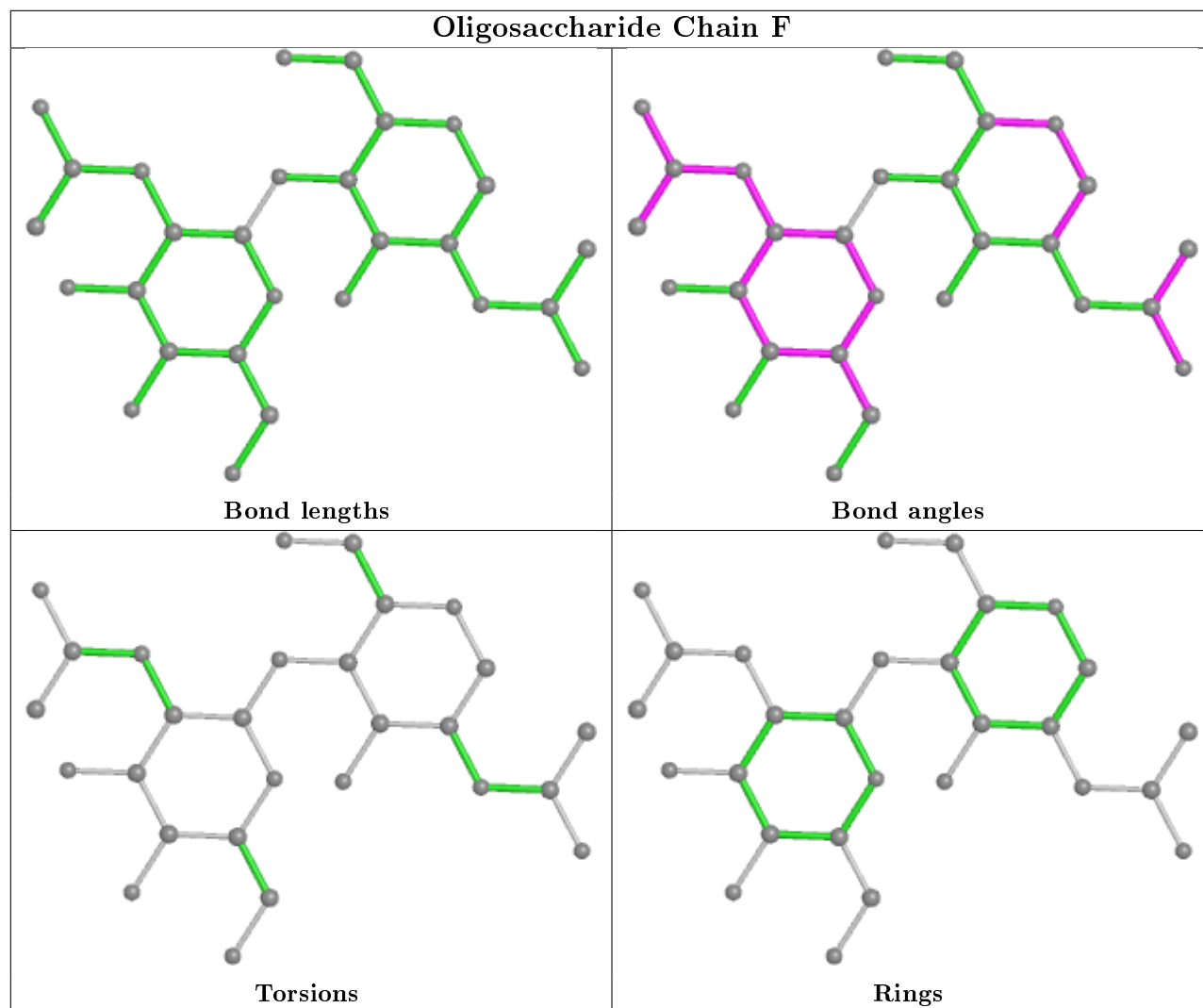
1 monomer is involved in 1 short contact:

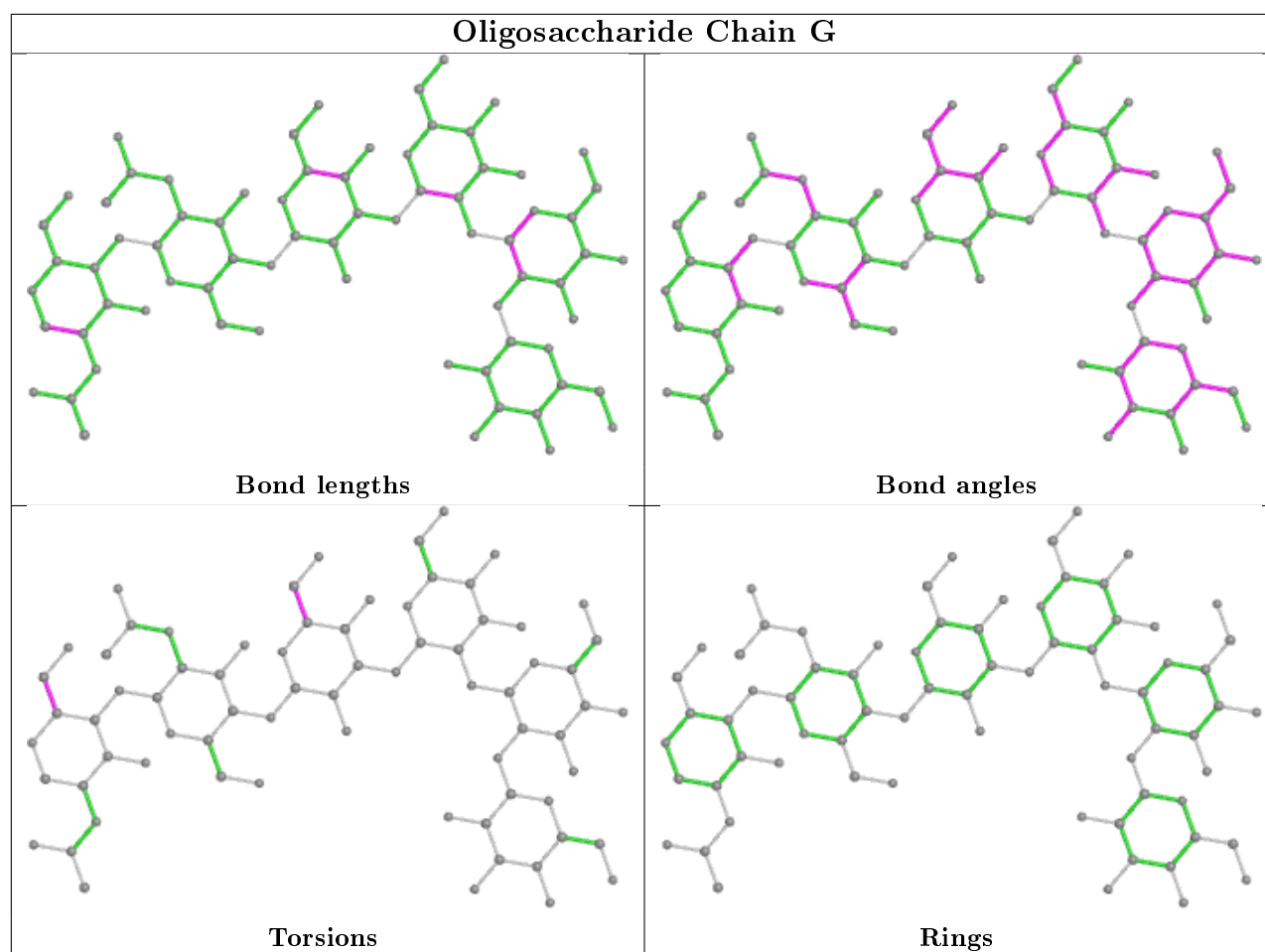
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	6	GAL	1	0

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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ACT	C	310	-	1,3,3	2.90	1 (100%)	0,3,3	0.00	-
7	ACT	A	514	-	1,3,3	4.02	1 (100%)	0,3,3	0.00	-
7	ACT	A	513	6	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
7	ACT	C	311	-	1,3,3	1.54	0	0,3,3	0.00	-
7	ACT	A	518	-	1,3,3	1.95	0	0,3,3	0.00	-
8	GOL	B	513	-	5,5,5	0.37	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACT	A	515	6	1,3,3	3.90	1 (100%)	0,3,3	0.00	-
7	ACT	B	512	6	1,3,3	1.71	0	0,3,3	0.00	-
7	ACT	A	516	-	1,3,3	0.71	0	0,3,3	0.00	-
8	GOL	A	519	-	5,5,5	0.33	0	5,5,5	0.57	0
7	ACT	A	517	-	1,3,3	2.64	1 (100%)	0,3,3	0.00	-

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
8	GOL	B	513	-	-	2/4/4/4	-
8	GOL	A	519	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	514	ACT	CH3-C	4.02	1.53	1.48
7	A	515	ACT	CH3-C	3.90	1.53	1.48
7	C	310	ACT	CH3-C	2.90	1.52	1.48
7	A	513	ACT	CH3-C	2.78	1.52	1.48
7	A	517	ACT	CH3-C	2.64	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	513	GOL	C1-C2-C3-O3
8	B	513	GOL	O2-C2-C3-O3
8	A	519	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	514	ACT	1	0
8	B	513	GOL	1	0

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	215/224 (95%)	-0.23	2 (0%) 84 82	26, 34, 51, 75	0
1	B	209/224 (93%)	-0.35	2 (0%) 82 80	27, 38, 55, 87	0
2	C	259/280 (92%)	0.18	24 (9%) 8 6	28, 40, 90, 119	0
All	All	683/728 (93%)	-0.11	28 (4%) 37 31	26, 37, 71, 119	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	50	GLY	7.1
2	C	64	GLN	7.0
2	C	51	SER	6.8
2	C	89	LEU	6.0
2	C	65	THR	5.2

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
3	NAG	E	8	14/15	0.72	0.30	92,102,114,115	0
4	NAG	F	2	14/15	0.79	0.35	83,92,100,101	0
5	NAG	G	2	14/15	0.81	0.27	59,66,71,72	0
3	NAG	D	8	14/15	0.83	0.24	78,88,102,107	0
3	GAL	D	6	11/12	0.83	0.24	37,49,58,64	0
5	MAN	G	5	11/12	0.86	0.17	46,52,56,57	0
5	NAG	G	1	14/15	0.87	0.19	53,64,72,78	0
5	MAN	G	6	11/12	0.89	0.13	49,53,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FUC	E	9	10/11	0.89	0.14	54,62,69,77	0
3	MAN	E	7	11/12	0.90	0.12	52,61,82,84	0
3	GAL	E	6	11/12	0.91	0.22	41,51,56,58	0
3	NAG	E	5	14/15	0.92	0.08	42,48,51,53	0
5	MAN	G	4	11/12	0.92	0.18	52,55,60,65	0
3	MAN	D	7	11/12	0.94	0.11	36,53,65,67	0
4	NAG	F	1	14/15	0.95	0.09	44,55,68,71	0
3	FUC	D	9	10/11	0.95	0.09	48,51,56,59	0
3	NAG	D	5	14/15	0.96	0.06	37,44,48,50	0
3	MAN	E	4	11/12	0.96	0.07	39,44,51,52	0
3	NAG	D	1	14/15	0.96	0.07	31,35,40,42	0
3	NAG	D	2	14/15	0.97	0.07	30,34,39,40	0
3	MAN	D	4	11/12	0.97	0.05	38,39,45,47	0
3	NAG	E	2	14/15	0.97	0.07	33,37,41,41	0
3	NAG	E	1	14/15	0.98	0.06	32,34,41,46	0

6.3 Carbohydrates

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

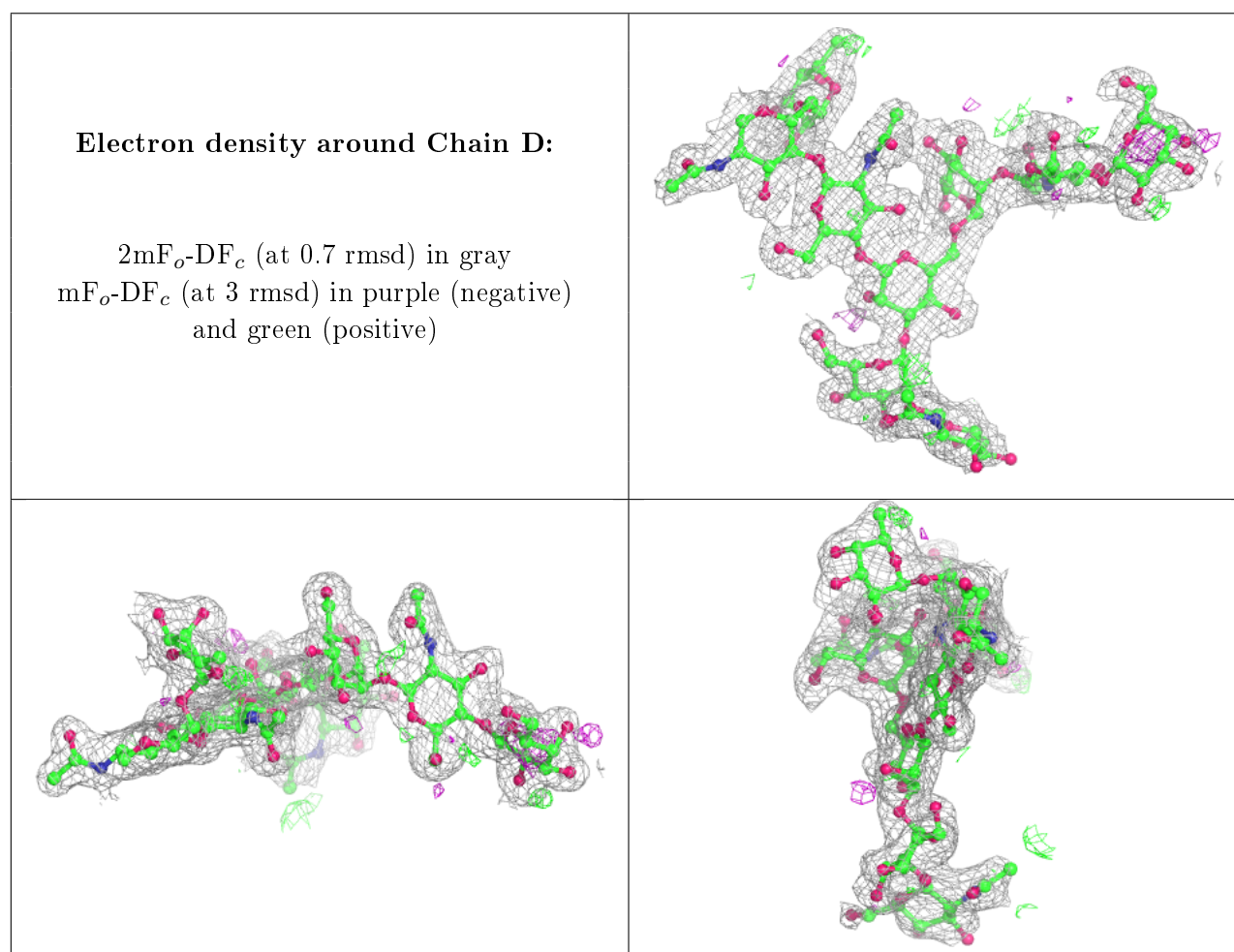
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	8	14/15	0.72	0.30	92,102,114,115	0
5	BMA	G	3	11/12	0.78	0.26	48,58,67,67	0
4	NAG	F	2	14/15	0.79	0.35	83,92,100,101	0
5	NAG	G	2	14/15	0.81	0.27	59,66,71,72	0
3	NAG	D	8	14/15	0.83	0.24	78,88,102,107	0
3	GAL	D	6	11/12	0.83	0.24	37,49,58,64	0
5	MAN	G	5	11/12	0.86	0.17	46,52,56,57	0
5	NAG	G	1	14/15	0.87	0.19	53,64,72,78	0
5	MAN	G	6	11/12	0.89	0.13	49,53,58,59	0
3	FUC	E	9	10/11	0.89	0.14	54,62,69,77	0
3	MAN	E	7	11/12	0.90	0.12	52,61,82,84	0
3	GAL	E	6	11/12	0.91	0.22	41,51,56,58	0
3	NAG	E	5	14/15	0.92	0.08	42,48,51,53	0
5	MAN	G	4	11/12	0.92	0.18	52,55,60,65	0
3	MAN	D	7	11/12	0.94	0.11	36,53,65,67	0
3	BMA	E	3	11/12	0.95	0.06	32,41,46,51	0
4	NAG	F	1	14/15	0.95	0.09	44,55,68,71	0
3	FUC	D	9	10/11	0.95	0.09	48,51,56,59	0

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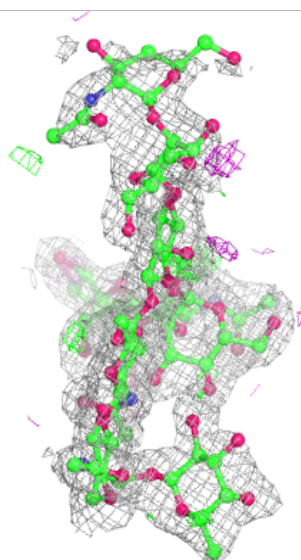
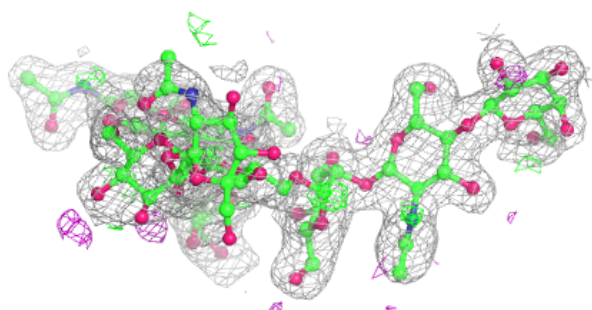
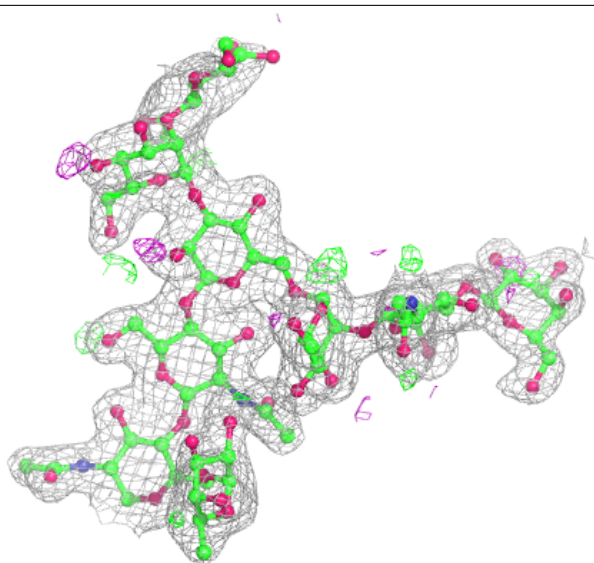
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	5	14/15	0.96	0.06	37,44,48,50	0
3	NAG	D	1	14/15	0.96	0.07	31,35,40,42	0
3	MAN	E	4	11/12	0.96	0.07	39,44,51,52	0
3	NAG	D	2	14/15	0.97	0.07	30,34,39,40	0
3	BMA	D	3	11/12	0.97	0.07	30,33,36,37	0
3	NAG	E	2	14/15	0.97	0.07	33,37,41,41	0
3	MAN	D	4	11/12	0.97	0.05	38,39,45,47	0
3	NAG	E	1	14/15	0.98	0.06	32,34,41,46	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.



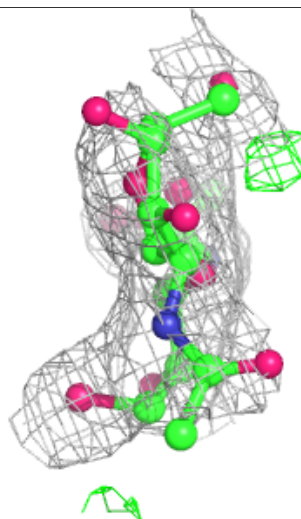
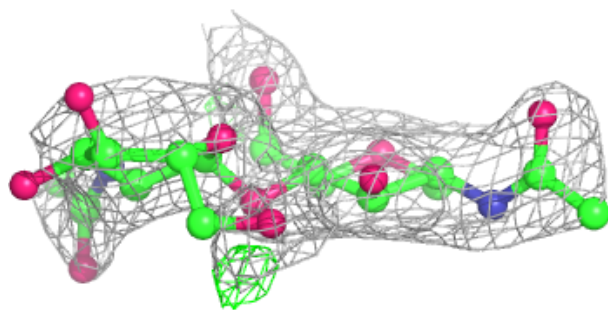
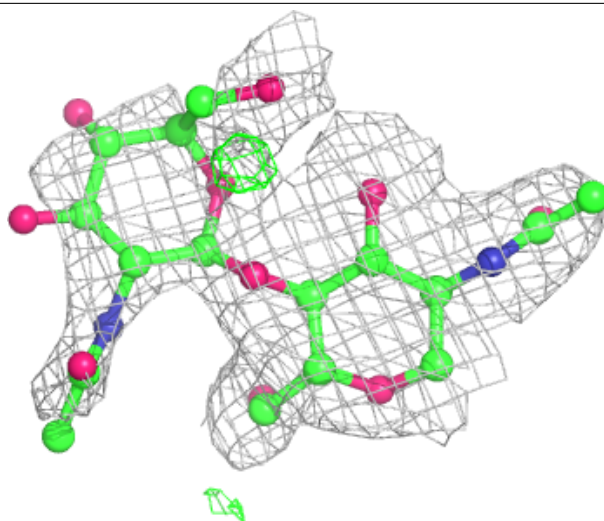
Electron density around Chain E:

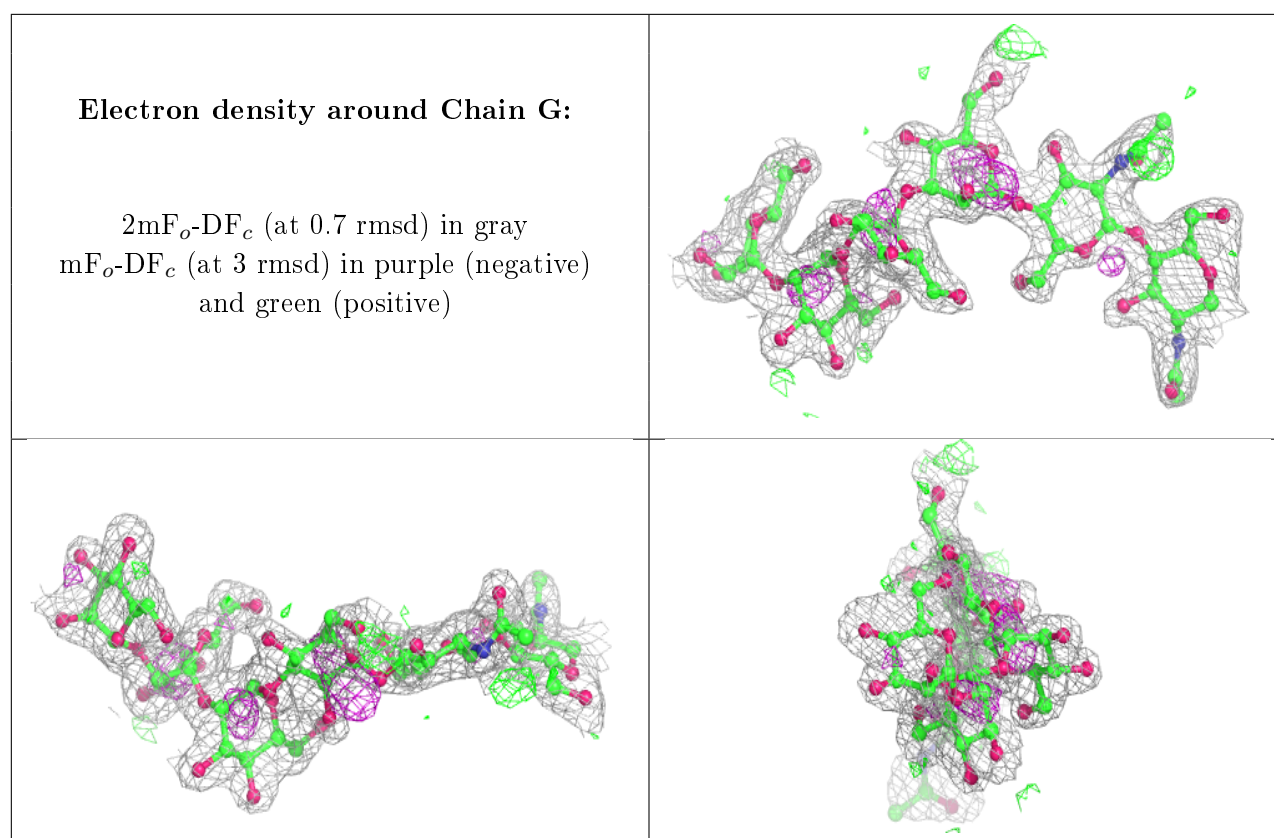
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o-DF_c$ (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
7	ACT	C	310	4/4	0.66	0.24	67,73,74,75	0
7	ACT	A	517	4/4	0.79	0.17	67,69,70,75	0
7	ACT	A	514	4/4	0.82	0.26	49,59,61,63	0
8	GOL	B	513	6/6	0.87	0.25	63,66,70,79	0
7	ACT	A	518	4/4	0.87	0.28	60,65,66,71	0
8	GOL	A	519	6/6	0.90	0.13	62,67,71,71	0
7	ACT	C	311	4/4	0.93	0.09	45,46,52,55	4
7	ACT	A	516	4/4	0.94	0.17	47,56,57,61	0
7	ACT	B	512	4/4	0.94	0.10	39,39,45,48	0
7	ACT	A	515	4/4	0.96	0.10	29,40,41,42	0
6	ZN	C	309	1/1	0.96	0.06	54,54,54,54	1
6	ZN	A	512	1/1	0.97	0.03	62,62,62,62	0
7	ACT	A	513	4/4	0.98	0.13	27,33,33,40	0
6	ZN	A	511	1/1	0.99	0.04	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ZN	A	510	1/1	0.99	0.09	34,34,34,34	0
6	ZN	B	511	1/1	1.00	0.10	30,30,30,30	0
6	ZN	B	510	1/1	1.00	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.