



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:00 PM UTC

PDB ID : 9GWT / pdb_00009gwt
Title : crystal structure of 23ME-00610 Fab in complex with human CD200R1
Authors : Huang, Y.M.; Ganichkin, O.M.
Deposited on : 2024-09-27
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

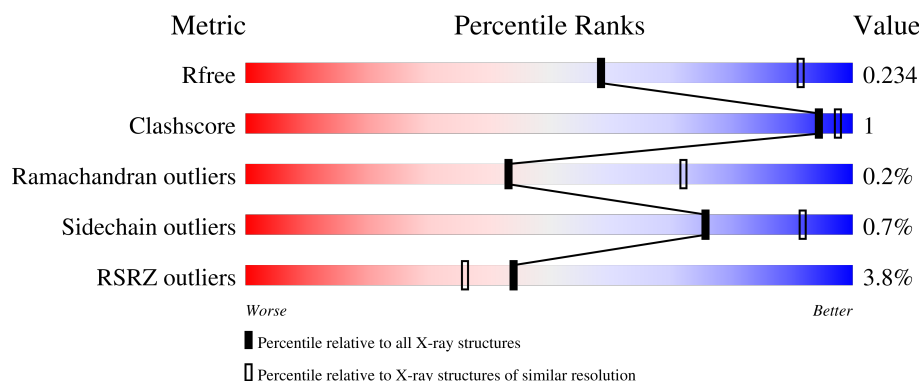
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	H	234	2% 91% 7%
2	L	218	% 95% 5%
3	P	268	6% 67% 6% 27%
4	A	2	50% 50%
4	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	B	3	67% 33%
6	C	7	43% 43% 14%
7	D	4	100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5128 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 23ME-00610 Fab (heavy).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	16	1	0
			1624	1025	270	322	7			

- Molecule 2 is a protein called 23ME-00610 Fab (light).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	29	2	0
			1693	1053	288	346	6			

- Molecule 3 is a protein called Isoform 1 of Cell surface glycoprotein CD200 receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	196	Total	C	N	O	S	44	0	0
			1552	977	275	289	11			

There are 53 discrepancies between the modelled and reference sequences:

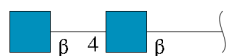
Chain	Residue	Modelled	Actual	Comment	Reference
P	10	MET	-	initiating methionine	UNP Q8TD46
P	11	GLY	-	expression tag	UNP Q8TD46
P	12	TRP	-	expression tag	UNP Q8TD46
P	13	SER	-	expression tag	UNP Q8TD46
P	14	CYS	-	expression tag	UNP Q8TD46
P	15	ILE	-	expression tag	UNP Q8TD46
P	16	ILE	-	expression tag	UNP Q8TD46
P	17	LEU	-	expression tag	UNP Q8TD46
P	18	PHE	-	expression tag	UNP Q8TD46
P	19	LEU	-	expression tag	UNP Q8TD46
P	20	VAL	-	expression tag	UNP Q8TD46
P	21	ALA	-	expression tag	UNP Q8TD46
P	22	THR	-	expression tag	UNP Q8TD46
P	23	ALA	-	expression tag	UNP Q8TD46

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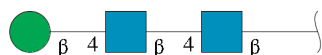
Chain	Residue	Modelled	Actual	Comment	Reference
P	24	THR	-	expression tag	UNP Q8TD46
P	25	GLY	-	expression tag	UNP Q8TD46
P	26	VAL	-	expression tag	UNP Q8TD46
P	27	HIS	-	expression tag	UNP Q8TD46
P	28	SER	-	expression tag	UNP Q8TD46
P	244	GLY	-	expression tag	UNP Q8TD46
P	245	GLY	-	expression tag	UNP Q8TD46
P	246	GLY	-	expression tag	UNP Q8TD46
P	247	SER	-	expression tag	UNP Q8TD46
P	248	GLY	-	expression tag	UNP Q8TD46
P	249	LEU	-	expression tag	UNP Q8TD46
P	250	ASN	-	expression tag	UNP Q8TD46
P	251	ASP	-	expression tag	UNP Q8TD46
P	252	ILE	-	expression tag	UNP Q8TD46
P	253	PHE	-	expression tag	UNP Q8TD46
P	254	GLU	-	expression tag	UNP Q8TD46
P	255	ALA	-	expression tag	UNP Q8TD46
P	256	GLN	-	expression tag	UNP Q8TD46
P	257	LYS	-	expression tag	UNP Q8TD46
P	258	ILE	-	expression tag	UNP Q8TD46
P	259	GLU	-	expression tag	UNP Q8TD46
P	260	TRP	-	expression tag	UNP Q8TD46
P	261	HIS	-	expression tag	UNP Q8TD46
P	262	GLU	-	expression tag	UNP Q8TD46
P	263	GLY	-	expression tag	UNP Q8TD46
P	264	GLY	-	expression tag	UNP Q8TD46
P	265	SER	-	expression tag	UNP Q8TD46
P	266	GLY	-	expression tag	UNP Q8TD46
P	267	SER	-	expression tag	UNP Q8TD46
P	268	GLY	-	expression tag	UNP Q8TD46
P	269	THR	-	expression tag	UNP Q8TD46
P	270	HIS	-	expression tag	UNP Q8TD46
P	271	HIS	-	expression tag	UNP Q8TD46
P	272	HIS	-	expression tag	UNP Q8TD46
P	273	HIS	-	expression tag	UNP Q8TD46
P	274	HIS	-	expression tag	UNP Q8TD46
P	275	HIS	-	expression tag	UNP Q8TD46
P	276	HIS	-	expression tag	UNP Q8TD46
P	277	HIS	-	expression tag	UNP Q8TD46

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



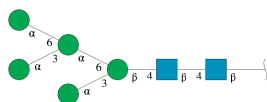
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 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	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
6	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 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
7	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	10	Total	O	0	0
			10	10		
9	L	8	Total	O	0	0
			8	8		
9	P	7	Total	O	0	0
			7	7		

Chain E:  50% 50%

MAG1
MAG2

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

Chain B:  67% 33%

MAG1
MAG2
BMA3

- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 C:  43% 43% 14%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 7: 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 D:  100%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.65Å 98.65Å 279.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.03 – 2.89 93.03 – 2.89	Depositor EDS
% Data completeness (in resolution range)	86.0 (93.03-2.89) 86.3 (93.03-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.202 , 0.236 0.203 , 0.234	Depositor DCC
R_{free} test set	1362 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	101.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5128	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, BMA, GOL

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	H	0.52	0/1661	0.77	1/2267 (0.0%)
2	L	0.55	2/1729 (0.1%)	0.79	1/2348 (0.0%)
3	P	0.62	3/1589 (0.2%)	0.86	2/2171 (0.1%)
All	All	0.56	5/4979 (0.1%)	0.81	4/6786 (0.1%)

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
2	L	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	225	LYS	CG-CD	-8.95	1.25	1.52
3	P	79	ARG	NE-CZ	8.22	1.42	1.33
2	L	72	ARG	NE-CZ	7.11	1.40	1.33
3	P	37	ASN	CB-CG	-5.91	1.37	1.52
2	L	169	GLU	CG-CD	-5.04	1.39	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	37	ASN	CA-CB-CG	13.75	126.35	112.60
3	P	225	LYS	CB-CG-CD	11.06	136.74	111.30
1	H	215	LYS	CG-CD-CE	5.86	124.78	111.30
2	L	151	GLN	CG-CD-NE2	5.70	124.95	116.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	72	ARG	Sidechain

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	H	1624	0	1610	2	0
2	L	1693	0	1627	3	0
3	P	1552	0	1526	8	0
4	A	28	0	25	0	0
4	E	28	0	25	0	0
5	B	39	0	34	0	0
6	C	83	0	70	1	0
7	D	50	0	43	0	0
8	L	6	0	8	0	0
9	H	10	0	0	0	0
9	L	8	0	0	0	0
9	P	7	0	0	0	0
All	All	5128	0	4968	13	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 1.

All (13) 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:P:81:GLN:HE21	3:P:82:PRO:HD2	1.69	0.56
3:P:76:ILE:HD13	3:P:105:ILE:HG21	1.86	0.56
2:L:4:LEU:HD22	2:L:37:MET:HE1	1.88	0.55
3:P:69:LEU:HD11	3:P:72:ILE:HB	1.89	0.54
3:P:181:ILE:HD12	3:P:217:HIS:NE2	2.27	0.49
1:H:18:LEU:HD13	1:H:114:VAL:HG11	1.94	0.49
2:L:87[B]:VAL:O	2:L:87[B]:VAL:HG23	2.11	0.49
3:P:208:VAL:HG12	3:P:210:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:LYS:N	1:H:207:PRO:CD	2.81	0.44
2:L:82:LEU:HD23	2:L:110:ILE:HD13	2.00	0.43
3:P:56:ASN:HD22	3:P:56:ASN:N	2.17	0.41
3:P:44:GLU:CG	6:C:1:NAG:H82	2.51	0.41
3:P:72:ILE:HD13	3:P:115:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

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	H	215/234 (92%)	211 (98%)	4 (2%)	0	100	100
2	L	218/218 (100%)	208 (95%)	9 (4%)	1 (0%)	24	54
3	P	194/268 (72%)	186 (96%)	8 (4%)	0	100	100
All	All	627/720 (87%)	605 (96%)	21 (3%)	1 (0%)	43	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	54	ARG

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	H	187/202 (93%)	187 (100%)	0	100	100
2	L	194/192 (101%)	192 (99%)	2 (1%)	68	89
3	P	176/232 (76%)	174 (99%)	2 (1%)	65	88
All	All	557/626 (89%)	553 (99%)	4 (1%)	76	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	13	VAL
2	L	76	THR
3	P	84	CYS
3	P	225	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	169	HIS
1	H	204	ASN
2	L	42	GLN
2	L	93	HIS
2	L	141	ASN
2	L	214	ASN
3	P	56	ASN
3	P	81	GLN
3	P	190	GLN

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 ⓘ

18 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	A	1	3,4	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
4	NAG	A	2	4	14,14,15	0.40	0	17,19,21	0.63	0
5	NAG	B	1	5,3	14,14,15	0.40	0	17,19,21	0.77	0
5	NAG	B	2	5	14,14,15	0.40	0	17,19,21	1.00	2 (11%)
5	BMA	B	3	5	11,11,12	0.39	0	15,15,17	0.60	0
6	NAG	C	1	6,3	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
6	NAG	C	2	6	14,14,15	0.41	0	17,19,21	0.67	0
6	BMA	C	3	6	11,11,12	0.34	0	15,15,17	0.53	0
6	MAN	C	4	6	11,11,12	0.34	0	15,15,17	0.90	1 (6%)
6	MAN	C	5	6	11,11,12	0.34	0	15,15,17	0.69	0
6	MAN	C	6	6	11,11,12	0.44	0	15,15,17	0.69	1 (6%)
6	MAN	C	7	6	11,11,12	0.39	0	15,15,17	0.81	1 (6%)
7	NAG	D	1	7,3	14,14,15	0.38	0	17,19,21	0.77	0
7	NAG	D	2	7	14,14,15	0.41	0	17,19,21	0.65	0
7	BMA	D	3	7	11,11,12	0.52	0	15,15,17	0.57	0
7	MAN	D	4	7	11,11,12	0.48	0	15,15,17	0.73	0
4	NAG	E	1	3,4	14,14,15	0.39	0	17,19,21	0.73	0
4	NAG	E	2	4	14,14,15	0.42	0	17,19,21	1.13	3 (17%)

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	A	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	1/6/23/26	0/1/1/1
5	NAG	B	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	2/6/23/26	0/1/1/1
5	BMA	B	3	5	-	0/2/19/22	0/1/1/1
6	NAG	C	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	C	4	6	-	0/2/19/22	0/1/1/1
6	MAN	C	5	6	-	0/2/19/22	0/1/1/1
6	MAN	C	6	6	-	1/2/19/22	0/1/1/1
6	MAN	C	7	6	-	0/2/19/22	0/1/1/1
7	NAG	D	1	7,3	-	1/6/23/26	0/1/1/1
7	NAG	D	2	7	-	0/6/23/26	0/1/1/1
7	BMA	D	3	7	-	2/2/19/22	0/1/1/1
7	MAN	D	4	7	-	1/2/19/22	0/1/1/1
4	NAG	E	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C1-C2-N2	3.34	115.70	110.43
6	C	1	NAG	C1-C2-N2	2.85	114.92	110.43
4	E	2	NAG	C1-C2-N2	2.72	114.73	110.43
4	A	1	NAG	C2-N2-C7	2.60	126.39	122.90
6	C	4	MAN	C1-O5-C5	2.50	115.54	112.19
5	B	2	NAG	C1-C2-N2	2.45	114.30	110.43
5	B	2	NAG	C2-N2-C7	2.41	126.12	122.90
4	E	2	NAG	O5-C1-C2	-2.39	107.60	111.29
4	E	2	NAG	C2-N2-C7	2.12	125.75	122.90
6	C	6	MAN	C1-O5-C5	2.11	115.02	112.19
6	C	7	MAN	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2	NAG	C1-C2-N2-C7
7	D	3	BMA	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
7	D	3	BMA	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
6	C	3	BMA	O5-C5-C6-O6
6	C	3	BMA	C4-C5-C6-O6
7	D	4	MAN	O5-C5-C6-O6
7	D	1	NAG	O5-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6

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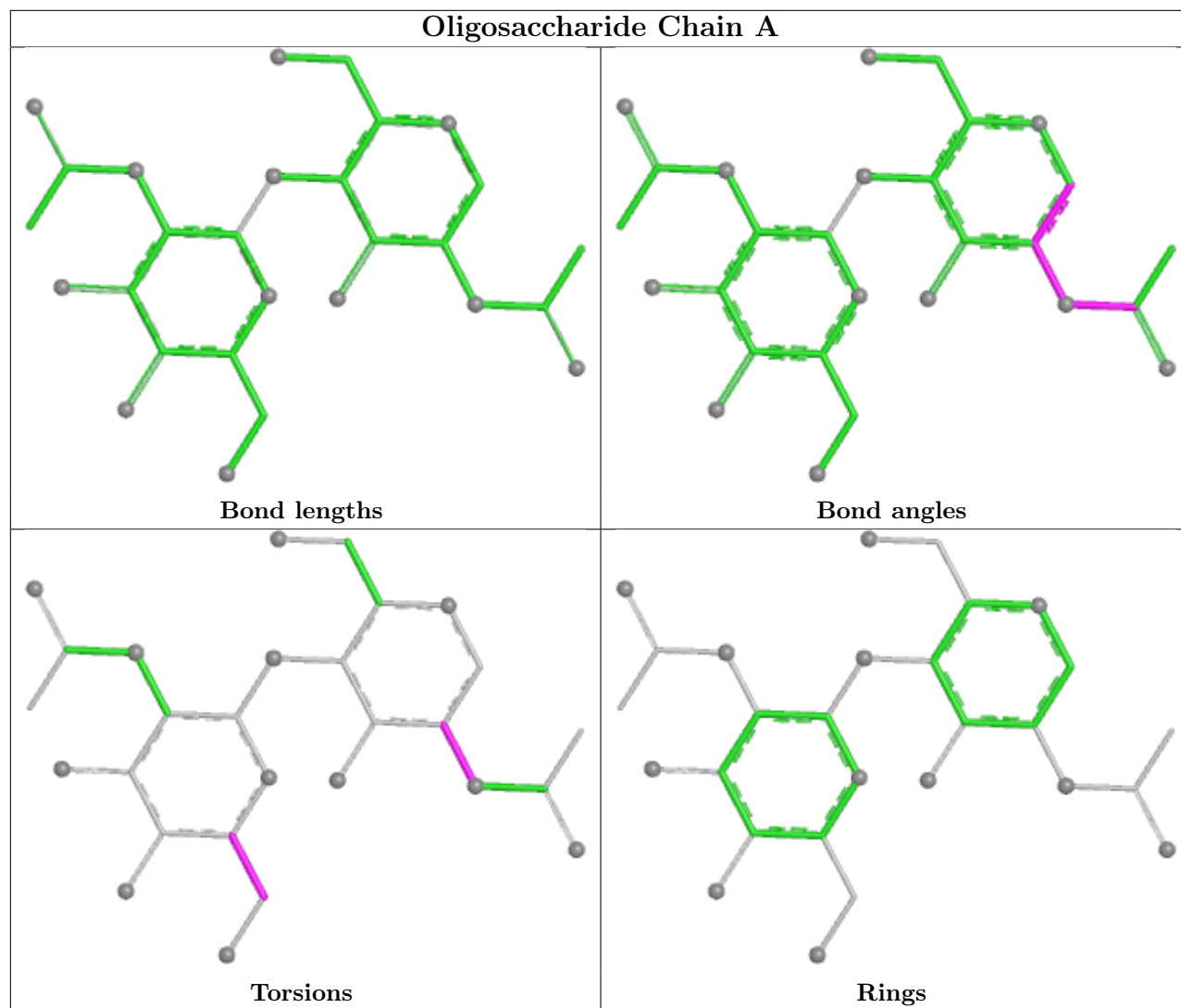
Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C1-C2-N2-C7
4	A	1	NAG	C3-C2-N2-C7
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
5	B	2	NAG	C3-C2-N2-C7
6	C	6	MAN	C4-C5-C6-O6

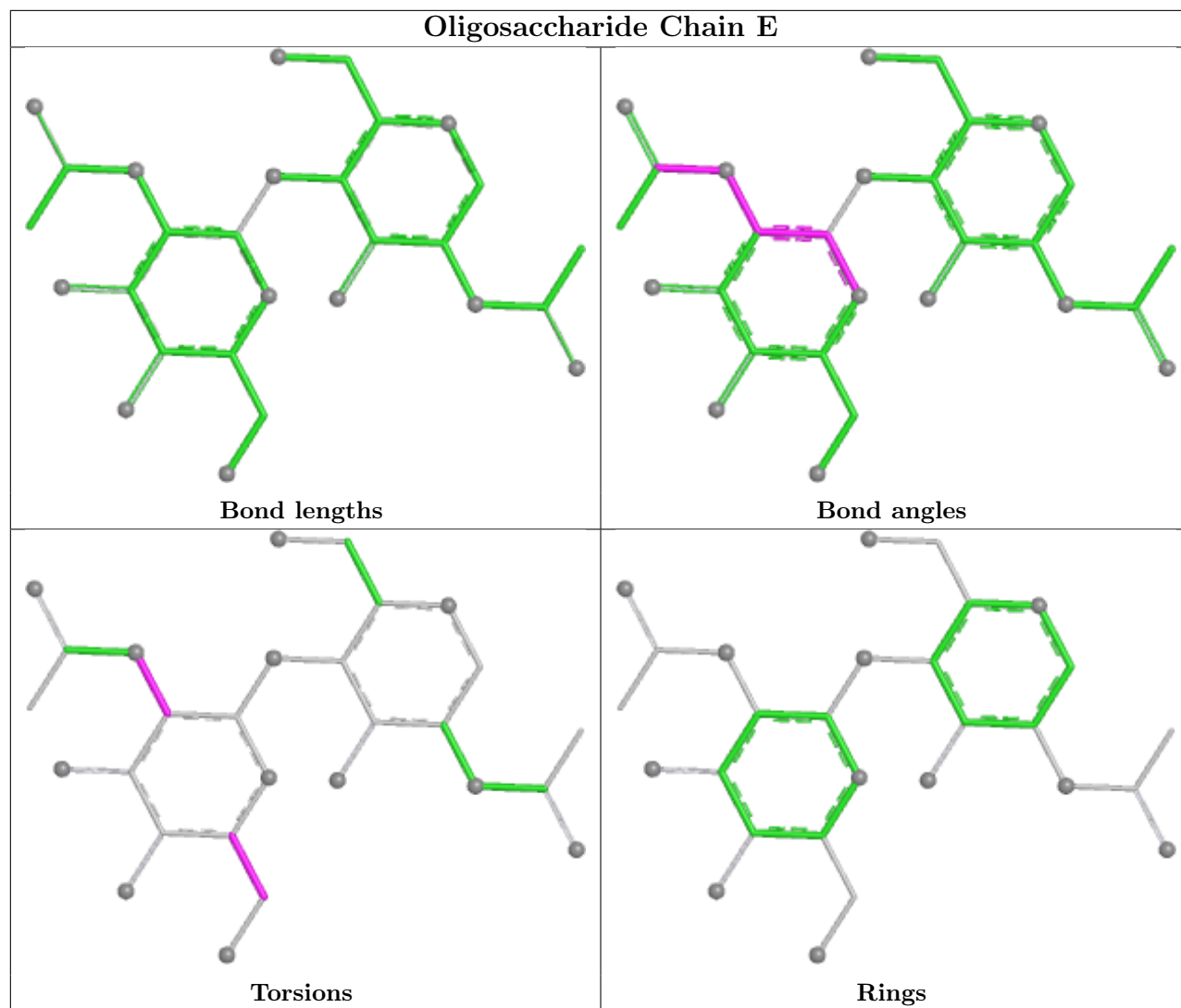
There are no ring outliers.

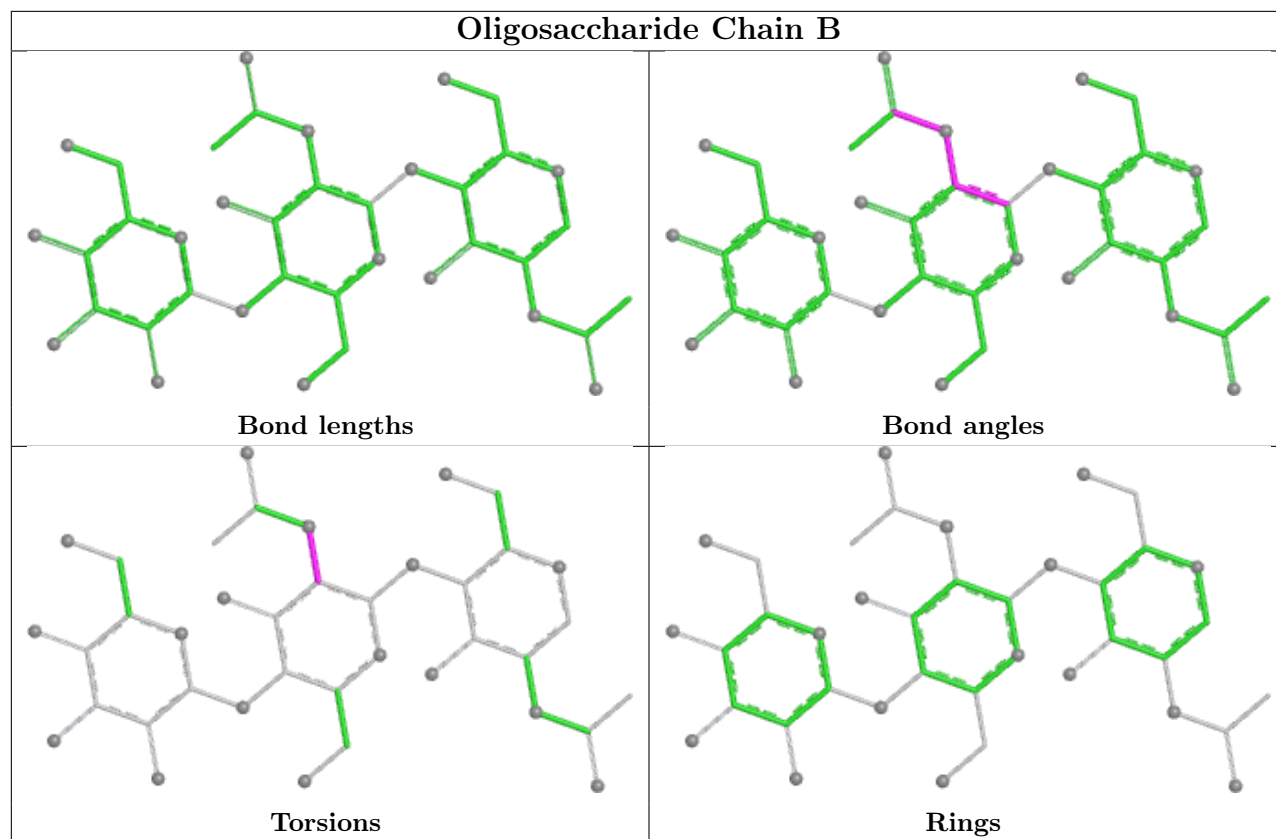
1 monomer is involved in 1 short contact:

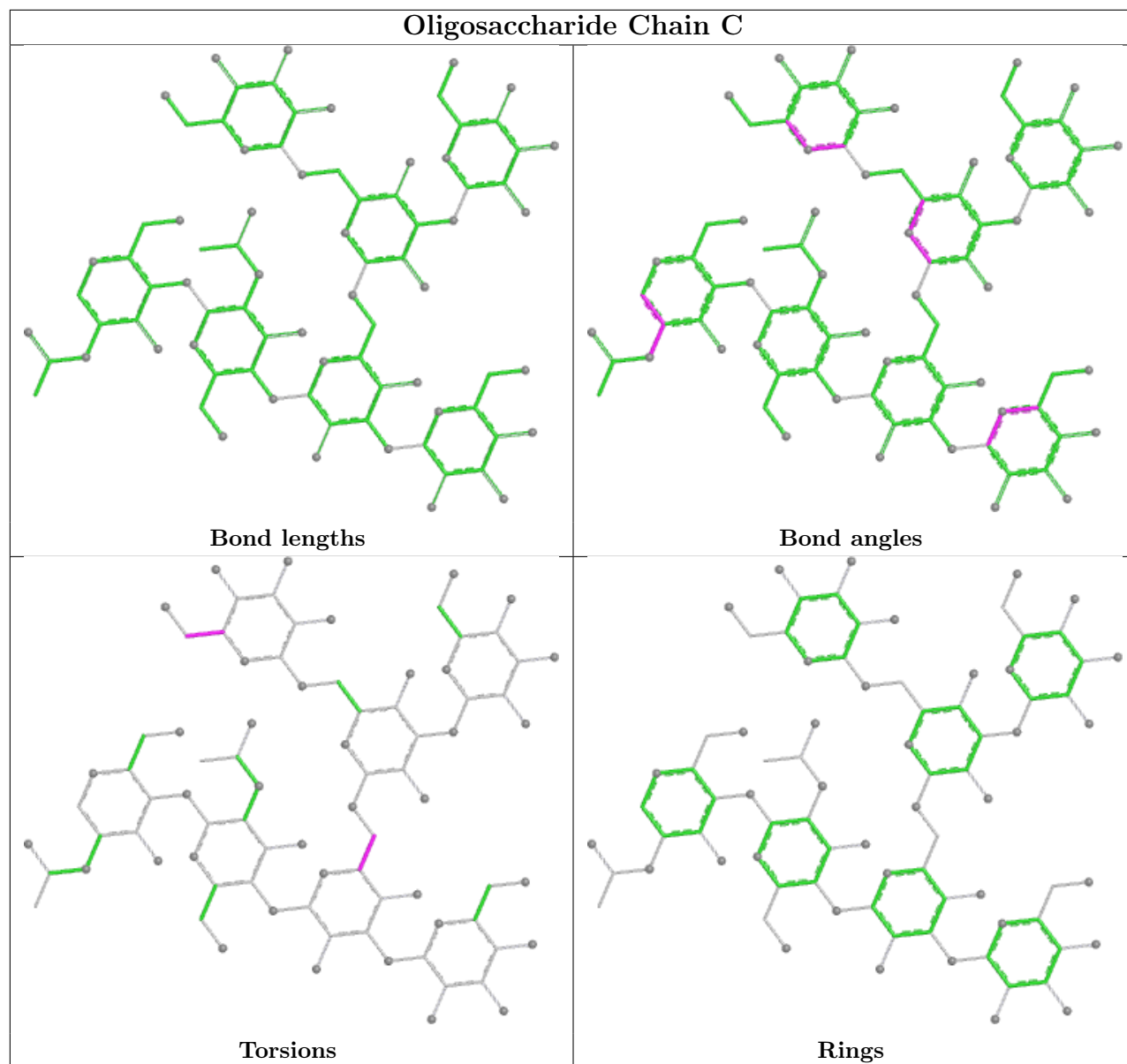
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	1	0

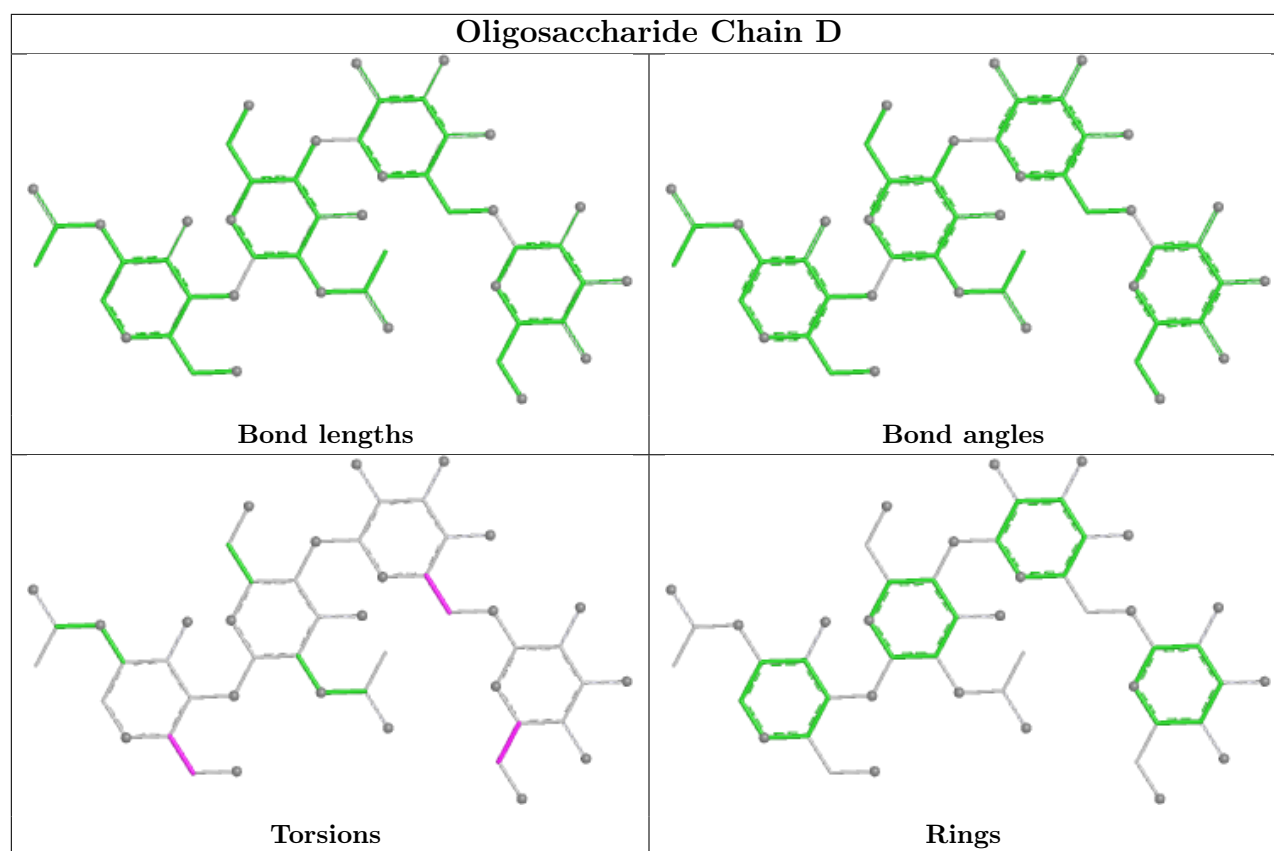
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
8	GOL	L	301	-	5,5,5	0.11	0	5,5,5	0.33	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
8	GOL	L	301	-	-	2/4/4/4	-

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
8	L	301	GOL	O2-C2-C3-O3
8	L	301	GOL	O1-C1-C2-C3

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	218/234 (93%)	0.03	4 (1%) 67 59	48, 100, 133, 206	9 (4%)
2	L	218/218 (100%)	-0.00	3 (1%) 73 65	44, 96, 131, 171	13 (5%)
3	P	196/268 (73%)	0.55	17 (8%) 16 13	52, 105, 140, 177	13 (6%)
All	All	632/720 (87%)	0.18	24 (3%) 44 36	44, 102, 135, 206	35 (5%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	37	ASN	4.6
3	P	159	GLN	4.1
3	P	41	VAL	4.1
3	P	38	TYR	3.8
3	P	162	ASN	3.2
3	P	207	GLU	3.1
2	L	156	ASN	3.0
3	P	230	GLU	2.8
3	P	167	CYS	2.8
3	P	42	LEU	2.8
1	H	133	SER	2.8
3	P	208	VAL	2.8
3	P	228	TYR	2.8
3	P	40	LYS	2.7
1	H	138	GLY	2.7
3	P	232	LEU	2.6
1	H	103	GLY	2.3
2	L	161	GLY	2.3
3	P	91	GLU	2.3
2	L	160	SER	2.2
1	H	54	GLY	2.1
3	P	121	THR	2.1
3	P	103	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	P	189	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

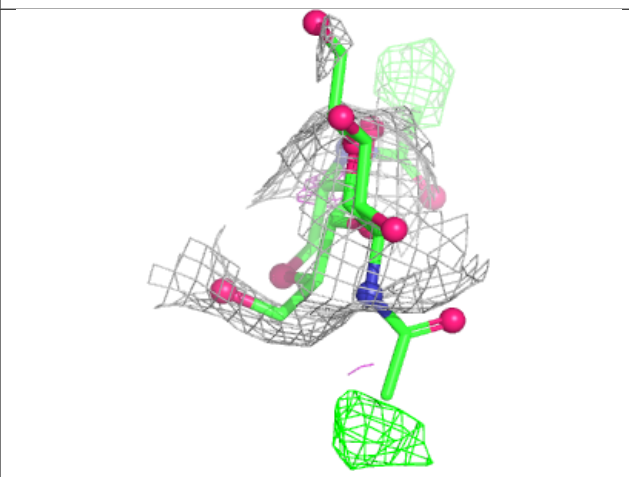
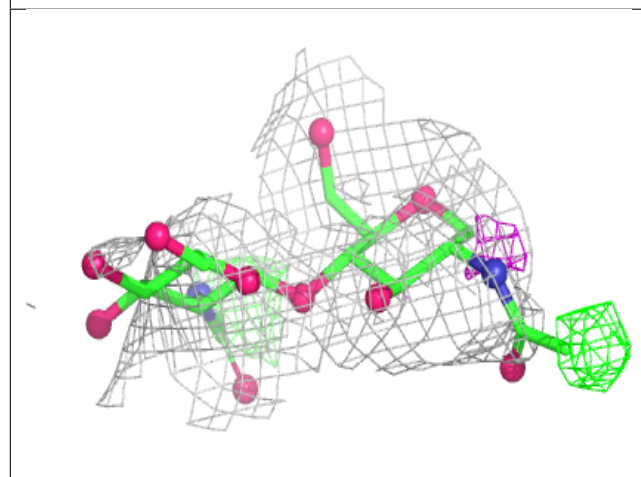
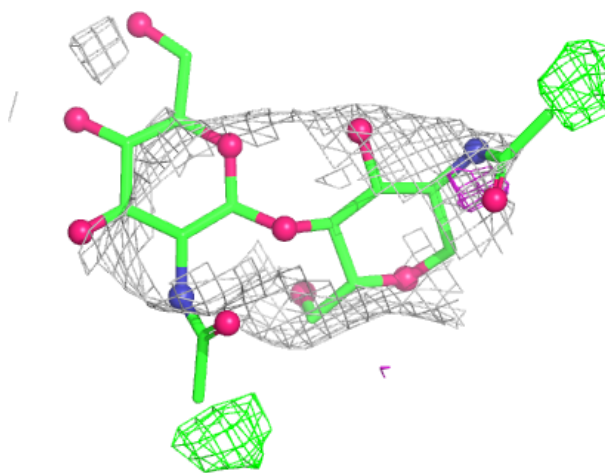
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	1	14/15	-	-	157,165,176,183	0
4	NAG	A	2	14/15	-	-	174,195,201,203	0
7	NAG	D	2	14/15	0.53	0.12	167,172,185,189	0
7	NAG	D	1	14/15	0.58	0.13	129,134,148,157	0
5	NAG	B	1	14/15	-	-	108,113,119,130	0
5	NAG	B	2	14/15	-	-	137,147,159,169	0
5	BMA	B	3	11/12	-	-	159,173,180,183	0
6	NAG	C	1	14/15	-	-	121,135,143,147	0
6	NAG	C	2	14/15	-	-	131,149,158,163	0
6	BMA	C	3	11/12	-	-	163,168,178,179	0
6	MAN	C	4	11/12	-	-	145,152,161,161	0
6	MAN	C	5	11/12	-	-	154,158,163,163	0
6	MAN	C	6	11/12	-	-	138,145,151,152	0
6	MAN	C	7	11/12	-	-	165,181,192,193	0
4	NAG	E	2	14/15	0.81	0.13	201,209,222,224	0
4	NAG	E	1	14/15	0.95	0.08	167,176,186,193	0
7	BMA	D	3	11/12	-	-	194,205,208,210	0
7	MAN	D	4	11/12	-	-	189,198,208,209	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.

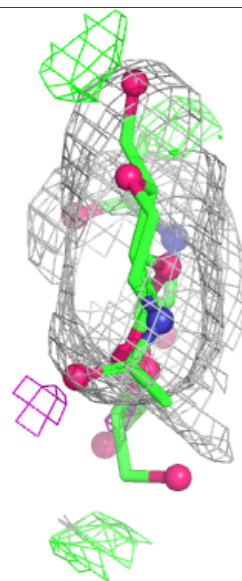
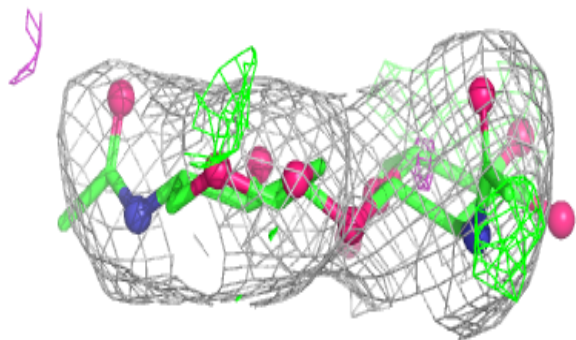
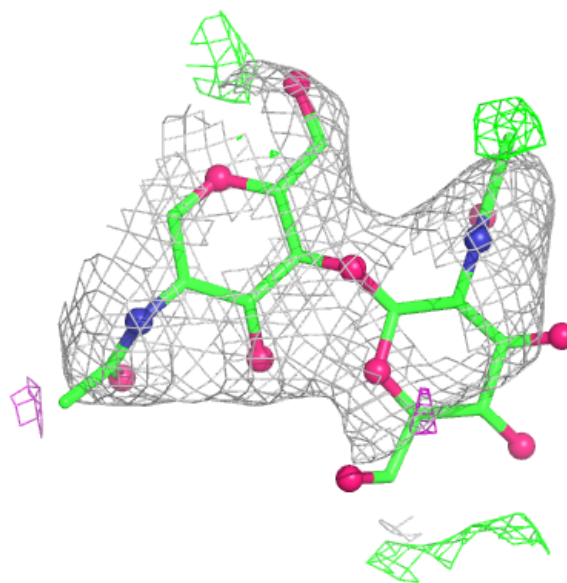
Electron density around Chain A:

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



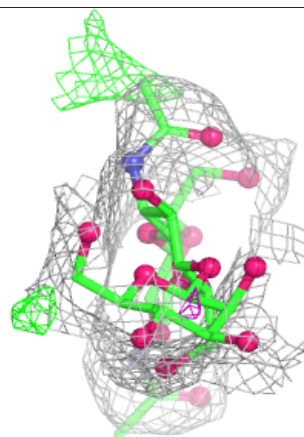
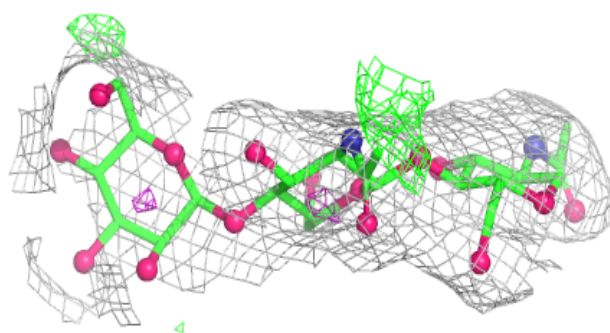
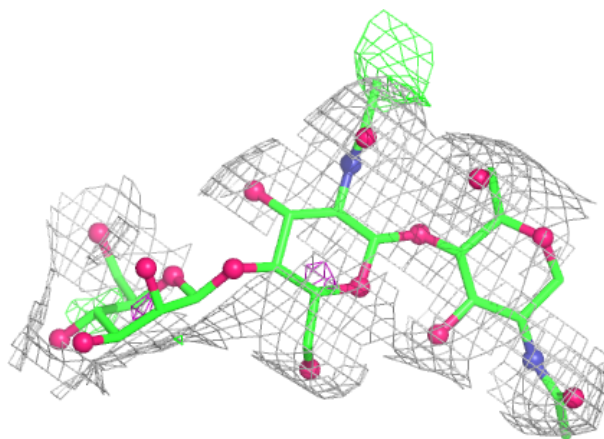
Electron density around Chain E:

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



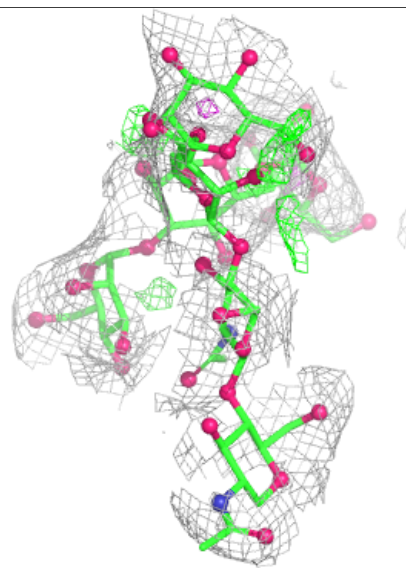
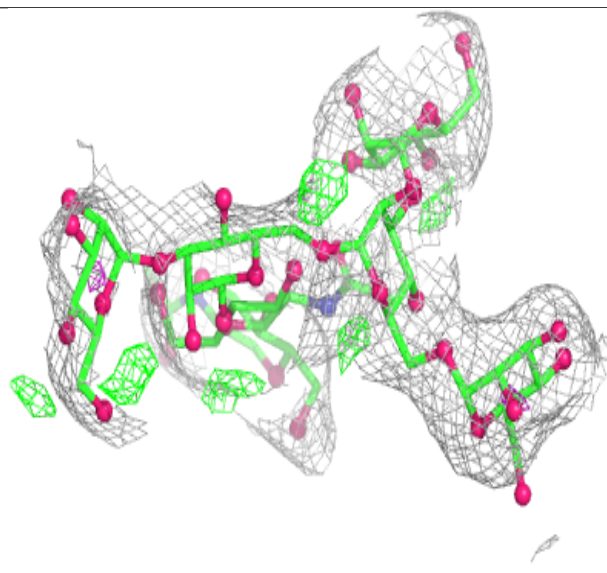
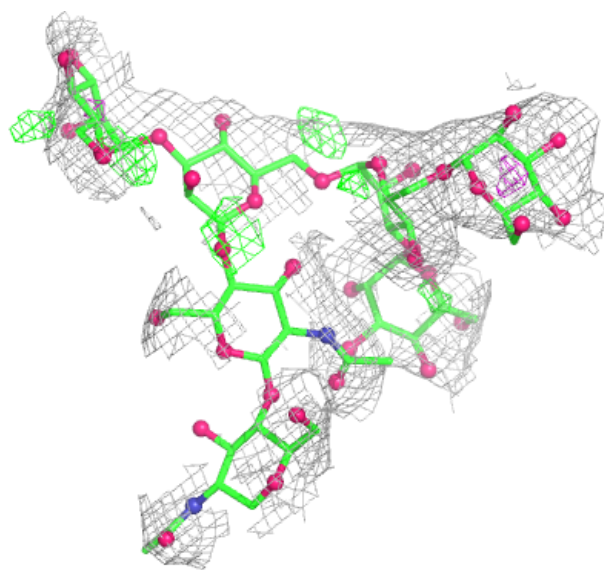
Electron density around Chain B:

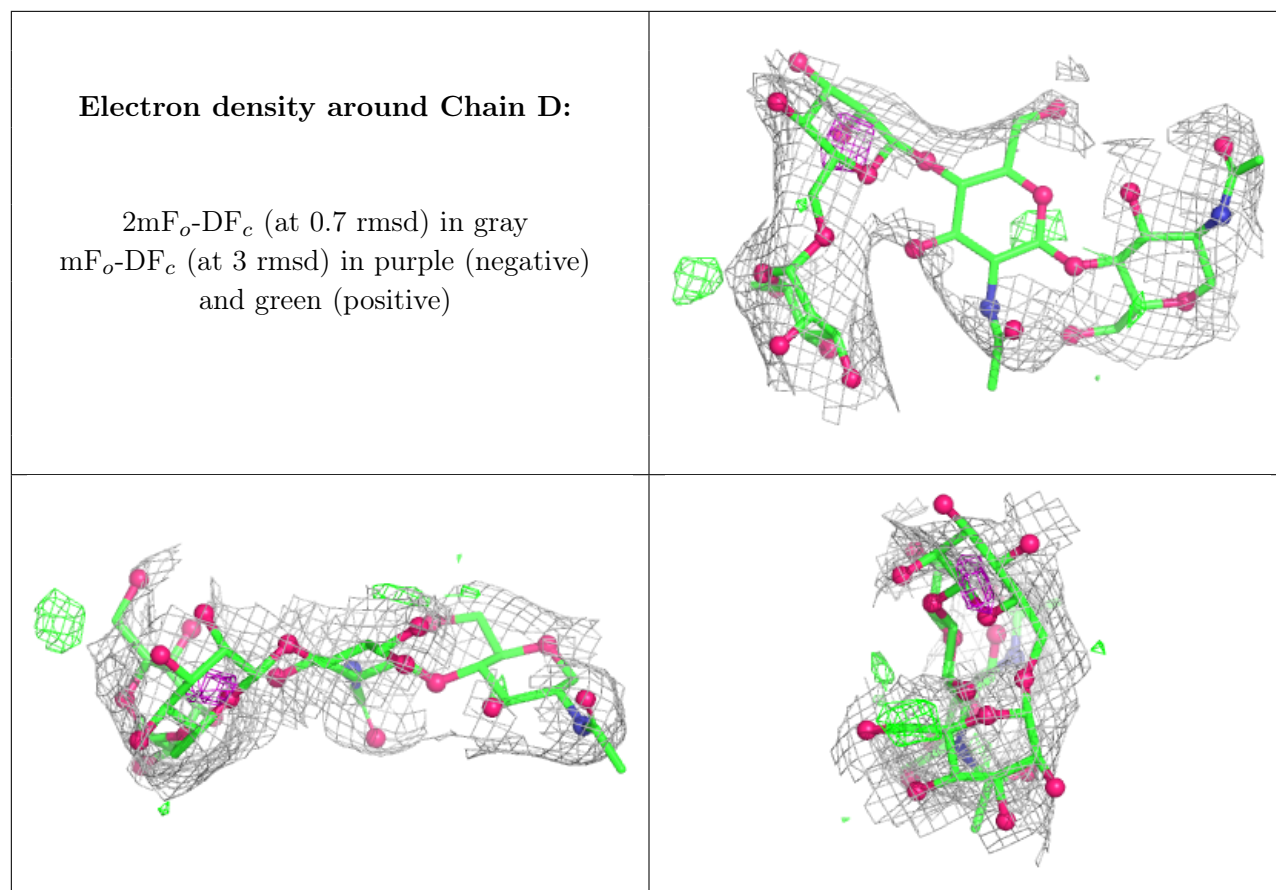
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

$2mF_o-DF_c$ (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
8	GOL	L	301	6/6	0.92	0.13	114,122,124,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.