



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 PM UTC

PDB ID : 8W0W / pdb_00008w0w
Title : Crystal structure of broadly neutralizing antibody hcab64 in complex with Hepatitis C virus envelope glycoprotein E2 ectodomain
Authors : Flyak, A.I.; Wilcox, X.E.
Deposited on : 2024-02-14
Resolution : 2.13 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

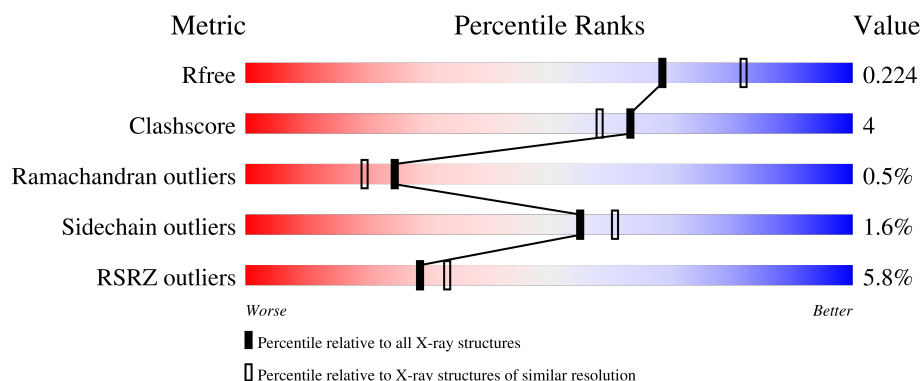
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	C	262	7% 74% 10% • 16%
2	H	237	5% 85% 8% • 5%
3	L	215	3% 93% 7% •
4	A	5	20% 80%
5	B	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	2	50% 50%
5	E	2	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5508 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	221	Total	C	N	O	S	0	0	0
			1738	1105	306	308	19			

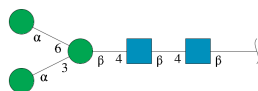
- Molecule 2 is a protein called hcab64 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1688	1053	292	334	9			

- Molecule 3 is a protein called hcab64 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1641	1029	278	330	4			

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	86	Total	O	0	0
			86	86		
7	H	107	Total	O	0	0
			107	107		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	75	Total	O	0	0
			75	75		

MAG1
MAG2

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.68Å 88.23Å 174.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.99 – 2.13 53.99 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.8 (53.99-2.13) 98.7 (53.99-2.13)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.195 , 0.224 0.196 , 0.224	Depositor DCC
R_{free} test set	2972 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	C	0.44	0/1802	0.62	0/2469
2	H	0.43	0/1726	0.59	0/2349
3	L	0.42	0/1679	0.59	0/2281
All	All	0.43	0/5207	0.60	0/7099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	1738	0	1604	16	0
2	H	1688	0	1650	18	0
3	L	1641	0	1586	8	0
4	A	61	0	52	0	0
5	B	28	0	25	0	0
5	D	28	0	25	0	0
5	E	28	0	25	1	0
6	C	28	0	26	1	0
7	C	86	0	0	2	1
7	H	107	0	0	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	75	0	0	1	1
All	All	5508	0	4993	41	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (41) 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:H:117:LYS:NZ	7:H:303:HOH:O	1.86	1.08
2:H:208:ASP:OD1	7:H:301:HOH:O	1.81	0.96
2:H:125:ALA:O	7:H:302:HOH:O	1.83	0.95
1:C:531:GLU:OE2	2:H:100(B):ARG:NE	2.01	0.92
2:H:81:GLU:OE2	7:H:304:HOH:O	1.89	0.91
2:H:43:GLN:O	7:H:305:HOH:O	2.01	0.78
1:C:449:ALA:HB1	6:C:702:NAG:H83	1.69	0.73
1:C:474:TYR:OH	7:C:801:HOH:O	2.08	0.72
1:C:584:ASP:OD1	7:C:802:HOH:O	2.10	0.70
2:H:54:ASP:HB3	2:H:56:SER:H	1.59	0.66
1:C:444:THR:O	1:C:445:HIS:HB2	1.98	0.62
2:H:60:THR:HG23	2:H:62:LYS:H	1.64	0.61
2:H:100(D):ARG:NH2	7:H:306:HOH:O	2.22	0.60
1:C:506:VAL:HG21	1:C:537:LEU:HD22	1.82	0.59
2:H:100(A):ARG:HG2	2:H:100(B):ARG:HD3	1.83	0.59
3:L:100:GLN:NE2	7:L:302:HOH:O	2.30	0.59
3:L:32:TYR:HB2	3:L:92:SER:HB3	1.85	0.58
3:L:149:LYS:NZ	3:L:195:GLU:OE2	2.37	0.57
2:H:1:GLN:OE1	2:H:1:GLN:N	2.29	0.57
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.39	0.56
3:L:35:TRP:HB2	3:L:48:VAL:HG22	1.86	0.56
2:H:131:THR:N	7:H:308:HOH:O	2.41	0.53
1:C:481:ASP:OD2	1:C:492:ARG:NH1	2.35	0.53
1:C:502:VAL:HG21	1:C:537:LEU:HD13	1.91	0.52
1:C:429:CYS:HB3	1:C:438:LEU:HD21	1.93	0.49
3:L:95:PHE:C	3:L:95:PHE:CD1	2.92	0.47
3:L:95:PHE:C	3:L:95:PHE:HD1	2.23	0.47
1:C:440:ALA:HB3	1:C:616:TRP:CD1	2.51	0.46
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.99	0.45
2:H:67:LEU:HD11	2:H:80:MET:HG2	2.00	0.43
2:H:60:THR:HG23	2:H:62:LYS:N	2.33	0.43
2:H:54:ASP:HB3	2:H:56:SER:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4:LEU:HD23	3:L:88:CYS:SG	2.59	0.42
1:C:624:PHE:CZ	1:C:645:ASN:HB2	2.54	0.42
2:H:131:THR:HG22	2:H:132:SER:H	1.83	0.42
1:C:482:GLN:HA	1:C:489:TYR:HE1	1.85	0.41
1:C:631:MET:HE3	1:C:631:MET:HB3	1.91	0.41
1:C:615:LEU:HD23	1:C:615:LEU:HA	1.79	0.41
1:C:562:LYS:NZ	5:E:1:NAG:O6	2.39	0.41
1:C:519:THR:HG22	1:C:525:PRO:HA	2.03	0.41
2:H:60:THR:HG22	2:H:63:PHE:HD1	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:868:HOH:O	7:C:875:HOH:O[4_445]	1.86	0.34
7:H:382:HOH:O	7:L:372:HOH:O[4_444]	2.04	0.16

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	C	217/262 (83%)	205 (94%)	10 (5%)	2 (1%)	14	8
2	H	220/237 (93%)	215 (98%)	5 (2%)	0	100	100
3	L	211/215 (98%)	205 (97%)	5 (2%)	1 (0%)	24	19
All	All	648/714 (91%)	625 (96%)	20 (3%)	3 (0%)	24	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	445	HIS
3	L	31	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	582	PRO

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	C	187/219 (85%)	184 (98%)	3 (2%)	55	61
2	H	193/206 (94%)	188 (97%)	5 (3%)	40	42
3	L	185/187 (99%)	184 (100%)	1 (0%)	81	86
All	All	565/612 (92%)	556 (98%)	9 (2%)	55	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	537	LEU
1	C	578	THR
1	C	640	LEU
2	H	37	VAL
2	H	60	THR
2	H	131	THR
2	H	178	LEU
2	H	199	ASN
3	L	56	THR

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

Mol	Chain	Res	Type
2	H	3	GLN
2	H	39	GLN
2	H	43	GLN
2	H	164	HIS
2	H	171	GLN
2	H	192	GLN
2	H	199	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	37	GLN
3	L	38	GLN
3	L	147	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 ⓘ

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	A	1	1,4	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
4	NAG	A	2	4	14,14,15	0.27	0	17,19,21	0.82	0
4	BMA	A	3	4	11,11,12	0.85	1 (9%)	15,15,17	1.75	2 (13%)
4	MAN	A	4	4	11,11,12	0.75	0	15,15,17	1.23	2 (13%)
4	MAN	A	5	4	11,11,12	0.86	0	15,15,17	1.45	2 (13%)
5	NAG	B	1	5,1	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
5	NAG	B	2	5	14,14,15	0.47	0	17,19,21	1.17	1 (5%)
5	NAG	D	1	5,1	14,14,15	0.50	0	17,19,21	1.02	0
5	NAG	D	2	5	14,14,15	0.52	0	17,19,21	0.91	1 (5%)
5	NAG	E	1	5,1	14,14,15	0.32	0	17,19,21	1.02	0
5	NAG	E	2	5	14,14,15	0.40	0	17,19,21	0.96	1 (5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	C2-C3	2.16	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	BMA	C1-O5-C5	4.74	118.54	112.19
4	A	5	MAN	C1-O5-C5	3.25	116.54	112.19
5	B	2	NAG	C2-N2-C7	-2.81	119.13	122.90
4	A	3	BMA	O5-C5-C6	2.79	113.10	107.66
5	D	2	NAG	O5-C5-C6	2.41	112.35	107.66
4	A	4	MAN	C2-C3-C4	2.30	114.90	110.86
4	A	4	MAN	C1-O5-C5	2.23	115.17	112.19
5	E	2	NAG	C2-N2-C7	2.17	125.80	122.90
5	B	1	NAG	C1-O5-C5	2.06	114.94	112.19
4	A	5	MAN	C2-C3-C4	2.05	114.46	110.86
4	A	1	NAG	C1-C2-N2	-2.05	107.21	110.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3	BMA	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

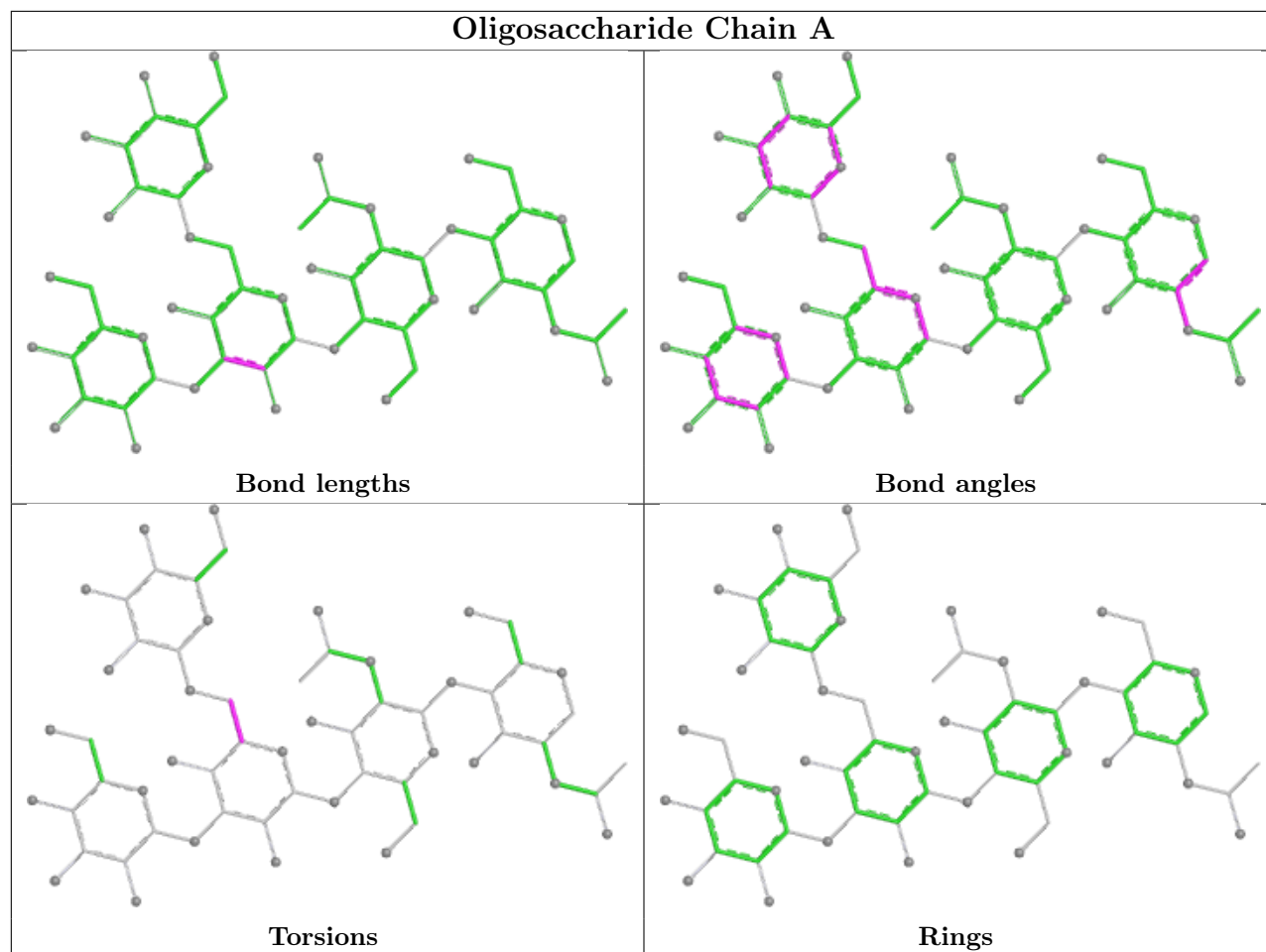
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
5	B	2	NAG	C8-C7-N2-C2
5	D	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
5	D	2	NAG	O7-C7-N2-C2
5	D	1	NAG	C3-C2-N2-C7
5	D	1	NAG	O5-C5-C6-O6
5	D	1	NAG	C1-C2-N2-C7

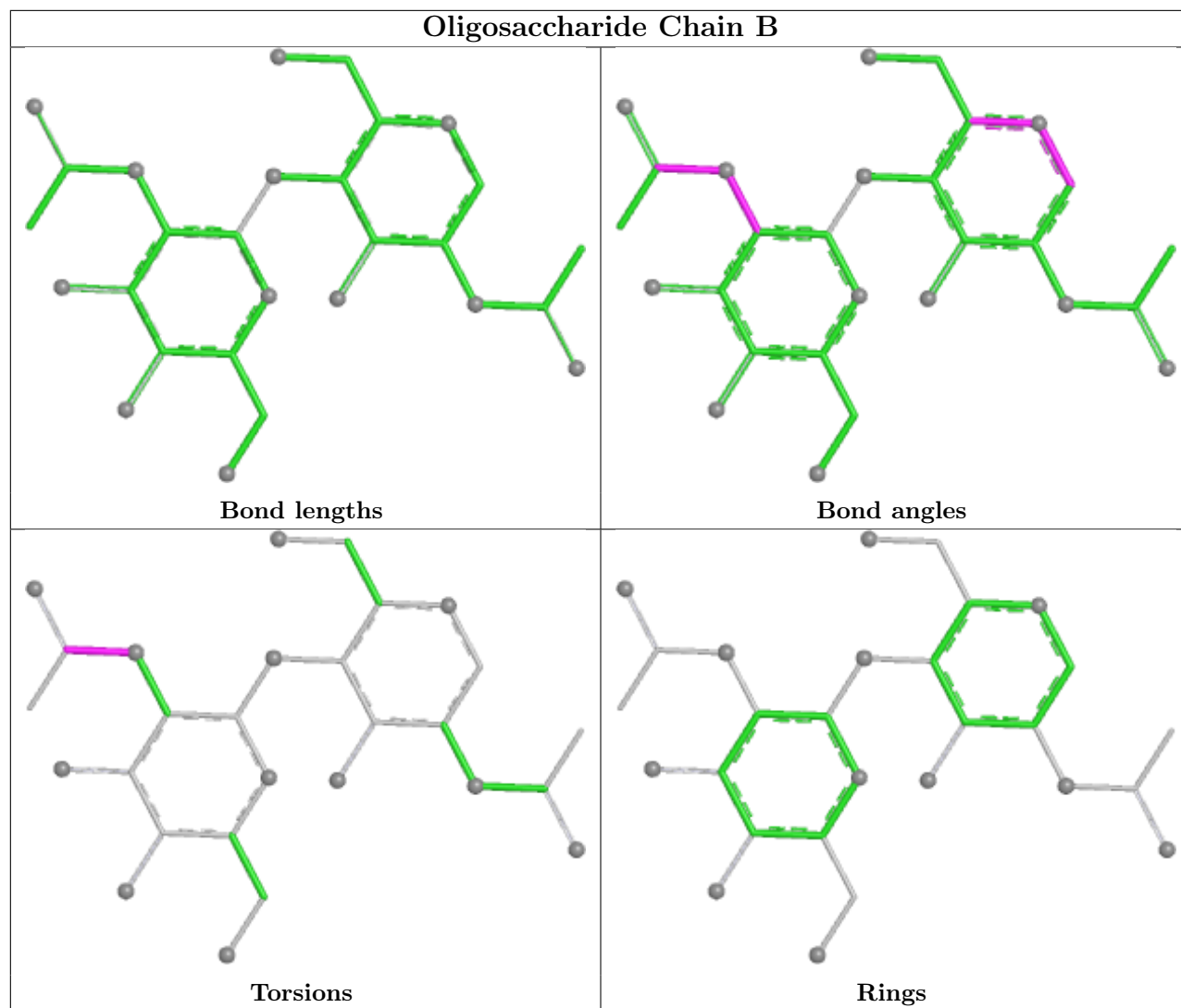
There are no ring outliers.

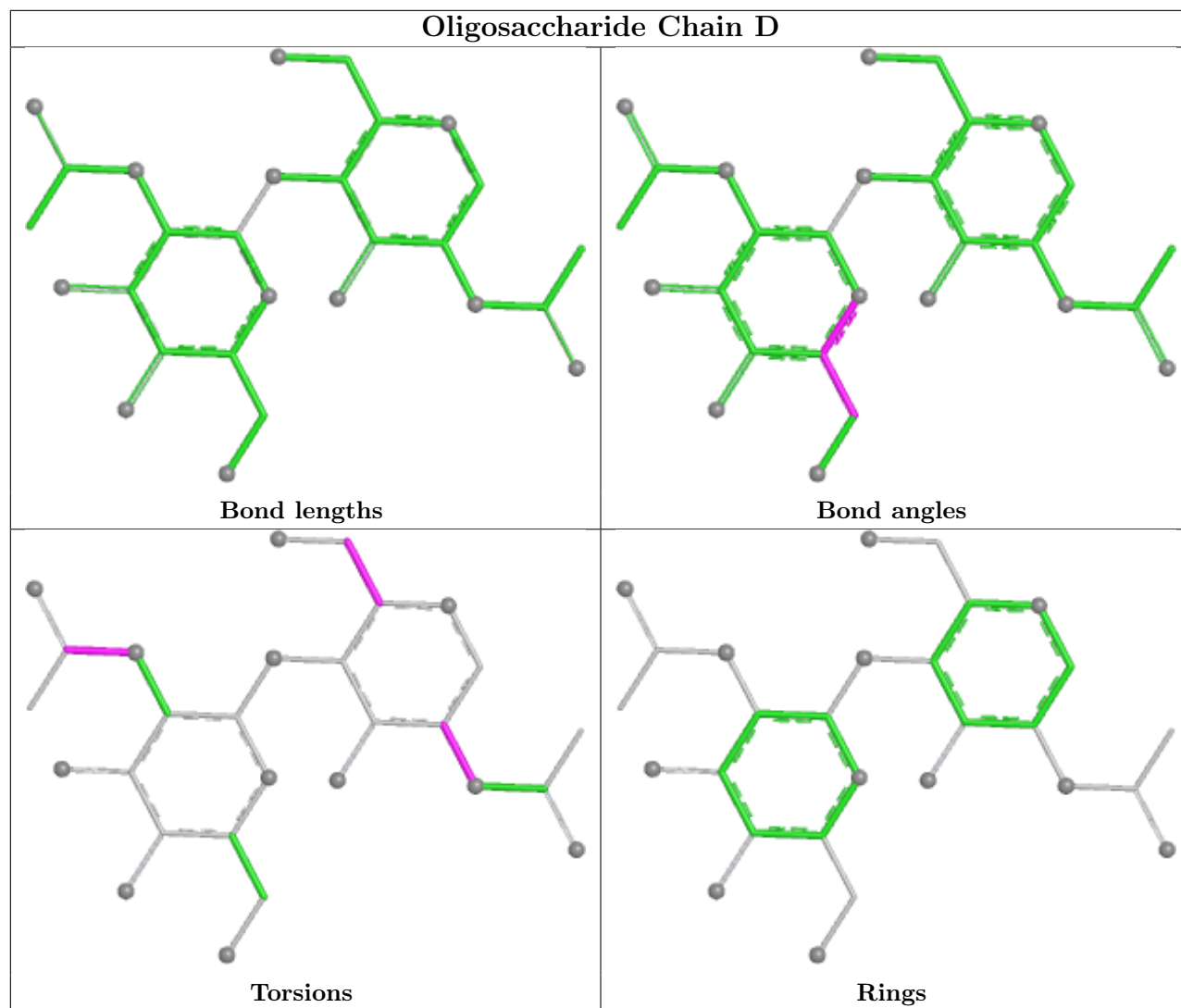
1 monomer is involved in 1 short contact:

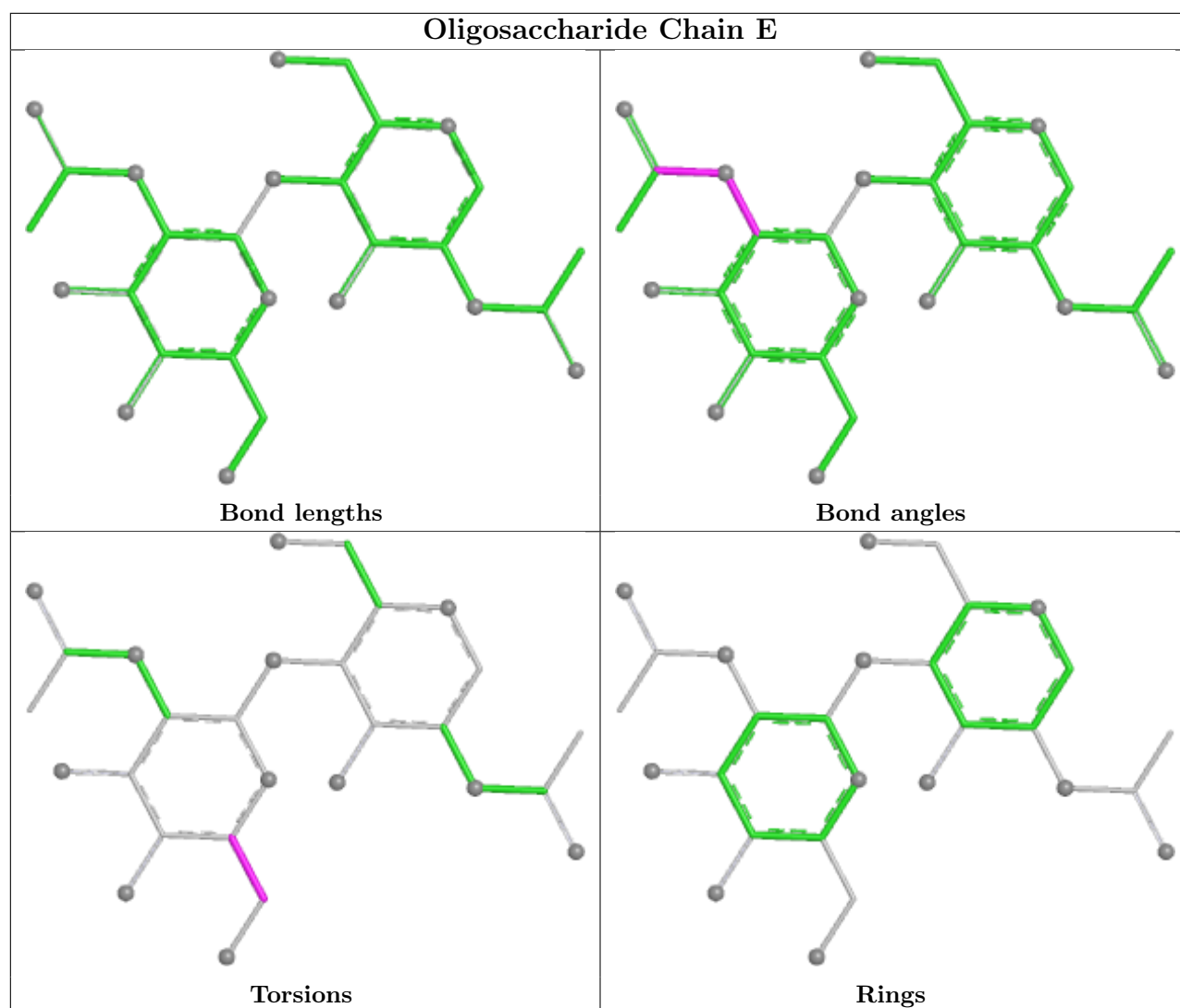
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	1	0

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	C	702	1	14,14,15	0.57	0	17,19,21	1.01	1 (5%)
6	NAG	C	701	1	14,14,15	0.34	0	17,19,21	1.22	2 (11%)

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
6	NAG	C	702	1	-	1/6/23/26	0/1/1/1
6	NAG	C	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	701	NAG	C1-O5-C5	2.82	115.97	112.19
6	C	702	NAG	C2-N2-C7	-2.29	119.83	122.90
6	C	701	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	702	NAG	O5-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	702	NAG	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

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	C	221/262 (84%)	0.35	18 (8%)	18 20	30, 42, 74, 98	0
2	H	224/237 (94%)	0.30	13 (5%)	29 33	27, 44, 76, 94	0
3	L	213/215 (99%)	0.30	7 (3%)	49 53	29, 49, 78, 88	0
All	All	658/714 (92%)	0.32	38 (5%)	29 33	27, 45, 78, 98	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	420	TRP	6.1
1	C	443	TYR	5.0
2	H	132	SER	4.0
1	C	481	ASP	3.9
1	C	442	PHE	3.8
2	H	131	THR	3.7
1	C	421	HIS	3.6
3	L	32	TYR	3.5
2	H	133	GLY	3.3
2	H	59	ASP	3.3
3	L	31	SER	3.3
3	L	95	PHE	3.2
1	C	441	LEU	3.1
1	C	444	THR	3.1
1	C	546	GLN	2.9
1	C	454	GLU	2.9
1	C	459	CYS	2.8
2	H	100(E)	CYS	2.8
3	L	60	ASP	2.7
3	L	94	SER	2.7
2	H	61	GLN	2.6
1	C	586	PHE	2.4
1	C	482	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	445	HIS	2.4
1	C	440	ALA	2.3
2	H	54	ASP	2.3
2	H	215	SER	2.2
2	H	57	THR	2.2
1	C	485	TYR	2.2
1	C	483	ARG	2.2
1	C	446	LYS	2.1
2	H	100(A)	ARG	2.1
2	H	100(D)	ARG	2.1
3	L	24	ARG	2.1
2	H	1	GLN	2.1
2	H	53	ASP	2.0
3	L	194	CYS	2.0
1	C	573	GLY	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.

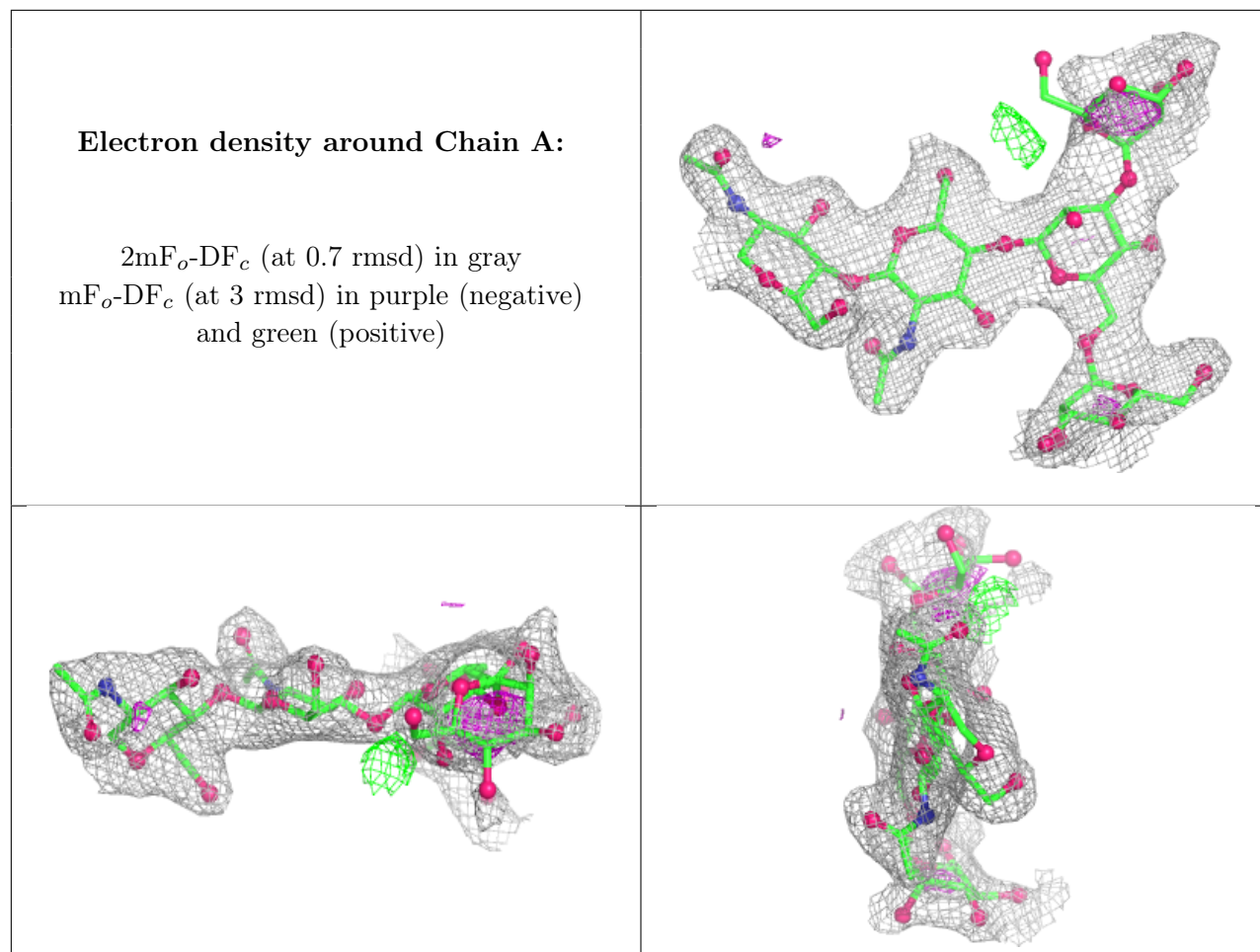
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
4	NAG	A	1	14/15	-	-	48,52,59,61	0
4	NAG	A	2	14/15	-	-	55,65,75,79	0
4	BMA	A	3	11/12	-	-	85,89,91,92	0
4	MAN	A	4	11/12	-	-	93,95,96,98	0
4	MAN	A	5	11/12	-	-	91,93,96,96	0
5	NAG	B	1	14/15	-	-	46,54,68,69	0
5	NAG	B	2	14/15	-	-	68,73,80,85	0
5	NAG	E	2	14/15	0.71	0.16	62,72,78,79	0
5	NAG	D	2	14/15	0.91	0.10	59,80,86,91	0
5	NAG	E	1	14/15	0.93	0.09	47,54,61,65	0
5	NAG	D	1	14/15	0.93	0.09	56,59,70,75	0

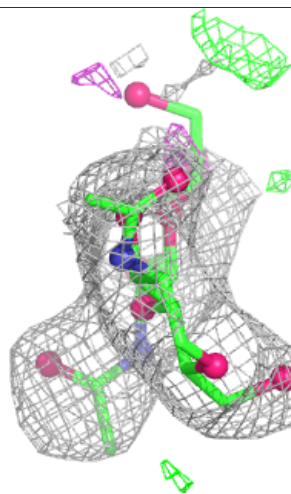
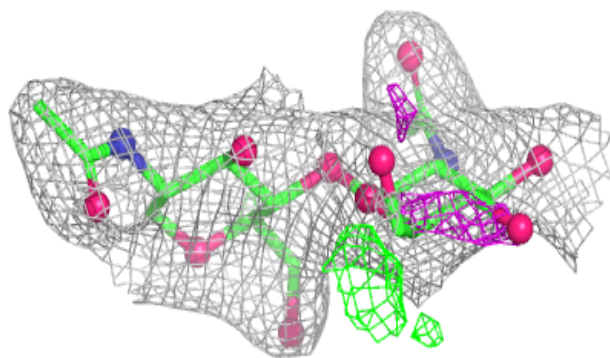
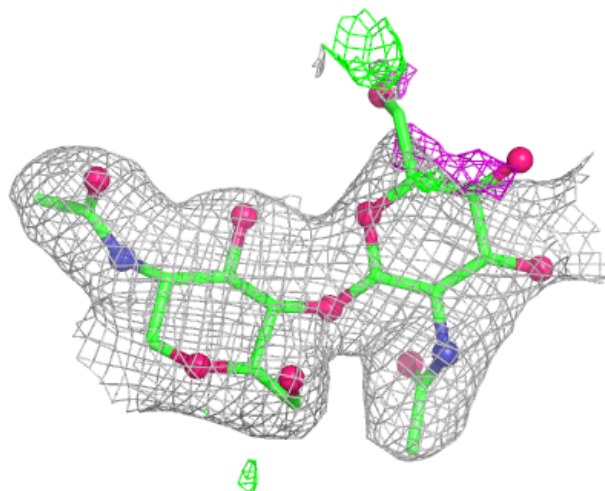
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



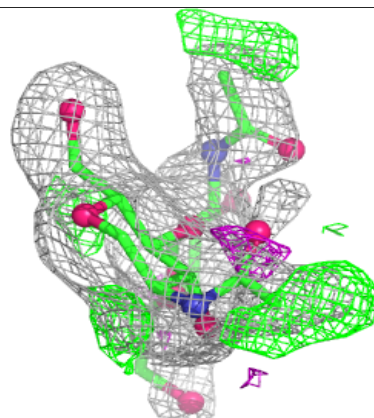
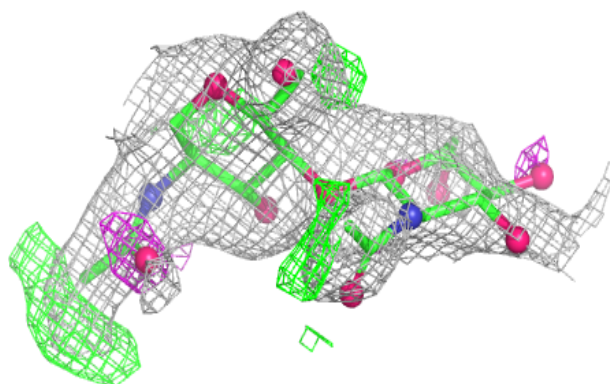
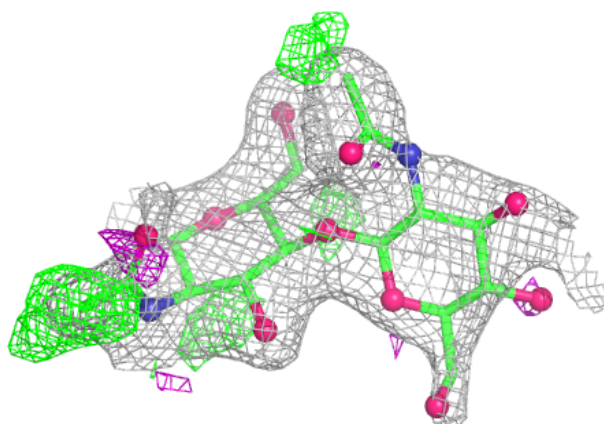
Electron density around Chain B:

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

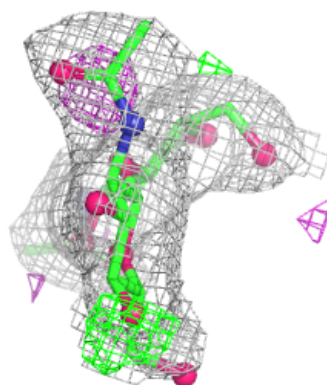
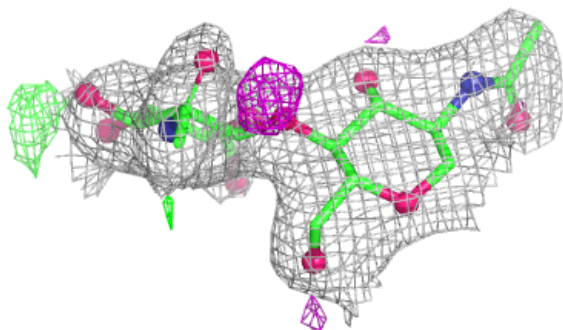
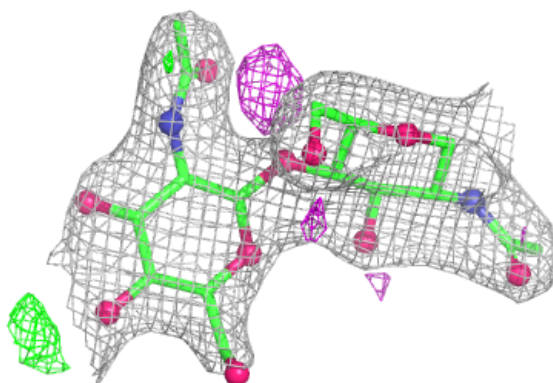


Electron density around Chain D:

$2mF_o - DF_c$ (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)



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(Å ²)	Q<0.9
6	NAG	C	702	14/15	0.67	0.18	67,77,89,95	0
6	NAG	C	701	14/15	0.69	0.15	72,76,78,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.