



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:02 PM UTC

PDB ID : 4GDJ / pdb_00004gdj
Title : A subtype N10 neuraminidase-like protein of A/little yellow-shouldered bat/
Guatemala/060/2010
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2012-07-31
Resolution : 2.00 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

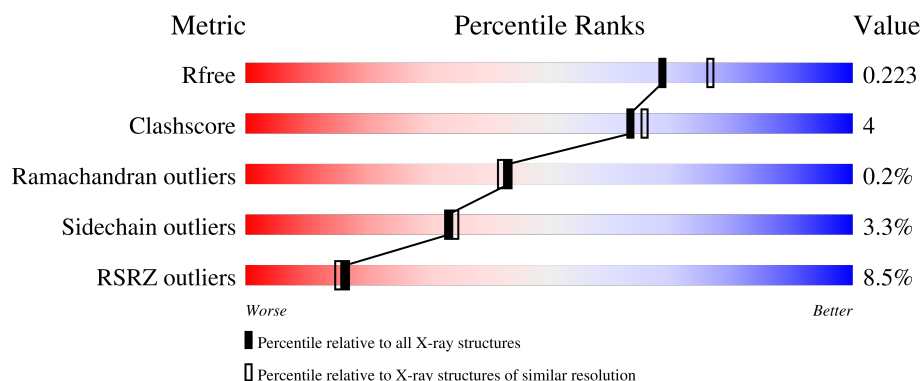
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

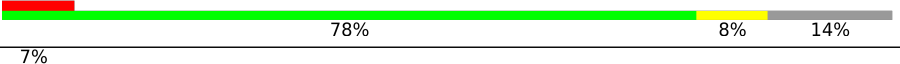
The reported resolution of this entry is 2.00 Å.

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.



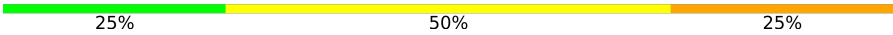
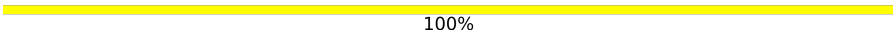
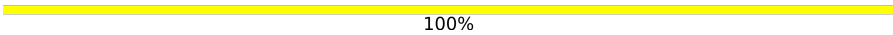
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	373	
1	B	373	
1	C	373	
1	D	373	
2	E	4	

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Mol	Chain	Length	Quality of chain
2	F	4	 25% 50% 25%
2	G	4	 100%
2	H	4	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20514 atoms, of which 9599 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.

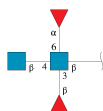
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	317	Total	C	H	N	O	S	0	0	0
			4874	1560	2396	421	479	18			
1	B	321	Total	C	H	N	O	S	0	0	0
			4942	1579	2435	426	484	18			
1	C	314	Total	C	H	N	O	S	0	0	0
			4839	1546	2383	418	474	18			
1	D	314	Total	C	H	N	O	S	0	0	0
			4841	1547	2385	418	474	17			

There are 20 discrepancies between the modelled and reference sequences:

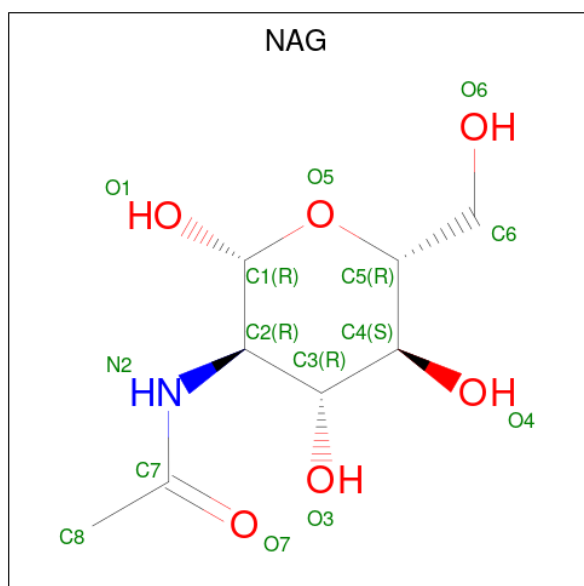
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP H6QM95
A	78	SER	-	expression tag	UNP H6QM95
A	79	PRO	-	expression tag	UNP H6QM95
A	80	SER	-	expression tag	UNP H6QM95
A	81	ARG	-	expression tag	UNP H6QM95
B	77	GLY	-	expression tag	UNP H6QM95
B	78	SER	-	expression tag	UNP H6QM95
B	79	PRO	-	expression tag	UNP H6QM95
B	80	SER	-	expression tag	UNP H6QM95
B	81	ARG	-	expression tag	UNP H6QM95
C	77	GLY	-	expression tag	UNP H6QM95
C	78	SER	-	expression tag	UNP H6QM95
C	79	PRO	-	expression tag	UNP H6QM95
C	80	SER	-	expression tag	UNP H6QM95
C	81	ARG	-	expression tag	UNP H6QM95
D	77	GLY	-	expression tag	UNP H6QM95
D	78	SER	-	expression tag	UNP H6QM95
D	79	PRO	-	expression tag	UNP H6QM95
D	80	SER	-	expression tag	UNP H6QM95
D	81	ARG	-	expression tag	UNP H6QM95

- Molecule 2 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[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
2	E	4	Total	C	N	O	0	0	0
			48	28	2	18			
2	F	4	Total	C	N	O	0	0	0
			48	28	2	18			
2	G	4	Total	C	N	O	0	0	0
			48	28	2	18			
2	H	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

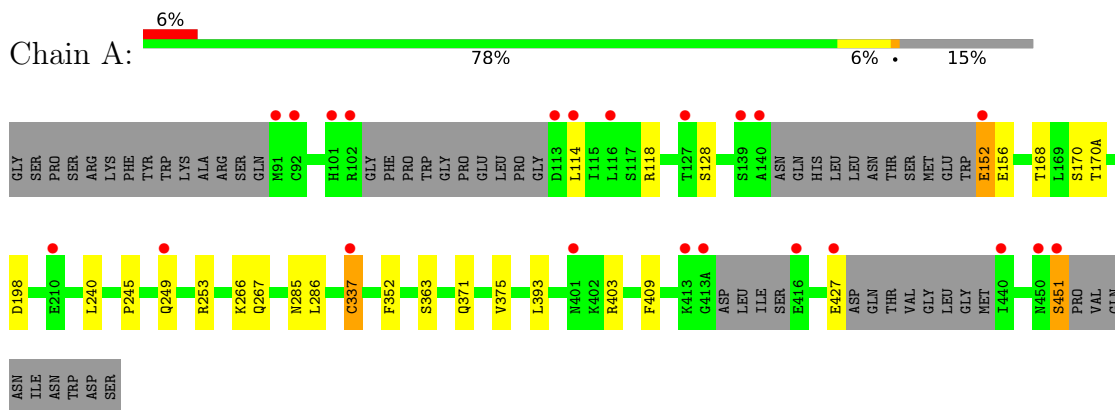
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total	O	0	0
			189	189		
5	B	195	Total	O	0	0
			195	195		
5	C	180	Total	O	0	0
			180	180		
5	D	174	Total	O	0	0
			174	174		

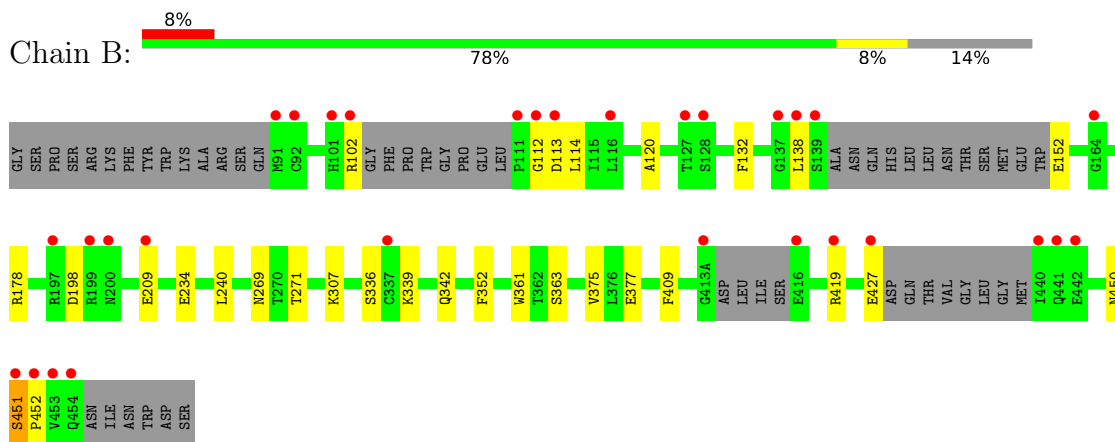
3 Residue-property plots [i](#)

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.

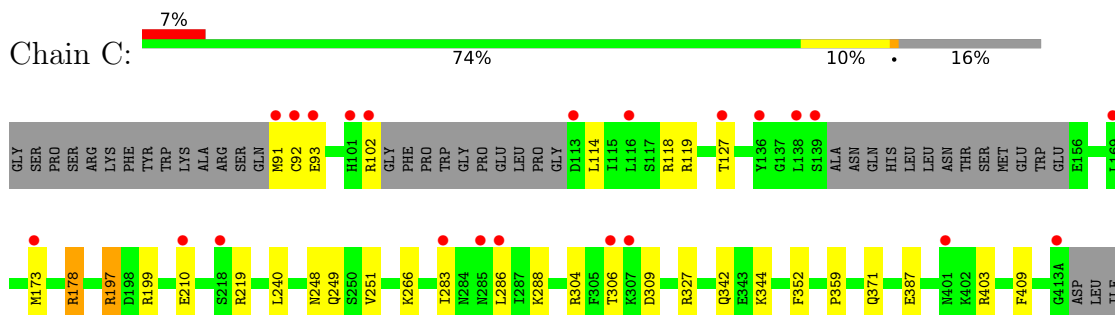
• Molecule 1: Neuraminidase

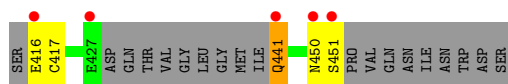


• Molecule 1: Neuraminidase

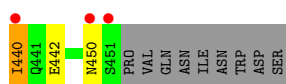
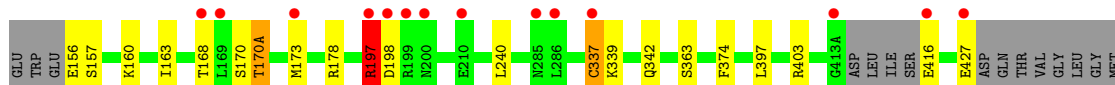
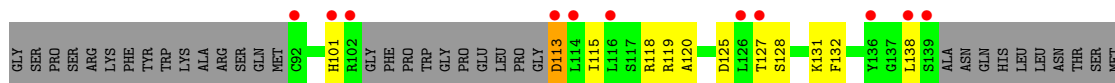
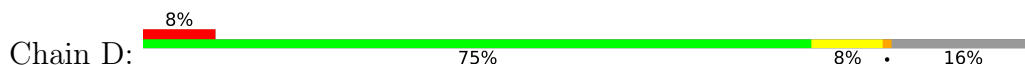


• Molecule 1: Neuraminidase





• Molecule 1: Neuraminidase



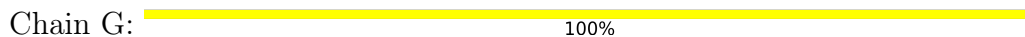
• Molecule 2: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 107.90Å 345.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.00 48.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.85-2.00) 97.7 (48.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.189 , 0.226 0.186 , 0.223	Depositor DCC
R_{free} test set	6812 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 53.1	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	0.96	EDS
Total number of atoms	20514	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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: NAG, CA, FUC, FUL

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	0.76	0/2527	0.92	4/3413 (0.1%)
1	B	0.76	0/2558	0.92	4/3456 (0.1%)
1	C	0.70	0/2505	0.93	4/3383 (0.1%)
1	D	0.70	0/2505	0.91	3/3384 (0.1%)
All	All	0.73	0/10095	0.92	15/13636 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	450	ASN	N-CA-C	8.98	122.75	110.35
1	A	337	CYS	CA-CB-SG	8.52	133.99	114.40
1	D	198	ASP	CB-CA-C	-7.03	108.48	116.63
1	A	198	ASP	CB-CA-C	-6.86	108.67	116.63
1	B	198	ASP	CB-CA-C	-6.16	109.48	116.63
1	D	197	ARG	N-CA-C	5.67	118.45	108.75
1	B	450	ASN	N-CA-C	5.65	118.79	110.59
1	A	337	CYS	CB-CA-C	5.50	120.32	110.81
1	D	450	ASN	N-CA-C	5.49	117.10	109.31
1	C	283	ILE	CB-CA-C	-5.45	103.07	110.42
1	A	337	CYS	N-CA-CB	5.36	117.96	110.56
1	C	197	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	C	178	ARG	CG-CD-NE	-5.08	100.83	112.00
1	B	451	SER	CA-C-N	-5.02	114.64	119.87
1	B	451	SER	C-N-CA	-5.02	114.64	119.87

There are no chirality outliers.

There are no planarity outliers.

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	2478	2396	2403	16	0
1	B	2507	2435	2433	15	0
1	C	2456	2383	2382	28	0
1	D	2456	2385	2384	23	0
2	E	48	0	43	0	0
2	F	48	0	43	1	0
2	G	48	0	43	0	0
2	H	48	0	43	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	189	0	0	3	0
5	B	195	0	0	1	0
5	C	180	0	0	5	0
5	D	174	0	0	2	0
All	All	10915	9599	9852	80	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 4.

All (80) 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)
1:B:178:ARG:NH1	5:B:707:HOH:O	1.59	1.32
1:A:118:ARG:NH2	1:A:156:GLU:OE2	1.97	0.96
1:C:178:ARG:CZ	1:C:197:ARG:HH12	1.79	0.96
1:B:336:SER:OG	1:B:339:LYS:HG2	1.69	0.93
1:C:306:THR:HG23	1:C:309:ASP:OD1	1.73	0.88
1:D:118:ARG:NH2	1:D:156:GLU:OE2	2.14	0.80
1:C:371:GLN:HB2	1:C:403:ARG:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:OE2	5:C:715:HOH:O	2.02	0.76
1:D:337:CYS:SG	5:D:663:HOH:O	2.43	0.76
1:B:451:SER:OG	1:B:452:PRO:HD3	1.85	0.76
1:B:451:SER:OG	1:B:452:PRO:CD	2.39	0.69
1:C:178:ARG:CZ	1:C:197:ARG:NH1	2.55	0.69
1:A:249:GLN:HG3	5:A:763:HOH:O	1.94	0.67
1:C:178:ARG:NH2	1:C:197:ARG:HH12	1.92	0.67
1:C:286:LEU:HD23	1:C:288:LYS:NZ	2.09	0.67
1:D:118:ARG:HH21	1:D:156:GLU:CD	2.03	0.66
1:D:157:SER:OG	1:D:173:MET:HE3	1.95	0.66
1:A:451:SER:O	1:A:451:SER:OG	2.07	0.66
1:C:327:ARG:O	1:C:344:LYS:HE3	1.95	0.65
1:C:93:GLU:HB2	1:C:359:PRO:HD2	1.78	0.64
1:A:427:GLU:N	1:A:427:GLU:OE1	2.31	0.64
1:B:271:THR:OG1	2:F:1:NAG:H5	1.98	0.63
1:A:118:ARG:NH2	1:A:156:GLU:CD	2.56	0.62
1:C:210:GLU:CD	5:C:715:HOH:O	2.44	0.61
1:D:403:ARG:HD3	1:D:427:GLU:CD	2.28	0.59
1:D:131:LYS:HG3	1:D:163:ILE:HD12	1.84	0.58
1:A:152:GLU:OE2	1:A:152:GLU:HA	2.04	0.57
1:A:403:ARG:O	1:A:427:GLU:OE1	2.22	0.57
1:D:197:ARG:CA	1:D:197:ARG:HE	2.18	0.54
1:B:209:GLU:H	1:B:209:GLU:CD	2.16	0.54
1:C:93:GLU:HG2	1:C:451:SER:O	2.08	0.54
1:C:118:ARG:NH1	1:C:119:ARG:HD2	2.23	0.53
1:C:288:LYS:CD	1:C:304:ARG:HG2	2.39	0.53
1:C:286:LEU:HD23	1:C:288:LYS:HZ2	1.71	0.53
1:C:441:GLN:OE1	1:C:441:GLN:HA	2.07	0.53
1:A:245:PRO:HD2	5:A:763:HOH:O	2.09	0.52
1:A:352:PHE:HB2	1:A:409:PHE:CE2	2.44	0.52
1:D:113:ASP:OD1	1:D:113:ASP:N	2.43	0.52
1:C:93:GLU:HB2	1:C:359:PRO:CD	2.41	0.51
1:B:114:LEU:O	1:B:138:LEU:HD12	2.10	0.51
1:D:440:ILE:HD11	1:D:442:GLU:OE2	2.11	0.51
1:D:440:ILE:CD1	1:D:442:GLU:OE2	2.59	0.51
1:B:209:GLU:CD	1:B:209:GLU:N	2.69	0.50
1:C:416:GLU:N	5:C:745:HOH:O	2.44	0.50
1:D:168:THR:HG22	1:D:170(A):THR:OG1	2.12	0.49
1:C:306:THR:CG2	1:C:309:ASP:OD1	2.54	0.49
1:D:118:ARG:NH1	1:D:119:ARG:HD2	2.28	0.49
1:C:91:MET:HG2	1:C:92:CYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD13	1:D:397:LEU:CD2	2.43	0.48
1:B:269:ASN:OD1	1:B:271:THR:HG23	2.14	0.48
1:C:219:ARG:HG3	1:C:251:VAL:HG21	1.95	0.47
1:C:248:ASN:OD1	1:C:249:GLN:HG3	2.14	0.47
1:C:288:LYS:HE3	1:C:304:ARG:HG2	1.97	0.47
1:C:327:ARG:C	1:C:344:LYS:HE3	2.39	0.46
1:D:197:ARG:HE	1:D:197:ARG:HA	1.78	0.46
1:D:120:ALA:HA	1:D:132:PHE:O	2.16	0.46
1:B:120:ALA:HA	1:B:132:PHE:O	2.16	0.46
1:C:199:ARG:NH1	5:C:697:HOH:O	2.49	0.46
1:A:249:GLN:CD	5:A:738:HOH:O	2.60	0.45
1:C:173:MET:HE1	5:C:743:HOH:O	2.16	0.45
1:B:113:ASP:OD1	1:B:113:ASP:N	2.46	0.45
1:C:327:ARG:O	1:C:344:LYS:CE	2.65	0.43
1:B:352:PHE:HB2	1:B:409:PHE:CE2	2.54	0.43
1:B:363:SER:HA	1:B:375:VAL:O	2.19	0.43
1:A:363:SER:HA	1:A:375:VAL:O	2.19	0.43
1:B:361:TRP:HA	1:B:377:GLU:O	2.18	0.42
1:D:115:ILE:HG13	1:D:168:THR:HA	2.00	0.42
1:B:234:GLU:OE1	1:B:307:LYS:NZ	2.41	0.42
1:D:363:SER:HB2	1:D:374:PHE:CZ	2.54	0.42
1:D:156:GLU:OE1	1:D:178:ARG:HG2	2.20	0.42
1:C:352:PHE:HB2	1:C:409:PHE:CE2	2.55	0.41
1:D:403:ARG:HD3	1:D:427:GLU:OE2	2.21	0.41
1:A:114:LEU:HD12	1:A:168:THR:HG22	2.03	0.41
1:C:178:ARG:NH2	1:C:197:ARG:NH1	2.63	0.41
1:D:339:LYS:HE3	5:D:721:HOH:O	2.20	0.41
1:A:253:ARG:HG2	1:A:267:GLN:HA	2.03	0.41
1:A:371:GLN:OE1	1:A:403:ARG:NH2	2.54	0.41
1:D:125:ASP:OD1	1:D:128:SER:N	2.50	0.41
1:D:197:ARG:HA	1:D:197:ARG:NE	2.36	0.41
1:A:393:LEU:HD13	1:D:397:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/373 (82%)	294 (96%)	12 (4%)	1 (0%)	36	35
1	B	311/373 (83%)	300 (96%)	10 (3%)	1 (0%)	36	35
1	C	304/373 (82%)	294 (97%)	10 (3%)	0	100	100
1	D	304/373 (82%)	292 (96%)	12 (4%)	0	100	100
All	All	1226/1492 (82%)	1180 (96%)	44 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	B	112	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	279/328 (85%)	270 (97%)	9 (3%)	34	35
1	B	283/328 (86%)	277 (98%)	6 (2%)	47	52
1	C	277/328 (84%)	268 (97%)	9 (3%)	34	35
1	D	277/328 (84%)	264 (95%)	13 (5%)	23	22
All	All	1116/1312 (85%)	1079 (97%)	37 (3%)	33	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	SER
1	A	152	GLU
1	A	170	SER
1	A	170(A)	THR

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	266	LYS
1	A	286	LEU
1	A	337	CYS
1	A	451	SER
1	B	102	ARG
1	B	152	GLU
1	B	240	LEU
1	B	342	GLN
1	B	419	ARG
1	B	427	GLU
1	C	102	ARG
1	C	114	LEU
1	C	127	THR
1	C	240	LEU
1	C	266	LYS
1	C	342	GLN
1	C	387	GLU
1	C	417	CYS
1	C	441	GLN
1	D	101	HIS
1	D	113	ASP
1	D	127	THR
1	D	138	LEU
1	D	160	LYS
1	D	170	SER
1	D	170(A)	THR
1	D	197	ARG
1	D	240	LEU
1	D	337	CYS
1	D	342	GLN
1	D	416	GLU
1	D	440	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	246	ASN
1	A	249	GLN
1	A	441	GLN
1	B	101	HIS

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Mol	Chain	Res	Type
1	B	167	ASN
1	B	263	GLN
1	C	246	ASN
1	C	249	GLN
1	C	258	GLN
1	C	378	GLN
1	C	450	ASN
1	D	167	ASN
1	D	342	GLN
1	D	378	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 ⓘ

16 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	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.80	0	17,19,21	1.15	1 (5%)
2	FUL	E	2	2	10,10,11	0.90	0	14,14,16	3.49	4 (28%)
2	NAG	E	3	2	14,14,15	0.46	0	17,19,21	1.00	0
2	FUC	E	4	2	10,10,11	0.77	0	14,14,16	0.99	0
2	NAG	F	1	1,2	14,14,15	0.75	0	17,19,21	1.18	2 (11%)
2	FUL	F	2	2	10,10,11	0.87	0	14,14,16	3.49	6 (42%)
2	NAG	F	3	2	14,14,15	0.64	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FUC	F	4	2	10,10,11	0.85	0	14,14,16	1.09	1 (7%)
2	NAG	G	1	1,2	14,14,15	0.58	0	17,19,21	1.40	2 (11%)
2	FUL	G	2	2	10,10,11	0.81	0	14,14,16	3.77	6 (42%)
2	NAG	G	3	2	14,14,15	0.58	0	17,19,21	1.33	4 (23%)
2	FUC	G	4	2	10,10,11	0.83	0	14,14,16	1.36	3 (21%)
2	NAG	H	1	1,2	14,14,15	0.70	0	17,19,21	1.13	2 (11%)
2	FUL	H	2	2	10,10,11	0.87	0	14,14,16	1.71	3 (21%)
2	NAG	H	3	2	14,14,15	0.60	0	17,19,21	1.15	1 (5%)
2	FUC	H	4	2	10,10,11	0.69	0	14,14,16	0.94	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	FUL	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	FUL	F	2	2	-	-	0/1/1/1
2	NAG	F	3	2	-	1/6/23/26	0/1/1/1
2	FUC	F	4	2	-	-	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	FUL	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
2	FUC	G	4	2	-	-	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	FUL	H	2	2	-	-	0/1/1/1
2	NAG	H	3	2	-	0/6/23/26	0/1/1/1
2	FUC	H	4	2	-	-	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	FUL	C1-C2-C3	-10.48	94.38	109.64
2	E	2	FUL	C1-C2-C3	-10.37	94.54	109.64
2	G	2	FUL	C1-O5-C5	-8.97	91.79	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	FUL	C1-C2-C3	-8.67	97.02	109.64
2	E	2	FUL	C1-O5-C5	-6.04	98.72	112.97
2	F	2	FUL	C1-O5-C5	-4.64	102.02	112.97
2	H	2	FUL	C1-C2-C3	-4.10	103.68	109.64
2	G	1	NAG	O3-C3-C2	-3.70	101.71	109.40
2	E	1	NAG	O3-C3-C2	-3.62	101.88	109.40
2	H	3	NAG	C1-O5-C5	3.56	116.96	112.19
2	G	2	FUL	C2-C3-C4	-3.55	104.63	110.86
2	F	2	FUL	O2-C2-C3	3.53	117.47	110.15
2	E	2	FUL	C3-C4-C5	3.35	114.91	109.81
2	H	2	FUL	O5-C1-C2	-2.75	104.22	110.79
2	G	2	FUL	O2-C2-C3	2.71	115.77	110.15
2	F	2	FUL	C3-C4-C5	2.70	113.92	109.81
2	H	1	NAG	C2-N2-C7	-2.67	119.32	122.90
2	G	4	FUC	C6-C5-C4	-2.55	108.42	113.08
2	F	2	FUL	C2-C3-C4	-2.52	106.43	110.86
2	G	3	NAG	C1-O5-C5	2.47	115.50	112.19
2	F	1	NAG	C1-O5-C5	2.47	115.49	112.19
2	G	1	NAG	C1-O5-C5	2.35	115.33	112.19
2	G	3	NAG	C3-C4-C5	2.30	114.41	110.23
2	H	1	NAG	O5-C1-C2	-2.30	107.73	111.29
2	F	1	NAG	O5-C1-C2	-2.28	107.76	111.29
2	G	3	NAG	C6-C5-C4	-2.26	107.46	113.02
2	F	4	FUC	O2-C2-C3	-2.25	105.48	110.15
2	E	2	FUL	O2-C2-C1	2.25	114.38	109.22
2	G	2	FUL	O2-C2-C1	2.22	114.31	109.22
2	G	4	FUC	O2-C2-C1	-2.20	104.18	109.22
2	G	3	NAG	O5-C5-C6	2.19	111.94	107.66
2	G	2	FUL	C3-C4-C5	2.19	113.14	109.81
2	F	2	FUL	O5-C1-C2	-2.18	105.59	110.79
2	G	4	FUC	O2-C2-C3	-2.18	105.63	110.15
2	H	4	FUC	O2-C2-C1	-2.15	104.31	109.22
2	H	2	FUL	C3-C4-C5	2.14	113.06	109.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

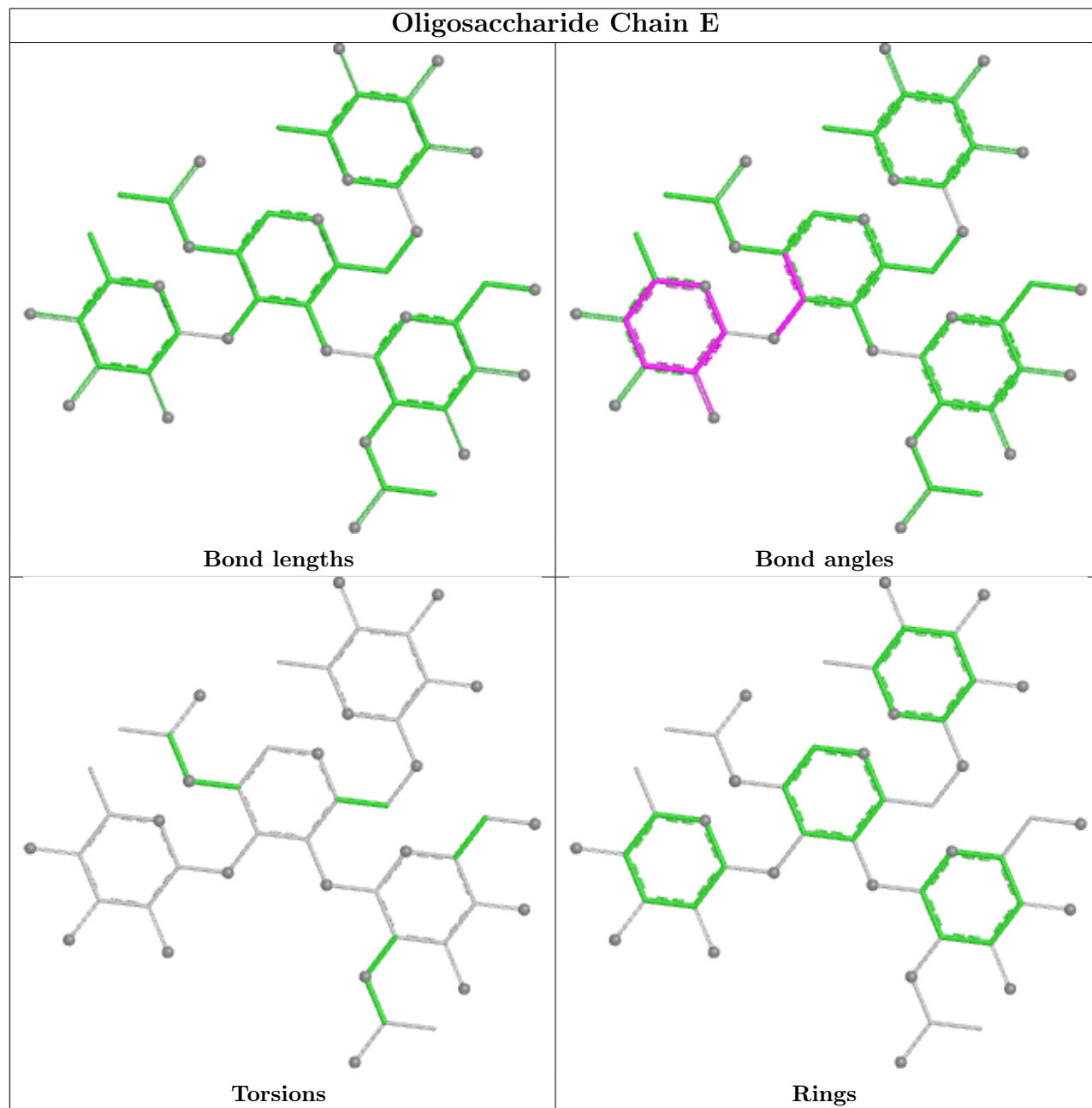
Mol	Chain	Res	Type	Atoms
2	F	3	NAG	C1-C2-N2-C7

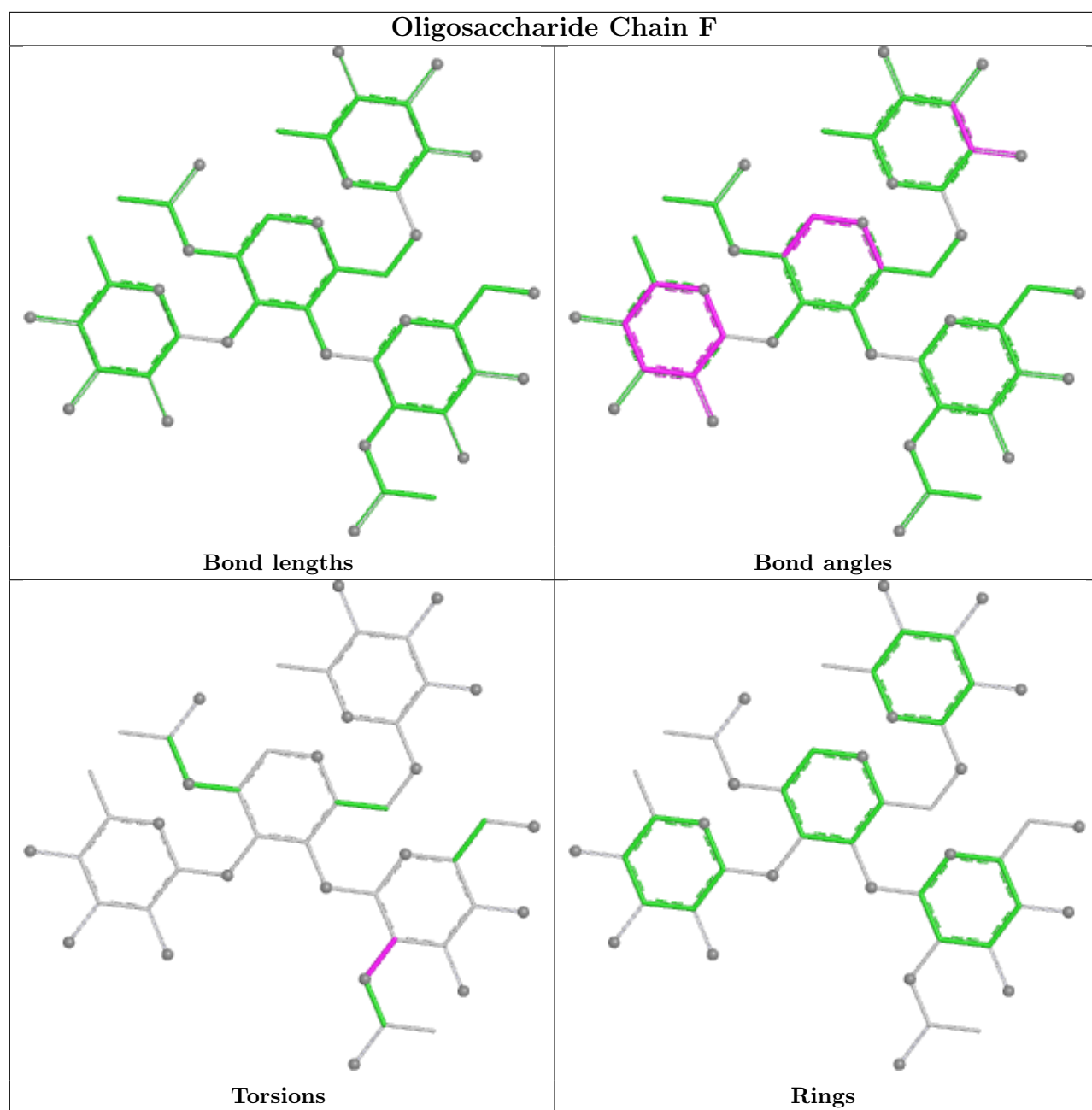
There are no ring outliers.

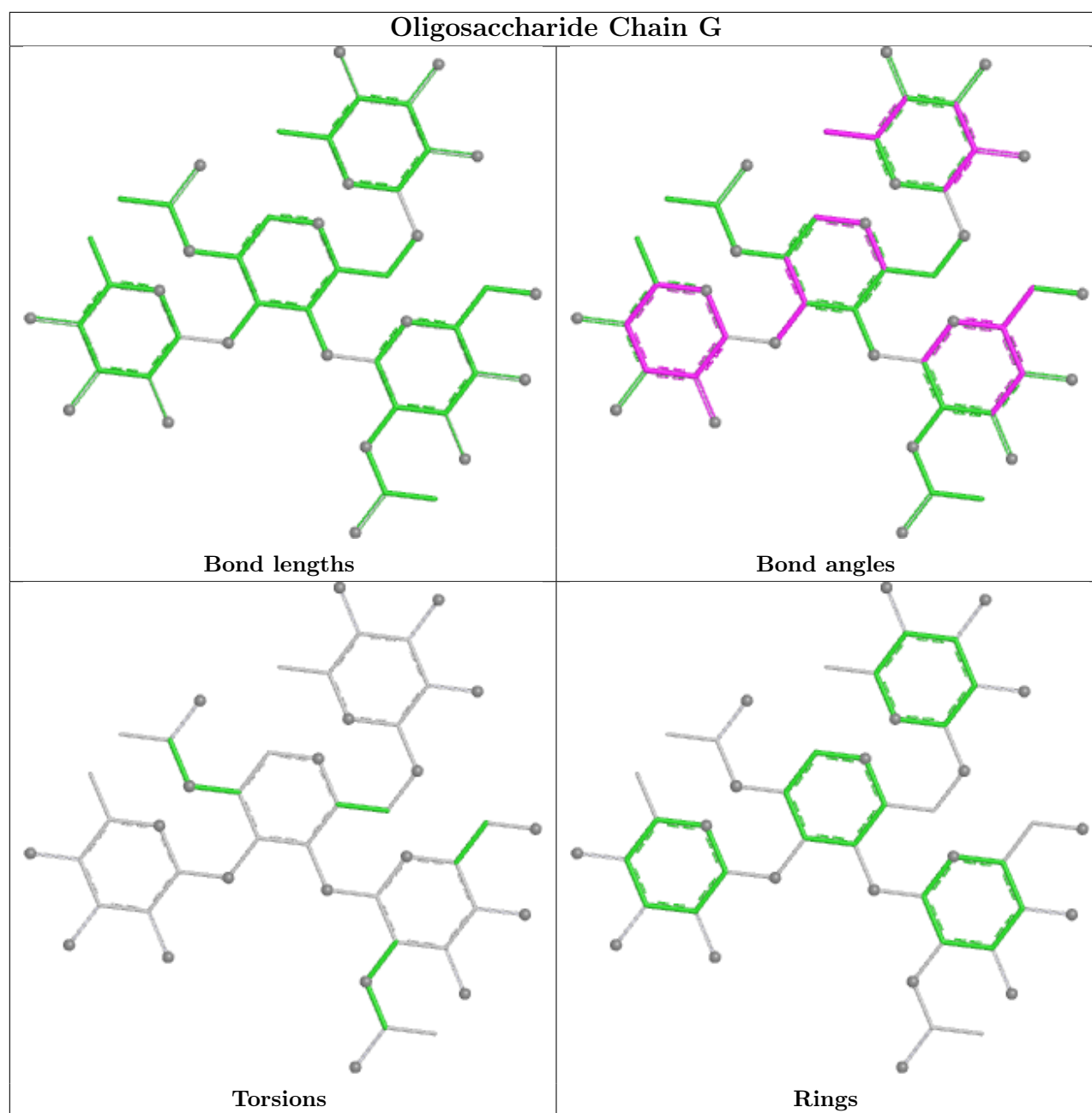
1 monomer is involved in 1 short contact:

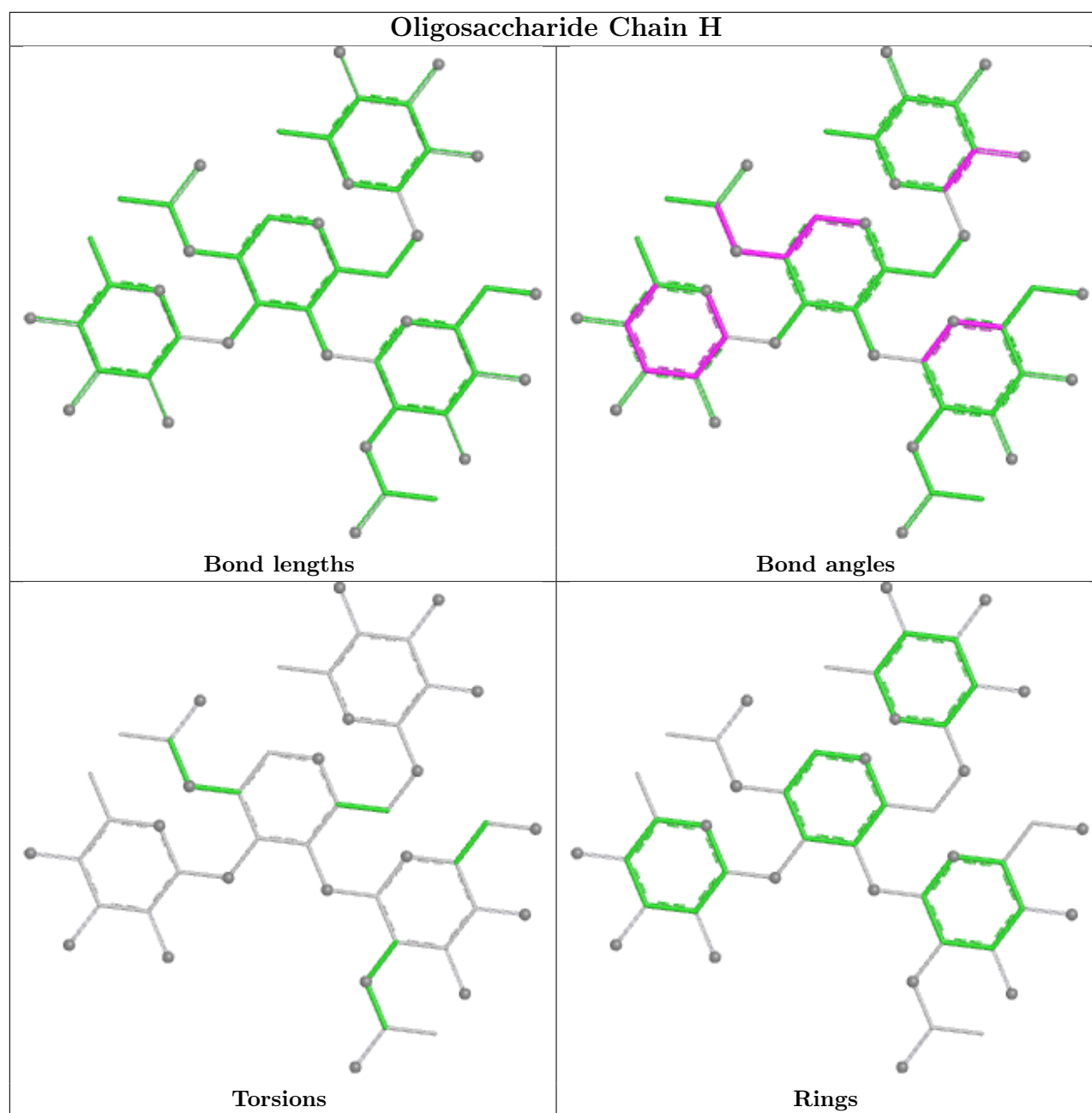
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0

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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
3	NAG	C	505	1	14,14,15	0.42	0	17,19,21	1.34	1 (5%)
3	NAG	D	505	1	14,14,15	0.55	0	17,19,21	0.87	0
3	NAG	A	505	1	14,14,15	0.56	0	17,19,21	1.19	1 (5%)
3	NAG	A	506	1	14,14,15	0.46	0	17,19,21	0.73	0
3	NAG	B	506	1	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
3	NAG	B	505	1	14,14,15	0.57	0	17,19,21	0.76	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	505	1	-	2/6/23/26	0/1/1/1
3	NAG	D	505	1	-	0/6/23/26	0/1/1/1
3	NAG	A	505	1	-	2/6/23/26	0/1/1/1
3	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	NAG	B	506	1	-	2/6/23/26	0/1/1/1
3	NAG	B	505	1	-	1/6/23/26	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(°)
3	C	505	NAG	C1-O5-C5	4.54	118.27	112.19
3	A	505	NAG	C1-O5-C5	-3.48	107.53	112.19
3	B	506	NAG	C1-O5-C5	2.98	116.18	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	505	NAG	C8-C7-N2-C2
3	C	505	NAG	O7-C7-N2-C2
3	A	505	NAG	C4-C5-C6-O6
3	B	506	NAG	C8-C7-N2-C2
3	A	505	NAG	O5-C5-C6-O6
3	B	506	NAG	O7-C7-N2-C2
3	B	505	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	317/373 (84%)	0.05	22 (6%)	23	21	20, 32, 72, 104	0
1	B	321/373 (86%)	0.09	30 (9%)	14	13	20, 33, 74, 117	0
1	C	314/373 (84%)	0.17	27 (8%)	16	15	21, 36, 74, 115	0
1	D	314/373 (84%)	0.19	28 (8%)	15	14	22, 36, 75, 115	0
All	All	1266/1492 (84%)	0.13	107 (8%)	16	15	20, 34, 74, 117	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	ILE	9.1
1	A	440	ILE	8.6
1	B	413(A)	GLY	8.0
1	C	451	SER	7.3
1	A	140	ALA	6.1
1	B	91	MET	6.0
1	D	451	SER	5.9
1	D	413(A)	GLY	5.8
1	A	413(A)	GLY	5.7
1	C	413(A)	GLY	5.7
1	D	337	CYS	5.2
1	A	451	SER	4.9
1	A	427	GLU	4.7
1	B	111	PRO	4.7
1	C	286	LEU	4.4
1	A	91	MET	4.3
1	C	91	MET	4.2
1	C	450	ASN	4.2
1	B	113	ASP	4.2
1	A	113	ASP	4.1
1	D	127	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	102	ARG	3.7
1	D	440	ILE	3.7
1	B	116	LEU	3.6
1	A	337	CYS	3.6
1	D	138	LEU	3.5
1	B	112	GLY	3.5
1	D	113	ASP	3.5
1	A	101	HIS	3.5
1	B	139	SER	3.5
1	C	113	ASP	3.5
1	D	102	ARG	3.5
1	D	139	SER	3.4
1	A	416	GLU	3.4
1	B	452	PRO	3.4
1	D	168	THR	3.4
1	D	286	LEU	3.4
1	C	92	CYS	3.3
1	B	454	GLN	3.3
1	B	101	HIS	3.3
1	D	169	LEU	3.3
1	C	101	HIS	3.3
1	D	198	ASP	3.3
1	B	416	GLU	3.2
1	D	450	ASN	3.2
1	D	136	TYR	3.2
1	D	200	ASN	3.2
1	C	401	ASN	3.2
1	D	92	CYS	3.1
1	D	116	LEU	3.1
1	C	139	SER	3.1
1	B	451	SER	3.0
1	B	442	GLU	3.0
1	D	416	GLU	2.9
1	B	427	GLU	2.9
1	D	114	LEU	2.9
1	C	218	SER	2.8
1	C	441	GLN	2.8
1	D	101	HIS	2.8
1	D	427	GLU	2.8
1	D	199	ARG	2.7
1	B	164	GLY	2.7
1	A	450	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	2.7
1	C	285	ASN	2.6
1	A	413	LYS	2.6
1	B	199	ARG	2.6
1	B	419	ARG	2.6
1	C	307	LYS	2.6
1	C	283	ILE	2.6
1	D	210	GLU	2.6
1	B	127	THR	2.5
1	C	127	THR	2.5
1	C	138	LEU	2.5
1	C	136	TYR	2.5
1	B	92	CYS	2.5
1	B	102	ARG	2.5
1	D	197	ARG	2.5
1	A	116	LEU	2.5
1	A	102	ARG	2.5
1	C	427	GLU	2.4
1	B	337	CYS	2.4
1	C	210	GLU	2.4
1	C	93	GLU	2.4
1	B	128	SER	2.3
1	A	152	GLU	2.3
1	A	127	THR	2.3
1	C	169	LEU	2.3
1	C	306	THR	2.3
1	B	197	ARG	2.2
1	D	173	MET	2.2
1	B	209	GLU	2.2
1	B	200	ASN	2.2
1	A	210	GLU	2.2
1	C	116	LEU	2.2
1	A	249	GLN	2.1
1	B	137	GLY	2.1
1	A	114	LEU	2.1
1	C	416	GLU	2.1
1	B	453	VAL	2.1
1	A	92	CYS	2.1
1	A	401	ASN	2.1
1	D	285	ASN	2.1
1	C	173	MET	2.0
1	D	126	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	441	GLN	2.0
1	A	139	SER	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](#)

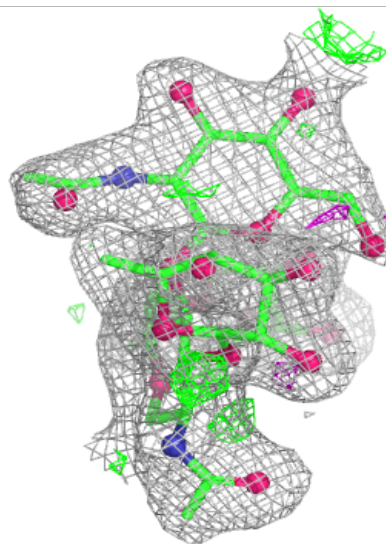
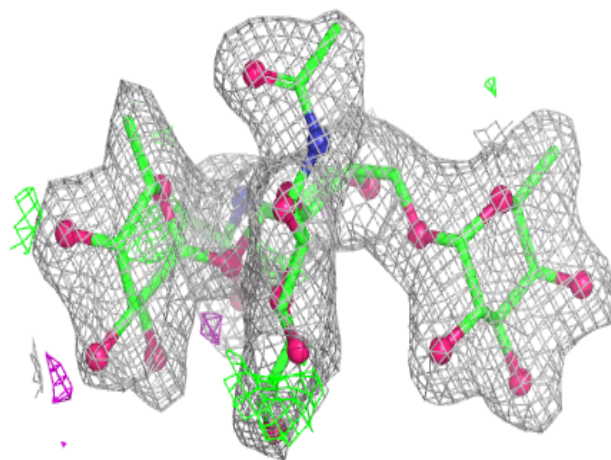
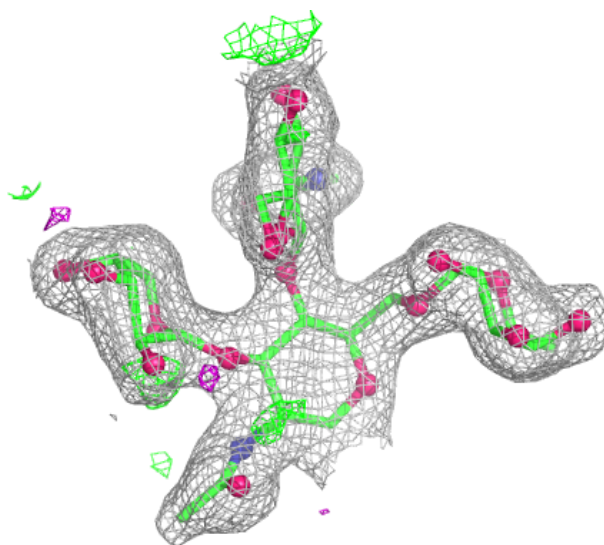
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUL	H	2	10/11	0.84	0.23	47,56,79,92	0
2	FUL	F	2	10/11	0.86	0.17	42,52,62,66	0
2	NAG	G	3	14/15	0.86	0.16	47,57,73,83	0
2	FUL	E	2	10/11	0.86	0.16	43,50,53,55	0
2	NAG	H	3	14/15	0.87	0.15	53,60,75,88	0
2	NAG	F	3	14/15	0.89	0.16	41,57,69,84	0
2	FUL	G	2	10/11	0.90	0.13	36,43,57,58	0
2	NAG	E	3	14/15	0.91	0.12	28,49,62,87	0
2	NAG	F	1	14/15	0.93	0.10	26,42,46,49	0
2	NAG	H	1	14/15	0.93	0.10	33,46,52,57	0
2	FUC	F	4	10/11	0.93	0.09	29,36,44,51	0
2	NAG	E	1	14/15	0.93	0.10	32,39,48,48	0
2	FUC	E	4	10/11	0.94	0.10	35,41,45,46	0
2	NAG	G	1	14/15	0.94	0.09	31,36,46,48	0
2	FUC	G	4	10/11	0.94	0.08	32,36,39,41	0
2	FUC	H	4	10/11	0.95	0.09	33,36,43,45	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.

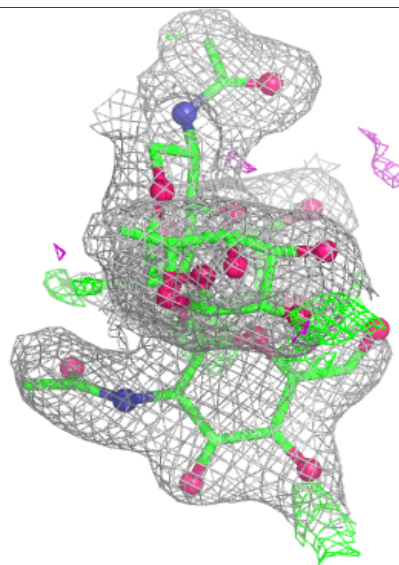
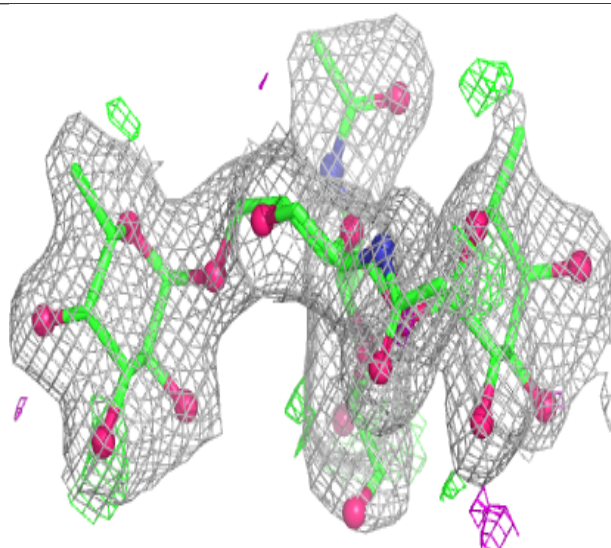
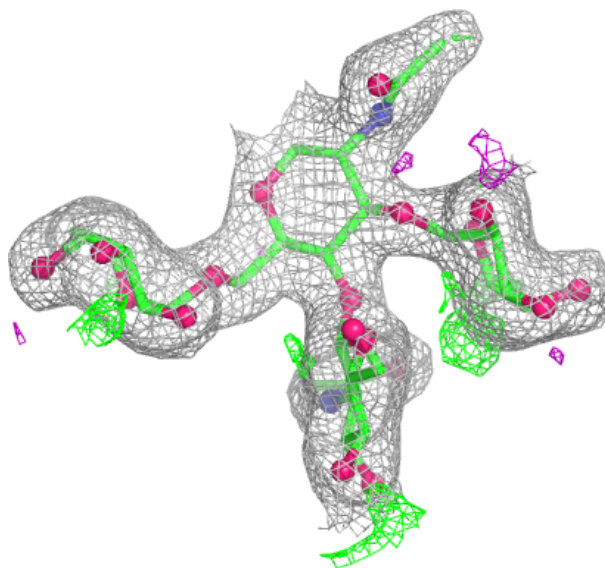
Electron density around Chain E:

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



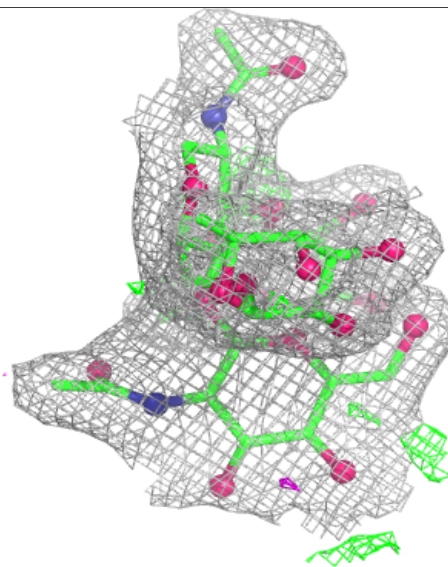
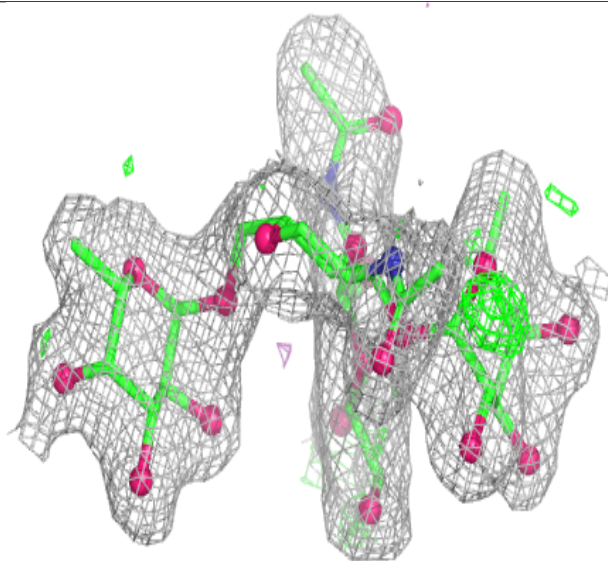
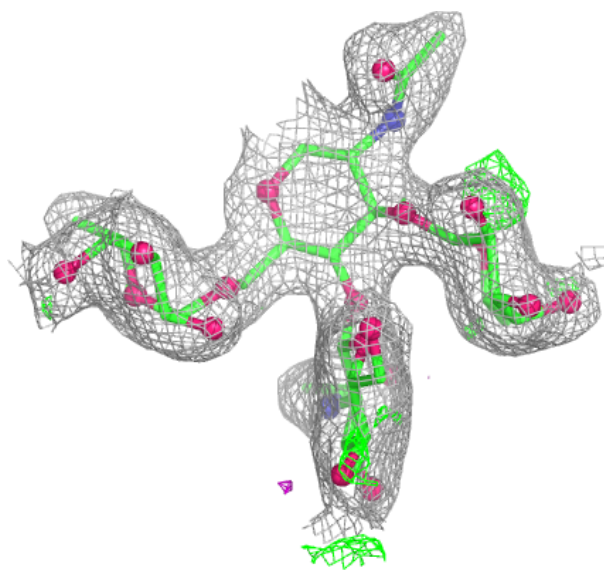
Electron density around Chain F:

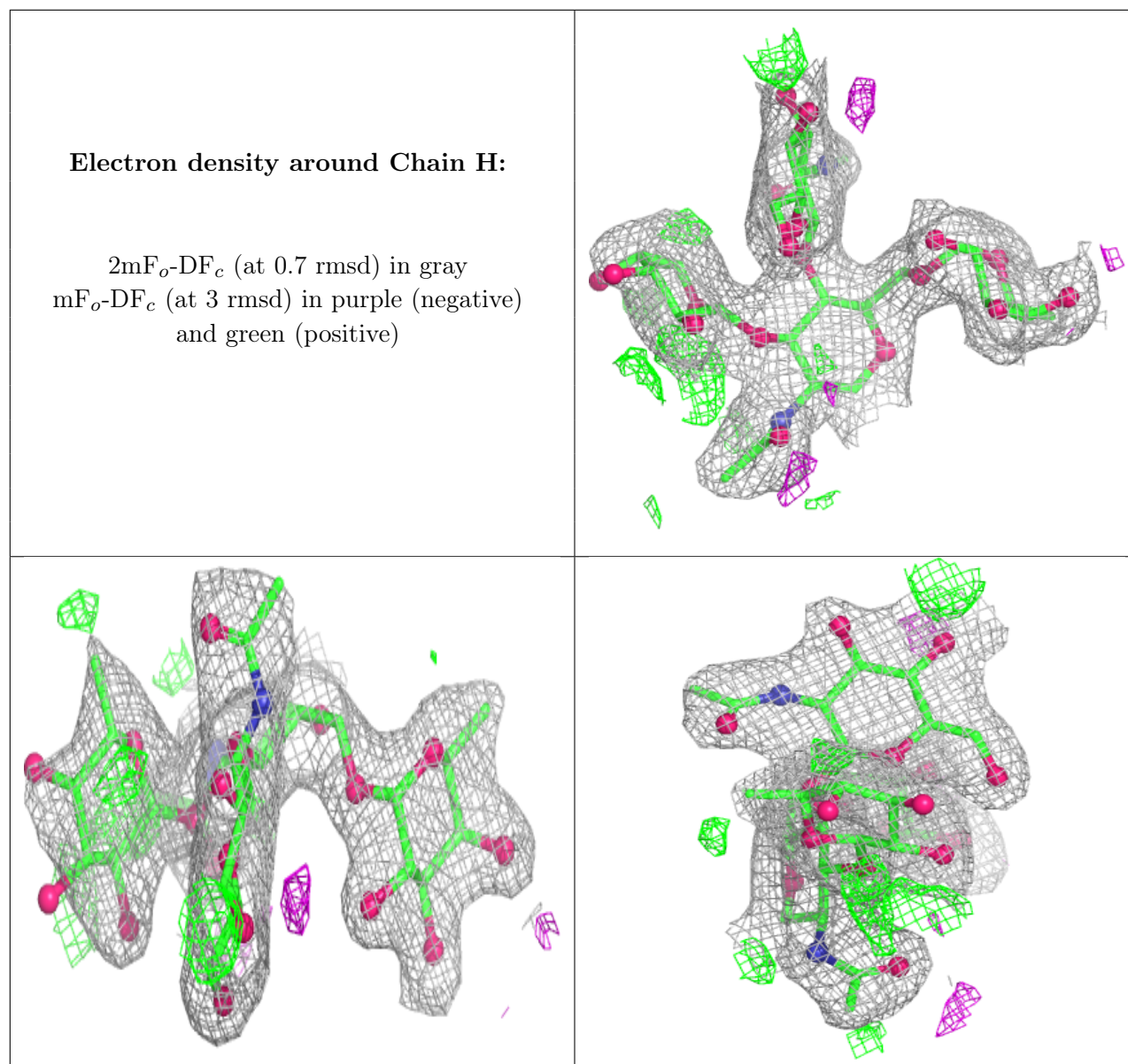
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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
3	NAG	B	506	14/15	0.60	0.23	72,85,96,99	0
3	NAG	C	505	14/15	0.72	0.21	73,84,92,102	0
3	NAG	D	505	14/15	0.74	0.19	67,81,86,90	0
3	NAG	A	505	14/15	0.76	0.21	68,86,96,97	0
3	NAG	B	505	14/15	0.79	0.22	76,88,100,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	506	14/15	0.81	0.21	71,84,95,103	0
4	CA	A	507	1/1	1.00	0.01	23,23,23,23	0
4	CA	B	507	1/1	1.00	0.02	22,22,22,22	0
4	CA	C	506	1/1	1.00	0.03	25,25,25,25	0
4	CA	D	506	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.