



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 8WSP / pdb_00008wsp
Title : Crystal structure of SFTSV Gn and antibody SF5
Authors : Chang, Z.; Gao, F.; Wu, Y.
Deposited on : 2023-10-17
Resolution : 2.51 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

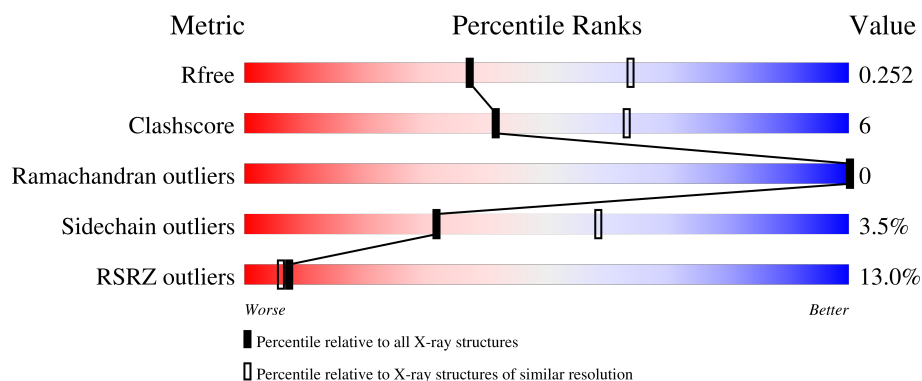
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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.



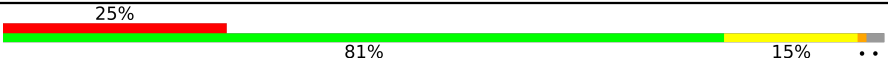
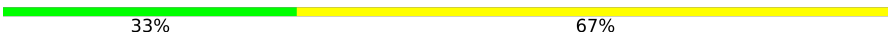
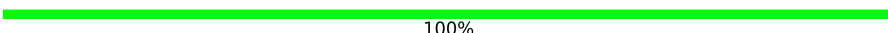
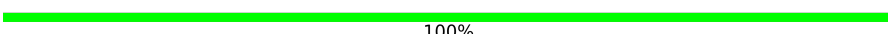
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	331	3% 86% 10% .
1	D	331	2% 81% 14% 5%
2	B	228	17% 78% 16% 5%
2	E	228	19% 77% 15% 7%
3	C	214	19% 83% 13% ...

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Mol	Chain	Length	Quality of chain
3	F	214	
4	G	3	
4	I	3	
5	H	2	
5	J	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11994 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 Gn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2445	1530	421	468	26			
1	D	316	Total	C	N	O	S	0	0	0
			2432	1523	418	465	26			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASP	-	expression tag	UNP F1BDJ0
A	17	GLY	-	expression tag	UNP F1BDJ0
A	18	ILE	-	expression tag	UNP F1BDJ0
A	19	GLN	-	expression tag	UNP F1BDJ0
A	341	HIS	-	expression tag	UNP F1BDJ0
A	342	HIS	-	expression tag	UNP F1BDJ0
A	343	HIS	-	expression tag	UNP F1BDJ0
A	344	HIS	-	expression tag	UNP F1BDJ0
A	345	HIS	-	expression tag	UNP F1BDJ0
A	346	HIS	-	expression tag	UNP F1BDJ0
D	16	ASP	-	expression tag	UNP F1BDJ0
D	17	GLY	-	expression tag	UNP F1BDJ0
D	18	ILE	-	expression tag	UNP F1BDJ0
D	19	GLN	-	expression tag	UNP F1BDJ0
D	341	HIS	-	expression tag	UNP F1BDJ0
D	342	HIS	-	expression tag	UNP F1BDJ0
D	343	HIS	-	expression tag	UNP F1BDJ0
D	344	HIS	-	expression tag	UNP F1BDJ0
D	345	HIS	-	expression tag	UNP F1BDJ0
D	346	HIS	-	expression tag	UNP F1BDJ0

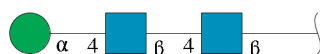
- Molecule 2 is a protein called Ab5-H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1630	1036	273	315	6			
2	E	212	Total	C	N	O	S	0	0	0
			1599	1015	268	310	6			

- Molecule 3 is a protein called Ab5-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1569	975	268	322	4			
3	F	209	Total	C	N	O	S	0	0	0
			1563	972	267	320	4			

- Molecule 4 is an oligosaccharide called alpha-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	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

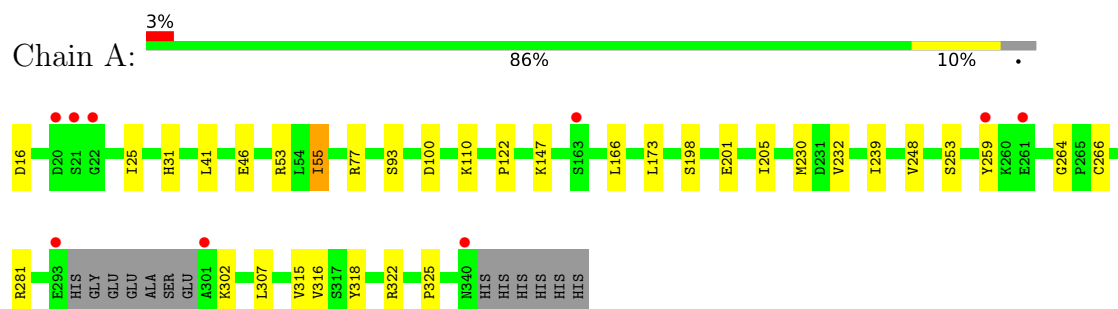
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	154	Total 154	O 154	0	0
6	B	58	Total 58	O 58	0	0
6	C	62	Total 62	O 62	0	0
6	D	204	Total 204	O 204	0	0
6	E	70	Total 70	O 70	0	0
6	F	74	Total 74	O 74	0	0

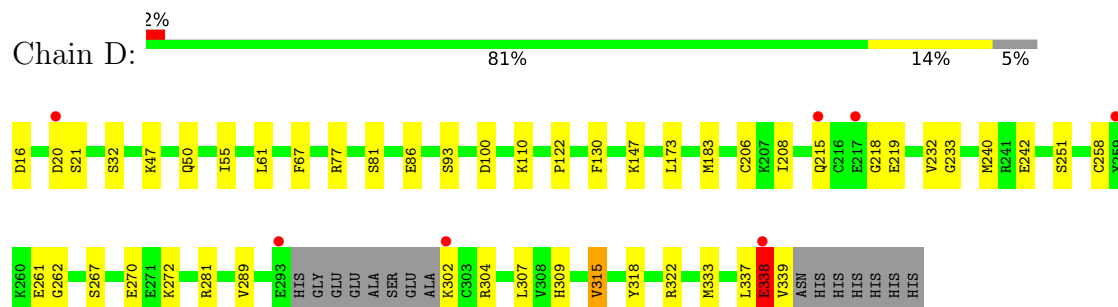
3 Residue-property plots [i](#)

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.

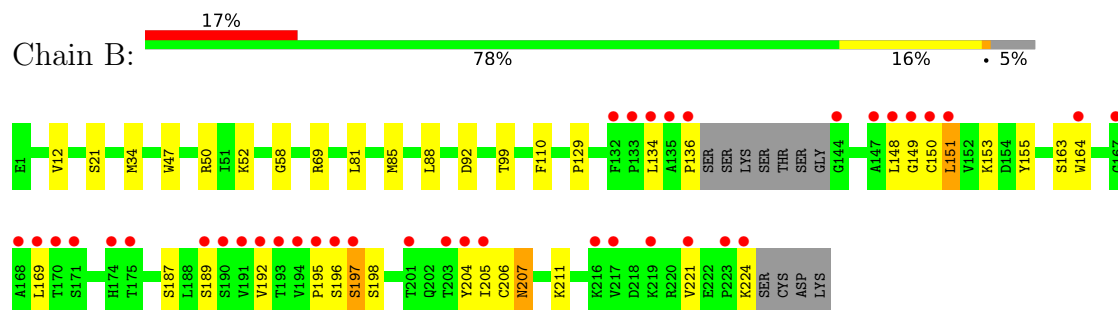
• Molecule 1: Gn



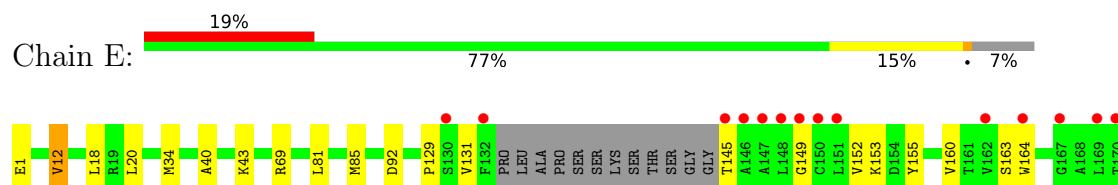
• Molecule 1: Gn

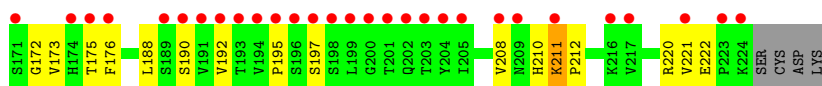


• Molecule 2: Ab5-H

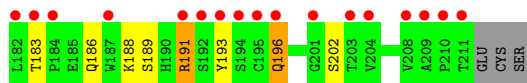
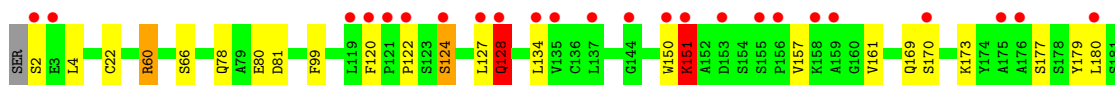
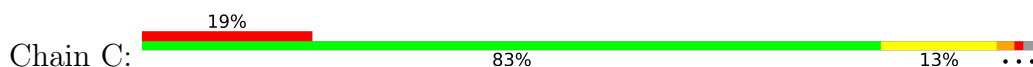


• Molecule 2: Ab5-H

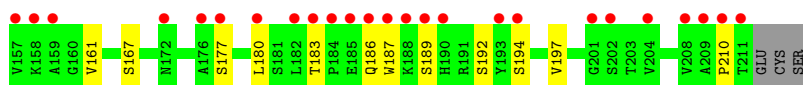
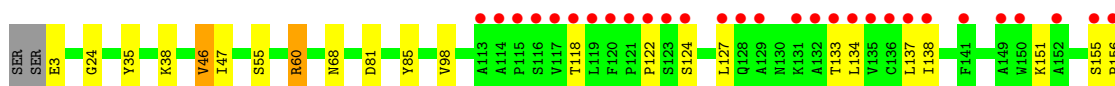
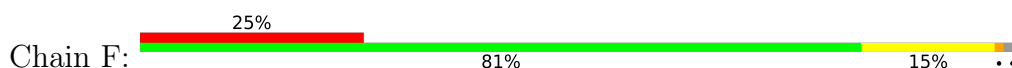




• Molecule 3: Ab5-L



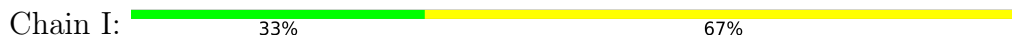
• Molecule 3: Ab5-L



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



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



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



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

Chain J:

100%

3MG1
3MG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.88Å 111.33Å 191.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 2.51 48.01 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.01-2.51) 98.4 (48.01-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.243 (Not available) , 0.252	Depositor DCC
R_{free} test set	3472 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11994	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5034e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, 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	0.41	0/2505	0.61	0/3377
1	D	0.45	0/2492	0.67	3/3359 (0.1%)
2	B	0.35	0/1671	0.62	3/2277 (0.1%)
2	E	0.37	0/1638	0.59	1/2230 (0.0%)
3	C	0.48	1/1605 (0.1%)	0.74	5/2191 (0.2%)
3	F	0.34	0/1599	0.56	0/2183
All	All	0.41	1/11510 (0.0%)	0.64	12/15617 (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	B	0	2
3	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	128	GLN	CD-OE1	5.22	1.33	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	196	GLN	CA-CB-CG	10.14	134.38	114.10
1	D	337	LEU	CA-C-N	-9.22	106.21	123.27
1	D	337	LEU	C-N-CA	-9.22	106.21	123.27
3	C	128	GLN	CB-CA-C	-7.08	96.32	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	151	LYS	CG-CD-CE	-7.05	95.08	111.30
2	B	151	LEU	CB-CG-CD1	-6.52	91.14	110.70
3	C	196	GLN	N-CA-CB	5.88	120.23	110.47
1	D	338	GLU	CA-CB-CG	5.79	125.68	114.10
2	B	150	CYS	CA-C-N	-5.46	115.31	123.00
2	B	150	CYS	C-N-CA	-5.46	115.31	123.00
2	E	211	LYS	CA-CB-CG	5.36	124.81	114.10
3	C	196	GLN	CB-CA-C	-5.28	102.19	110.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	196	SER	Peptide
2	B	197	SER	Peptide
3	C	128	GLN	Sidechain

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	A	2445	0	2343	18	0
1	D	2432	0	2332	30	0
2	B	1630	0	1607	24	0
2	E	1599	0	1574	23	0
3	C	1569	0	1513	28	0
3	F	1563	0	1508	22	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0
5	H	28	0	25	0	0
5	J	28	0	25	0	0
6	A	154	0	0	1	0
6	B	58	0	0	0	0
6	C	62	0	0	1	0
6	D	204	0	0	4	0
6	E	70	0	0	0	0
6	F	74	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11994	0	10995	142	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 6.

All (142) 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:C:128:GLN:HE21	3:C:128:GLN:HA	1.38	0.88
3:C:151:LYS:HG3	3:C:196:GLN:NE2	1.91	0.85
3:C:99:PHE:O	6:C:301:HOH:O	1.98	0.82
2:B:195:PRO:HB2	2:B:197:SER:HB3	1.63	0.81
2:B:151:LEU:C	2:B:151:LEU:HD12	2.07	0.79
3:C:60:ARG:NH2	3:C:81:ASP:OD2	2.15	0.79
2:E:69:ARG:NH2	2:E:92:ASP:OD2	2.17	0.76
2:B:69:ARG:NH2	2:B:92:ASP:OD2	2.18	0.75
3:F:124:SER:HA	3:F:127:LEU:HD12	1.70	0.74
1:A:230:MET:HE1	1:A:316:VAL:HB	1.71	0.72
1:D:215:GLN:NE2	6:D:401:HOH:O	2.23	0.69
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.25	0.69
3:C:122:PRO:HD3	3:C:134:LEU:HD23	1.74	0.68
1:A:77:ARG:NH2	1:A:93:SER:O	2.22	0.68
2:E:152:VAL:HB	2:E:188:LEU:HD23	1.78	0.66
1:A:31:HIS:HB2	1:A:166:LEU:HD22	1.79	0.65
3:F:46:VAL:HG12	3:F:47:ILE:HG12	1.79	0.65
2:B:12:VAL:HG11	2:B:88:LEU:HD13	1.79	0.64
2:E:210:HIS:CD2	2:E:212:PRO:HD2	2.34	0.63
2:B:129:PRO:HB3	2:B:155:TYR:HB3	1.79	0.63
3:C:186:GLN:HA	3:C:189:SER:HB3	1.81	0.63
2:E:129:PRO:HB3	2:E:155:TYR:HB3	1.81	0.62
3:F:134:LEU:HD12	3:F:180:LEU:HB3	1.81	0.61
1:D:338:GLU:HG2	1:D:339:VAL:N	2.16	0.61
3:C:188:LYS:O	3:C:191:ARG:NH2	2.33	0.61
1:D:206:CYS:SG	1:D:338:GLU:HB3	2.41	0.59
1:D:208:ILE:HG21	1:D:333:MET:HE3	1.84	0.59
1:D:77:ARG:NH2	1:D:93:SER:O	2.33	0.58
3:C:150:TRP:C	3:C:151:LYS:HG2	2.29	0.58
1:A:259:TYR:CZ	1:A:264:GLY:HA2	2.40	0.57
3:C:124:SER:HA	3:C:127:LEU:HD12	1.87	0.57
2:E:210:HIS:HD2	2:E:212:PRO:HD2	1.69	0.57
3:F:24:GLY:O	3:F:68:ASN:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:38:LYS:NZ	6:F:301:HOH:O	2.37	0.57
3:C:78:GLN:HB3	3:C:80:GLU:OE1	2.05	0.57
3:F:3:GLU:HB3	3:F:98:VAL:HG11	1.87	0.56
1:A:230:MET:HG3	1:A:232:VAL:HG13	1.87	0.56
3:C:60:ARG:HH22	3:C:81:ASP:CG	2.12	0.56
1:D:315:VAL:CG1	1:D:322:ARG:HD3	2.36	0.56
2:B:204:TYR:HB2	2:B:221:VAL:HG22	1.87	0.56
1:D:315:VAL:HG11	1:D:322:ARG:HD3	1.86	0.56
2:B:204:TYR:HB2	2:B:221:VAL:CG2	2.36	0.55
3:C:157:VAL:HG11	3:C:180:LEU:HD21	1.89	0.55
2:B:195:PRO:C	2:B:197:SER:H	2.13	0.55
1:D:281:ARG:HE	1:D:302:LYS:HB2	1.72	0.55
3:C:151:LYS:CD	3:C:196:GLN:HE22	2.20	0.55
2:E:34:MET:HB3	2:E:81:LEU:HD22	1.89	0.54
3:C:151:LYS:CG	3:C:196:GLN:NE2	2.68	0.54
1:D:16:ASP:HB2	1:D:307:LEU:HD13	1.89	0.54
1:D:183:MET:HE1	1:D:232:VAL:C	2.33	0.54
1:D:218:GLY:O	1:D:338:GLU:HB2	2.08	0.53
3:F:122:PRO:HB2	3:F:127:LEU:HD21	1.91	0.53
2:E:69:ARG:HH22	2:E:92:ASP:CG	2.17	0.53
3:C:151:LYS:HE2	3:C:196:GLN:HE22	1.75	0.52
2:E:40:ALA:HB3	2:E:43:LYS:HD2	1.91	0.51
1:D:86:GLU:HG3	6:F:356:HOH:O	2.09	0.51
2:B:34:MET:HB3	2:B:81:LEU:HD22	1.92	0.51
1:D:47:LYS:HA	1:D:50:GLN:HE21	1.75	0.51
1:D:77:ARG:NH1	1:D:100:ASP:OD2	2.41	0.51
1:D:242:GLU:HA	6:D:520:HOH:O	2.10	0.51
2:B:134:LEU:HB3	3:C:120:PHE:CD1	2.45	0.51
3:F:161:VAL:HG22	3:F:180:LEU:HD13	1.91	0.51
1:D:267:SER:OG	1:D:270:GLU:HG3	2.10	0.51
1:D:20:ASP:HB2	1:D:309:HIS:CG	2.46	0.50
3:C:4:LEU:HB3	3:C:22:CYS:SG	2.52	0.49
1:A:16:ASP:HB2	1:A:307:LEU:HD13	1.94	0.49
3:F:186:GLN:HA	3:F:189:SER:OG	2.13	0.49
2:B:47:TRP:HZ2	2:B:50:ARG:HG2	1.77	0.49
3:C:128:GLN:HA	3:C:128:GLN:NE2	2.17	0.49
2:E:195:PRO:C	2:E:197:SER:H	2.20	0.49
2:E:173:VAL:HG12	2:E:192:VAL:HG22	1.95	0.49
1:A:230:MET:HE2	1:A:325:PRO:HB3	1.94	0.49
1:A:198:SER:OG	1:A:239:ILE:O	2.28	0.48
3:C:151:LYS:CG	3:C:196:GLN:HE22	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HE3	6:A:487:HOH:O	2.13	0.48
2:E:12:VAL:CG2	2:E:18:LEU:HD22	2.43	0.48
2:E:149:GLY:HA2	2:E:164:TRP:CH2	2.49	0.48
1:D:338:GLU:CG	1:D:339:VAL:H	2.28	0.47
2:E:172:GLY:O	2:E:192:VAL:HA	2.13	0.47
2:B:195:PRO:C	2:B:197:SER:N	2.73	0.47
1:D:147:LYS:NZ	6:D:411:HOH:O	2.47	0.47
3:F:151:LYS:HB2	3:F:194:SER:HB2	1.96	0.47
2:E:220:ARG:CZ	2:E:222:GLU:HG2	2.44	0.47
1:D:130:PHE:HA	1:D:173:LEU:O	2.14	0.47
2:E:131:VAL:HG11	2:E:208:VAL:HG21	1.97	0.47
2:E:18:LEU:HB3	2:E:85:MET:HE3	1.96	0.47
2:E:149:GLY:HA2	2:E:164:TRP:HH2	1.79	0.47
1:D:77:ARG:HB3	6:D:446:HOH:O	2.15	0.47
3:F:151:LYS:HA	3:F:151:LYS:HE2	1.97	0.47
3:C:151:LYS:O	3:C:193:TYR:HA	2.16	0.46
3:C:128:GLN:HE21	3:C:128:GLN:CA	2.19	0.46
3:F:183:THR:OG1	3:F:186:GLN:HG3	2.16	0.46
2:B:149:GLY:HA2	2:B:164:TRP:CZ2	2.51	0.46
2:E:160:VAL:HG22	2:E:210:HIS:HB2	1.98	0.46
1:A:281:ARG:HD3	1:A:302:LYS:HB2	1.98	0.45
1:A:315:VAL:HG11	1:A:322:ARG:HD3	1.97	0.45
2:B:85:MET:HB3	2:B:88:LEU:HD21	1.98	0.45
3:F:151:LYS:N	3:F:194:SER:O	2.42	0.45
2:E:12:VAL:HG21	2:E:18:LEU:HD22	1.98	0.45
2:B:153:LYS:HA	2:B:187:SER:OG	2.16	0.45
3:C:151:LYS:CE	3:C:196:GLN:HE22	2.29	0.45
1:D:122:PRO:HB3	1:D:173:LEU:HD21	1.98	0.45
1:D:258:CYS:HA	1:D:304:ARG:O	2.17	0.45
1:D:261:GLU:OE1	1:D:262:GLY:N	2.50	0.45
2:E:175:THR:HG22	2:E:190:SER:OG	2.16	0.45
1:D:110:LYS:HB2	1:D:110:LYS:HE2	1.64	0.44
1:A:77:ARG:NH1	1:A:100:ASP:OD2	2.50	0.44
3:C:122:PRO:HD3	3:C:134:LEU:CD2	2.46	0.44
2:B:52:LYS:O	2:B:58:GLY:HA2	2.18	0.44
2:B:136:PRO:HD3	2:B:148:LEU:HB3	1.99	0.44
3:C:151:LYS:HG2	3:C:151:LYS:HZ3	1.52	0.44
1:A:201:GLU:OE1	1:A:318:TYR:OH	2.36	0.44
1:A:53:ARG:HB2	1:A:55:ILE:HD12	1.98	0.44
3:C:161:VAL:HA	3:C:179:TYR:O	2.18	0.44
2:E:153:LYS:NZ	3:F:133:THR:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:GLU:H	3:C:80:GLU:CD	2.26	0.43
1:D:183:MET:HE1	1:D:233:GLY:N	2.34	0.43
1:A:25:ILE:HG12	1:A:259:TYR:CD1	2.54	0.43
3:C:169:GLN:HG3	3:C:173:LYS:O	2.18	0.43
1:D:218:GLY:O	1:D:338:GLU:HG3	2.19	0.43
3:F:35:TYR:O	3:F:85:TYR:HA	2.18	0.43
3:F:138:ILE:HG12	3:F:197:VAL:HG11	2.01	0.43
1:A:110:LYS:HB2	1:A:110:LYS:HE2	1.84	0.42
3:F:60:ARG:H	3:F:60:ARG:HG3	1.57	0.42
2:B:163:SER:OG	2:B:207:ASN:OD1	2.37	0.42
2:B:198:SER:O	2:B:198:SER:OG	2.35	0.42
1:A:122:PRO:HB3	1:A:173:LEU:HD21	2.01	0.42
3:F:187:TRP:O	3:F:210:PRO:HG3	2.19	0.42
2:B:149:GLY:HA2	2:B:164:TRP:CH2	2.53	0.42
2:B:169:LEU:HD12	2:B:169:LEU:HA	1.91	0.41
3:F:155:SER:HA	3:F:156:PRO:HD3	1.96	0.41
3:F:167:SER:HB2	6:F:304:HOH:O	2.20	0.41
2:E:20:LEU:HG	2:E:85:MET:HE2	2.01	0.41
2:B:99:THR:OG1	2:B:110:PHE:HB3	2.20	0.41
3:C:150:TRP:CD1	3:C:161:VAL:HG21	2.55	0.41
1:A:41:LEU:HD13	1:A:46:GLU:HB3	2.03	0.41
2:B:169:LEU:HD22	2:B:204:TYR:CD1	2.56	0.41
1:D:240:MET:HG2	1:D:318:TYR:CZ	2.56	0.41
2:E:176:PHE:CE1	3:F:137:LEU:HD23	2.56	0.41
1:D:219:GLU:HA	1:D:338:GLU:HA	2.02	0.41
1:D:61:LEU:HB3	1:D:67:PHE:HB3	2.03	0.40
2:B:205:ILE:O	2:B:205:ILE:HG13	2.20	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	314/331 (95%)	302 (96%)	12 (4%)	0	100	100
1	D	312/331 (94%)	301 (96%)	11 (4%)	0	100	100
2	B	213/228 (93%)	206 (97%)	7 (3%)	0	100	100
2	E	208/228 (91%)	200 (96%)	8 (4%)	0	100	100
3	C	208/214 (97%)	203 (98%)	5 (2%)	0	100	100
3	F	207/214 (97%)	203 (98%)	4 (2%)	0	100	100
All	All	1462/1546 (95%)	1415 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	274/285 (96%)	269 (98%)	5 (2%)	51	77
1	D	273/285 (96%)	264 (97%)	9 (3%)	33	61
2	B	181/191 (95%)	174 (96%)	7 (4%)	28	55
2	E	178/191 (93%)	172 (97%)	6 (3%)	32	60
3	C	175/179 (98%)	164 (94%)	11 (6%)	16	34
3	F	174/179 (97%)	168 (97%)	6 (3%)	32	60
All	All	1255/1310 (96%)	1211 (96%)	44 (4%)	32	58

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	205	ILE
1	A	248	VAL
1	A	253	SER
1	A	266	CYS
2	B	21	SER
2	B	189	SER

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Mol	Chain	Res	Type
2	B	192	VAL
2	B	206	CYS
2	B	207	ASN
2	B	211	LYS
2	B	224	LYS
3	C	2	SER
3	C	60	ARG
3	C	66	SER
3	C	124	SER
3	C	128	GLN
3	C	151	LYS
3	C	170	SER
3	C	177	SER
3	C	183	THR
3	C	191	ARG
3	C	202	SER
1	D	21	SER
1	D	32	SER
1	D	55	ILE
1	D	81	SER
1	D	251	SER
1	D	272	LYS
1	D	289	VAL
1	D	315	VAL
1	D	338	GLU
2	E	1	GLU
2	E	12	VAL
2	E	145	THR
2	E	163	SER
2	E	211	LYS
2	E	221	VAL
3	F	46	VAL
3	F	55	SER
3	F	60	ARG
3	F	118	THR
3	F	177	SER
3	F	192	SER

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

Mol	Chain	Res	Type
2	B	31	ASN

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Mol	Chain	Res	Type
2	B	84	GLN
2	B	86	ASN
2	B	181	GLN
3	C	16	GLN
3	C	128	GLN
3	C	196	GLN
3	C	199	HIS
1	D	50	GLN
2	E	39	GLN
2	E	209	ASN
3	F	37	GLN
3	F	172	ASN
3	F	190	HIS
3	F	199	HIS

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 ⓘ

10 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	G	1	4,1	14,14,15	0.47	0	17,19,21	0.69	0
4	NAG	G	2	4	14,14,15	0.50	0	17,19,21	0.64	0
4	MAN	G	3	4	11,11,12	1.47	2 (18%)	15,15,17	1.10	1 (6%)
5	NAG	H	1	5,1	14,14,15	0.30	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	H	2	5	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	I	1	4,1	14,14,15	0.26	0	17,19,21	0.73	0
4	NAG	I	2	4	14,14,15	0.92	1 (7%)	17,19,21	0.76	1 (5%)
4	MAN	I	3	4	11,11,12	1.87	4 (36%)	15,15,17	1.67	3 (20%)
5	NAG	J	1	5,1	14,14,15	0.32	0	17,19,21	0.74	0
5	NAG	J	2	5	14,14,15	0.40	0	17,19,21	0.45	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
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	MAN	G	3	4	-	1/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	MAN	I	3	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	MAN	O5-C5	3.90	1.51	1.43
4	I	2	NAG	O5-C1	-3.19	1.38	1.43
4	G	3	MAN	O5-C5	3.08	1.49	1.43
4	I	3	MAN	C6-C5	2.45	1.60	1.51
4	G	3	MAN	C4-C5	2.45	1.58	1.53
4	I	3	MAN	C4-C5	2.37	1.58	1.53
4	I	3	MAN	C4-C3	2.16	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	3	MAN	C1-O5-C5	4.54	118.27	112.19
4	G	3	MAN	O2-C2-C3	-2.84	104.28	110.15
4	I	3	MAN	O2-C2-C3	-2.45	105.07	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C1-O5-C5	2.07	114.96	112.19
4	I	3	MAN	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

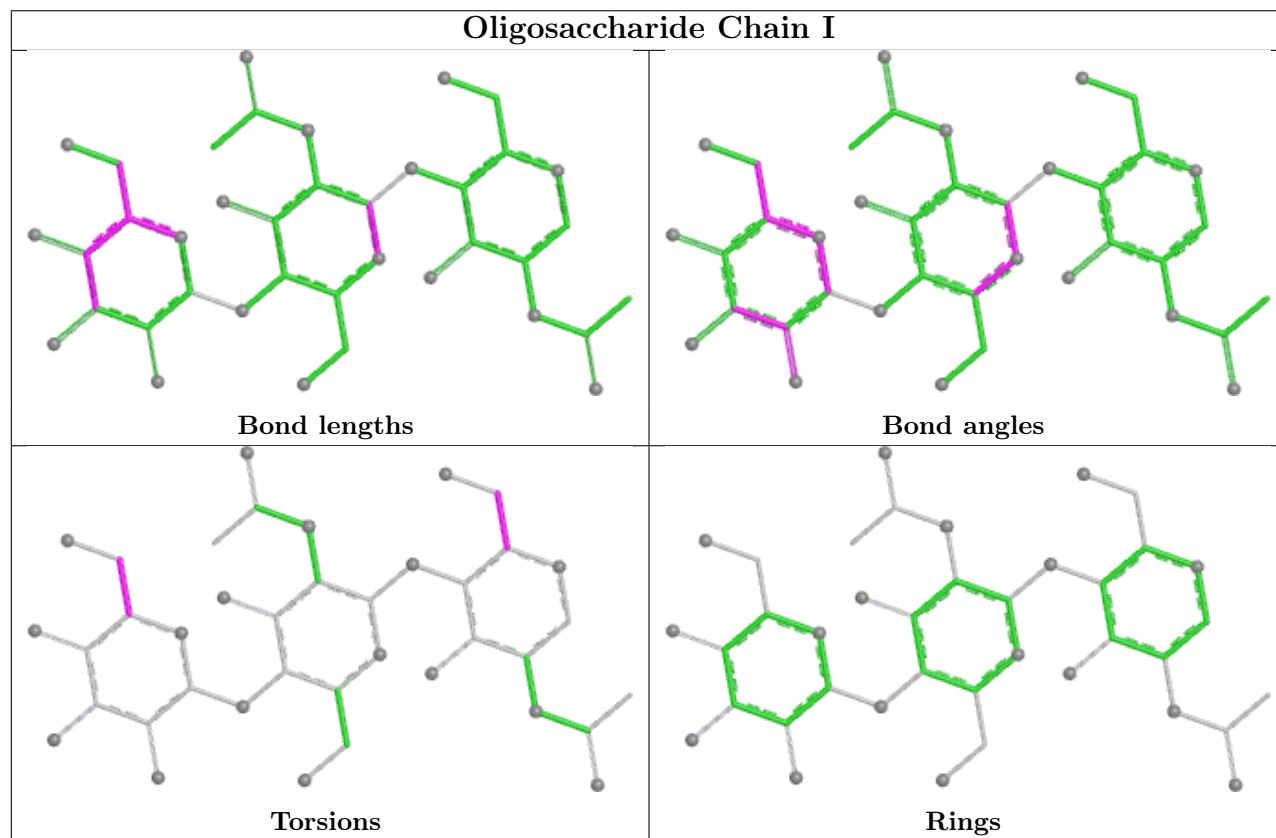
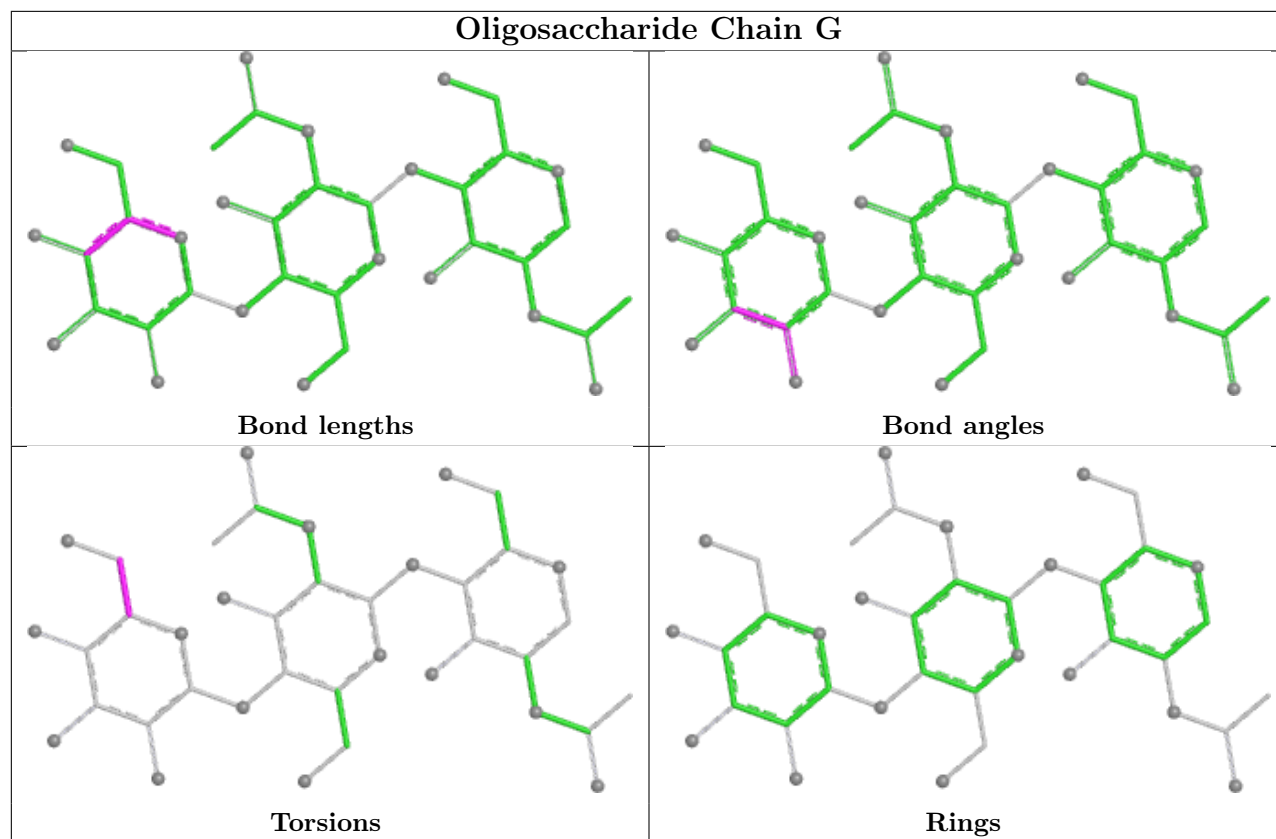
All (14) torsion outliers are listed below:

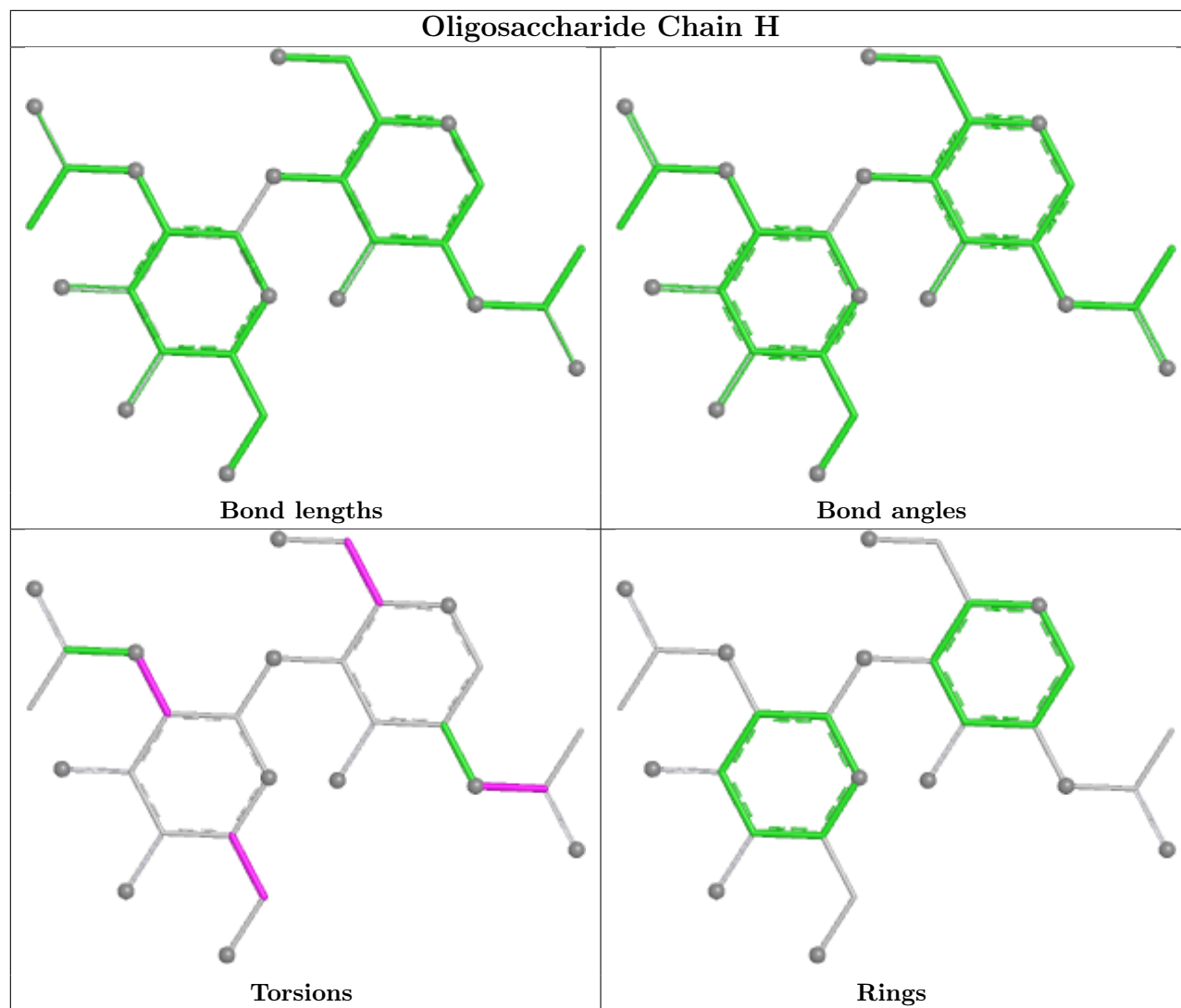
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C4-C5-C6-O6
4	I	3	MAN	C4-C5-C6-O6
4	G	3	MAN	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C1-C2-N2-C7
5	J	2	NAG	C4-C5-C6-O6

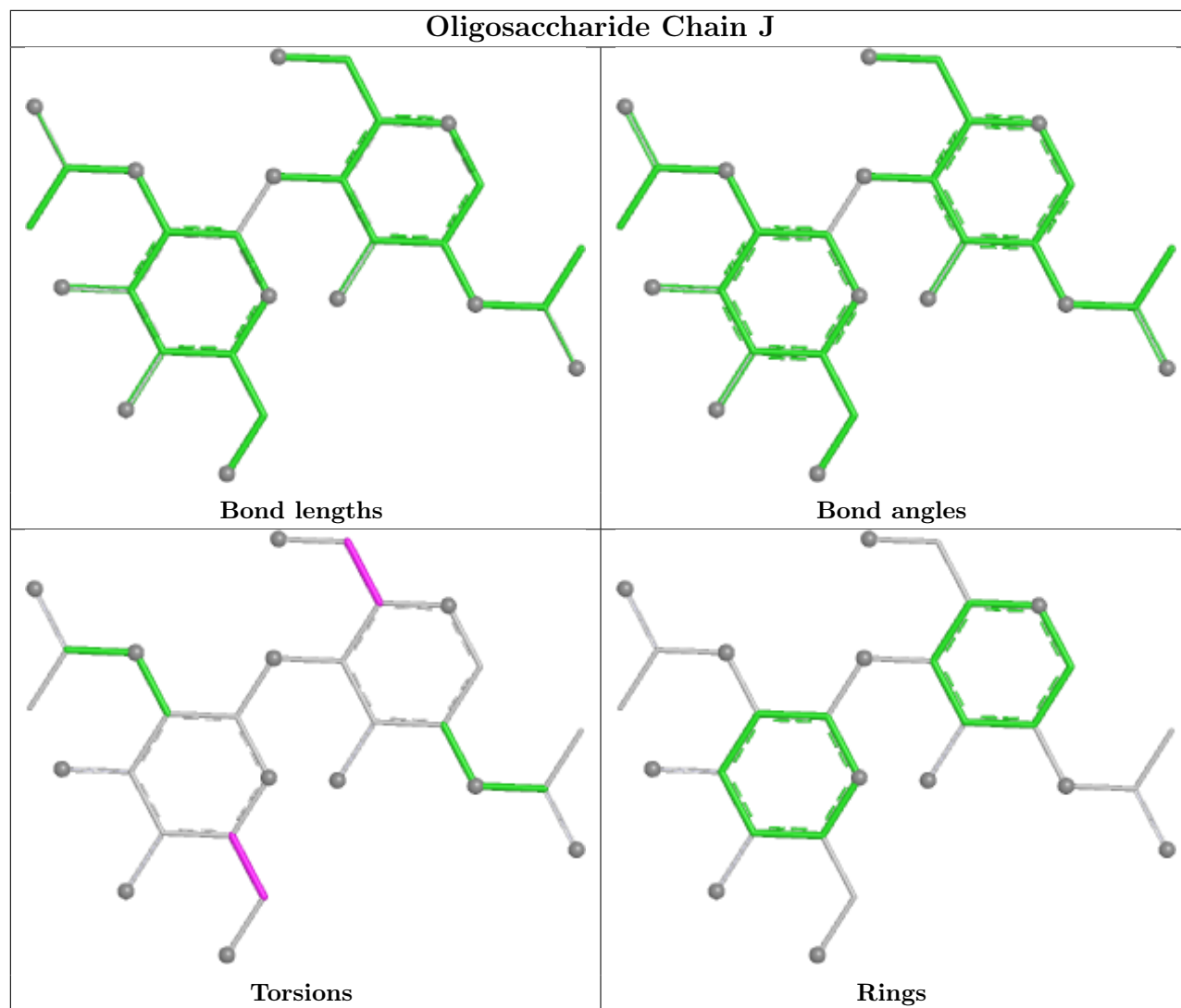
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

There are no ligands in this entry.

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	A	318/331 (96%)	-0.08	9 (2%)	55	50	25, 35, 63, 134	0
1	D	316/331 (95%)	-0.18	7 (2%)	62	58	22, 32, 55, 91	0
2	B	217/228 (95%)	0.53	38 (17%)	4	3	27, 44, 118, 153	0
2	E	212/228 (92%)	0.67	43 (20%)	3	2	23, 35, 120, 149	0
3	C	210/214 (98%)	0.83	41 (19%)	3	2	25, 55, 104, 124	0
3	F	209/214 (97%)	0.96	54 (25%)	1	1	23, 51, 111, 133	0
All	All	1482/1546 (95%)	0.37	192 (12%)	7	6	22, 37, 105, 153	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	148	LEU	7.3
2	E	199	LEU	7.0
2	E	149	GLY	6.7
3	F	211	THR	5.9
3	F	187	TRP	5.3
3	F	121	PRO	5.3
2	E	204	TYR	5.1
3	C	3	GLU	4.8
3	F	123	SER	4.8
2	E	147	ALA	4.8
2	E	194	VAL	4.8
2	E	195	PRO	4.8
3	F	193	TYR	4.8
2	E	191	VAL	4.7
2	B	147	ALA	4.7
1	D	338	GLU	4.6
3	F	182	LEU	4.6
1	A	301	ALA	4.6
3	F	209	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
3	F	135	VAL	4.5
2	E	190	SER	4.4
3	C	201	GLY	4.4
3	F	157	VAL	4.4
2	B	190	SER	4.3
2	B	136	PRO	4.2
3	C	211	THR	4.2
3	F	120	PHE	4.2
3	F	210	PRO	4.1
2	E	217	VAL	4.1
2	B	194	VAL	4.0
2	B	135	ALA	3.8
2	E	164	TRP	3.8
3	F	149	ALA	3.8
3	F	133	THR	3.8
3	F	208	VAL	3.8
2	B	175	THR	3.7
2	B	193	THR	3.7
2	B	191	VAL	3.7
2	B	192	VAL	3.7
3	C	128	GLN	3.7
2	B	168	ALA	3.6
3	C	156	PRO	3.6
2	B	204	TYR	3.5
3	F	137	LEU	3.5
2	B	195	PRO	3.5
3	F	122	PRO	3.5
3	F	184	PRO	3.5
2	E	170	THR	3.5
2	E	221	VAL	3.5
3	F	117	VAL	3.4
3	C	182	LEU	3.4
2	E	203	THR	3.4
3	C	119	LEU	3.3
3	F	150	TRP	3.3
2	E	197	SER	3.3
3	F	119	LEU	3.3
2	E	189	SER	3.3
2	E	192	VAL	3.2
3	F	129	ALA	3.2
2	E	223	PRO	3.2
3	C	158	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	191	ARG	3.1
3	C	121	PRO	3.1
2	E	169	LEU	3.1
2	B	144	GLY	3.1
2	E	132	PHE	3.1
3	C	194	SER	3.1
1	D	302	LYS	3.1
1	A	21	SER	3.1
2	B	217	VAL	3.1
2	E	201	THR	3.0
3	F	183	THR	3.0
2	E	151	LEU	3.0
1	A	293	GLU	3.0
3	C	193	TYR	3.0
3	F	190	HIS	3.0
1	A	340	ASN	3.0
2	E	196	SER	2.9
3	F	124	SER	2.9
2	B	197	SER	2.9
3	C	196	GLN	2.9
2	B	205	ILE	2.8
3	C	155	SER	2.8
3	F	132	ALA	2.8
3	C	208	VAL	2.8
3	F	156	PRO	2.8
3	F	128	GLN	2.8
2	B	169	LEU	2.8
3	F	131	LYS	2.8
2	B	174	HIS	2.8
2	B	132	PHE	2.8
3	F	204	VAL	2.7
3	F	134	LEU	2.7
3	C	120	PHE	2.7
2	E	208	VAL	2.7
2	E	193	THR	2.7
3	F	118	THR	2.7
2	E	174	HIS	2.7
2	E	209	ASN	2.7
1	D	20	ASP	2.7
2	B	223	PRO	2.7
3	C	209	ALA	2.7
3	F	188	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	221	VAL	2.6
3	F	114	ALA	2.6
2	E	150	CYS	2.6
3	C	195	CYS	2.6
3	F	155	SER	2.6
3	F	113	ALA	2.6
2	E	202	GLN	2.6
3	F	116	SER	2.6
3	C	187	TRP	2.5
2	E	205	ILE	2.5
2	E	176	PHE	2.5
2	B	219	LYS	2.5
2	E	200	GLY	2.5
3	C	122	PRO	2.5
3	F	189	SER	2.5
2	B	150	CYS	2.5
2	B	151	LEU	2.5
3	F	172	ASN	2.5
2	E	211	LYS	2.5
3	F	141	PHE	2.5
2	E	145	THR	2.5
1	A	259	TYR	2.4
1	D	217	GLU	2.4
2	E	167	GLY	2.4
3	C	176	ALA	2.4
2	B	201	THR	2.4
2	B	203	THR	2.4
2	E	171	SER	2.4
3	F	115	PRO	2.4
2	B	149	GLY	2.4
2	E	175	THR	2.4
2	B	134	LEU	2.4
1	D	259	TYR	2.4
1	A	261	GLU	2.4
2	B	216	LYS	2.3
2	B	224	LYS	2.3
3	F	158	LYS	2.3
3	F	159	ALA	2.3
3	C	134	LEU	2.3
3	F	138	ILE	2.3
2	E	216	LYS	2.3
3	C	151	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	204	VAL	2.3
1	A	22	GLY	2.3
2	B	167	GLY	2.3
1	D	293	GLU	2.3
3	F	176	ALA	2.3
2	B	170	THR	2.3
3	F	201	GLY	2.2
3	F	180	LEU	2.2
1	A	20	ASP	2.2
3	C	210	PRO	2.2
3	F	186	GLN	2.2
3	C	2	SER	2.2
3	C	175	ALA	2.2
3	F	127	LEU	2.2
2	E	198	SER	2.2
3	C	150	TRP	2.2
3	C	184	PRO	2.2
2	E	146	ALA	2.2
3	F	152	ALA	2.2
1	D	215	GLN	2.2
2	E	130	SER	2.2
2	B	133	PRO	2.2
2	E	224	LYS	2.2
3	C	159	ALA	2.1
2	B	148	LEU	2.1
2	B	196	SER	2.1
3	C	124	SER	2.1
3	F	177	SER	2.1
3	F	194	SER	2.1
2	E	162	VAL	2.1
2	B	189	SER	2.1
3	F	202	SER	2.1
3	C	127	LEU	2.1
3	C	183	THR	2.1
1	A	163	SER	2.1
3	F	136	CYS	2.1
3	C	180	LEU	2.1
3	F	185	GLU	2.1
2	B	171	SER	2.1
3	C	144	GLY	2.0
3	C	153	ASP	2.0
3	C	170	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	192	SER	2.0
3	C	135	VAL	2.0
3	C	137	LEU	2.0
3	C	203	THR	2.0
2	B	164	TRP	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](#)

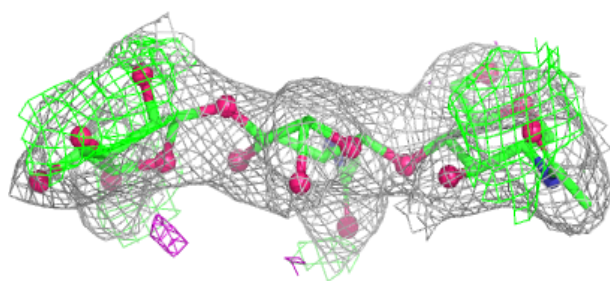
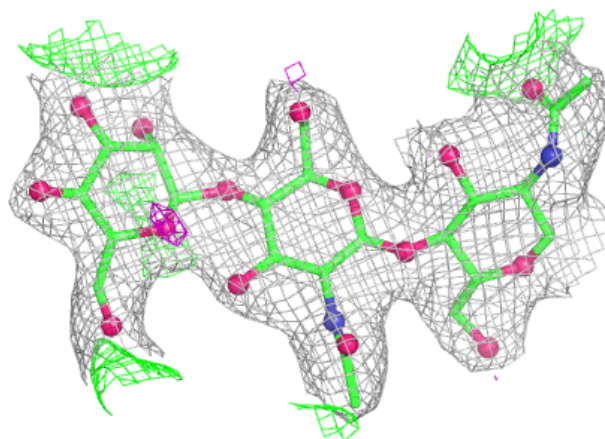
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	H	1	14/15	0.48	0.20	79,88,98,108	0
5	NAG	H	2	14/15	0.52	0.17	105,118,124,124	0
4	MAN	I	3	11/12	0.71	0.14	47,51,54,55	0
4	MAN	G	3	11/12	0.75	0.14	47,50,60,60	0
5	NAG	J	1	14/15	0.76	0.12	43,47,55,60	0
5	NAG	J	2	14/15	0.78	0.13	63,67,69,71	0
4	NAG	G	1	14/15	0.88	0.09	31,35,42,45	0
4	NAG	I	1	14/15	0.89	0.12	29,35,41,45	0
4	NAG	G	2	14/15	0.92	0.09	36,45,49,49	0
4	NAG	I	2	14/15	0.94	0.07	38,41,45,46	0

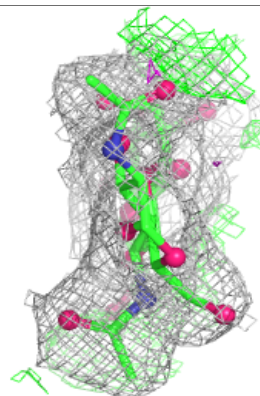
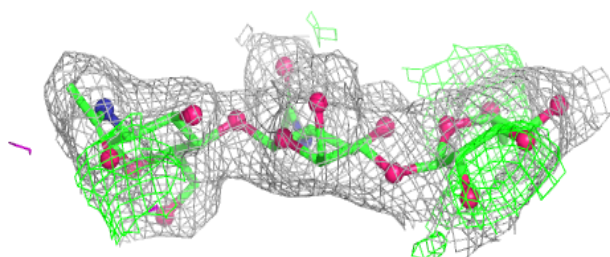
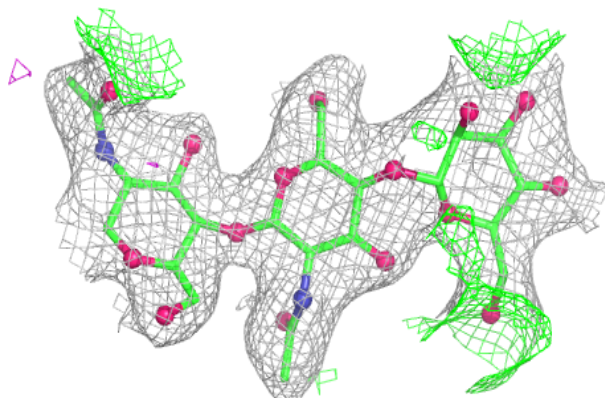
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

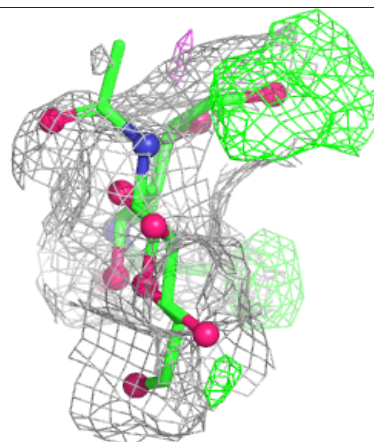
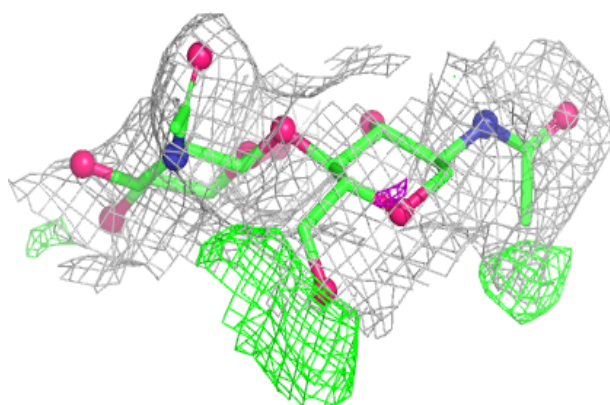
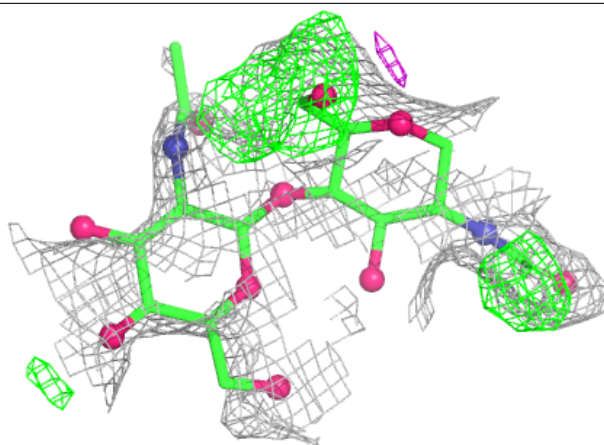
**Electron density around Chain I:**

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

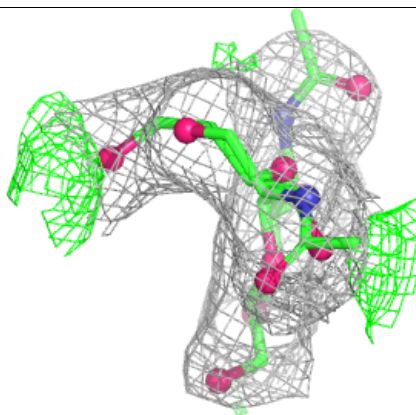
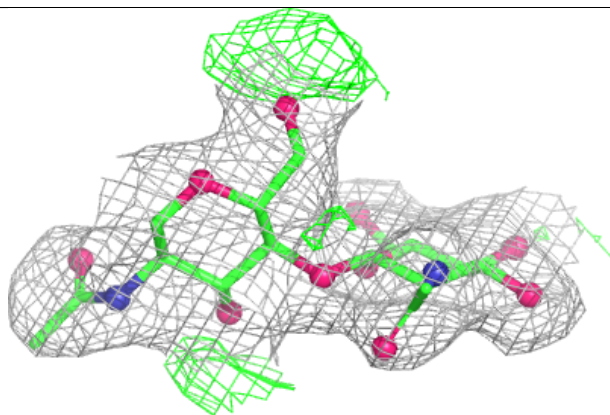
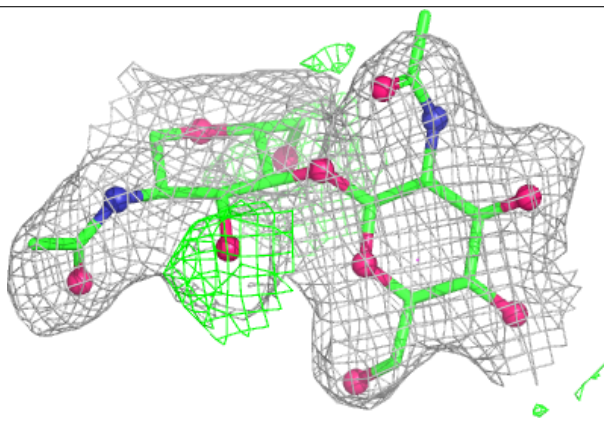


Electron density around Chain H:

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

**Electron density around Chain J:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.