



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:09 AM UTC

PDB ID : 6MF0 / pdb_00006mf0
Title : Crystal Structure Determination of Human/Porcine Chimera Coagulation Factor VIII
Authors : Smith, I.W.; Spiegel, P.C.
Deposited on : 2018-09-07
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

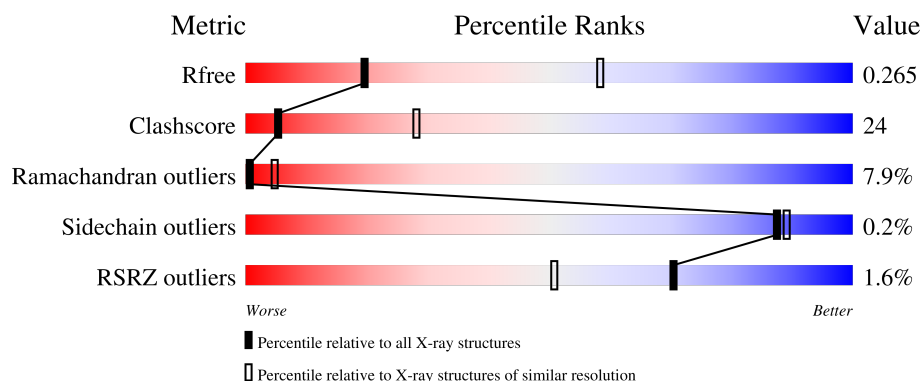
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	1467	45% 36% 14%
1	B	1467	42% 39% 15%
2	C	5	80% 20%
2	E	5	20% 60% 20%
2	F	5	20% 60% 20%

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Mol	Chain	Length	Quality of chain
3	D	3	 100%
4	G	7	 71% 29%
5	H	6	 50% 50%

2 Entry composition [i](#)

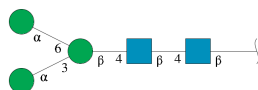
There are 9 unique types of molecules in this entry. The entry contains 20622 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coagulation factor VIII chimera.

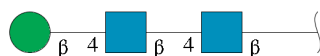
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1256	Total	C	N	O	S	0	0	0
			10147	6520	1738	1837	52			
1	B	1247	Total	C	N	O	S	0	0	0
			10084	6476	1729	1827	52			

- Molecule 2 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.



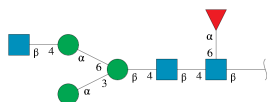
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



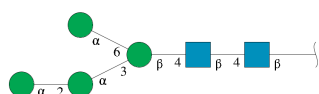
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			85	48	3	34			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
5	H	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		

- Molecule 8 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Cu 1	0	0
8	B	1	Total 1	Cu 1	0	0

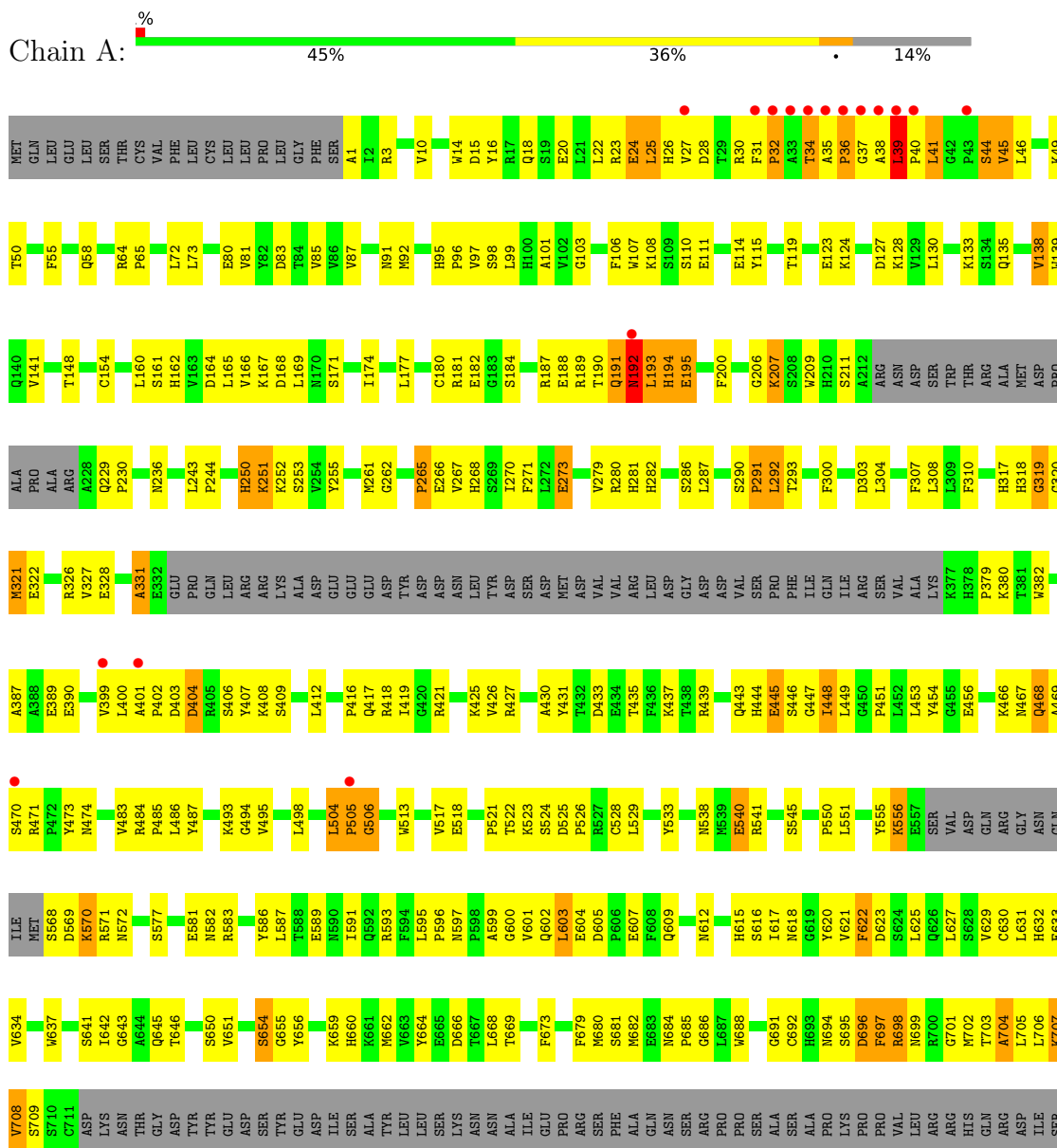
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total 5	O 5	0	0
9	B	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

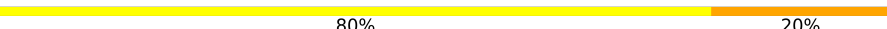
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Coagulation factor VIII chimera



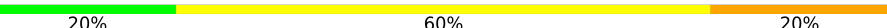
R2320	T2244	S2089	G1832	H1755	GLU	GLU	PRO	ASP	T514	T436	ASP
M2321	T2245	Q2100	K1833	L1756	ASP	ASP	PRO	GLU	V515	F436	GLY
E2322	Q2246	F2101	A1834	G1757	GLU	GLU	ARG	ASN	E518	K437	ASP
C2325	G2247	I2102	V1835	L1758	GLN	ASN	ARG	GLN	E519	T438	ASP
G2326	M2104	M1926	A1836	G1759	ASP	ALA	PHE	ALA	G520	R439	VAL
E2327	M2105	D1927	Y1837	L1760	ASP	ALA	ALA	GLN	P521	P440	SER
A2328	S2106	L1928	V1841	P1761	PRO	PRO	GLN	ASN	P522	A441	PRO
Q2329	L2107	P1930	V1842	Y1762	ARG	ARG	ASN	SER	T523	L442	PHE
ASP	L2108	G1931	D1846	I1763	SER	SER	SER	SER	K443	ILE	ILE
LEU	L1932	L1932	S1849	A1765	GLN	GLN	PRO	ARG	S446	GLN	GLN
TYR	Q2036	Q1936	G1850	E1766	K1693	K1694	PRO	PRO	P526	ARG	ARG
	T2037	I2037	G1850	D1769	R1694	R1695	SER	SER	S611	SER	SER
	A2039	N1937	L1851	I1770	T1696	T1696	ALA	ALA	R527	VAL	VAL
			G1852	I1771	R1696	R1696	SER	SER	L449	ALA	ALA
			G1853	M1772	F1699	F1699	PRO	PRO	L452	LYS	LYS
			L1854	V1773	G691	G691	LYS	LYS	L453		
			L1855	T1774	I1700	I1700	PRO	PRO	L456		
			L1856	F1775	H693	H693	PRO	PRO	V457		
			L1857	K1776	M1707	M1707	VAL	VAL	L461		
			G1858	L1777	D1708	D1708	LEU	LEU	L462		
			L1863	Q1778	Y1709	Y1709	ARG	ARG	L463		
			E1875	R1781	E1713	E1713	HIS	HIS	L464		
			F1876	P1782	S1714	S1714	GLN	GLN	F485		
			V1965	Y1783	P1715	P1715	ASP	ASP	K466		
			R1966	S1784	ALA	ALA	ASP	ASP	R471		
			K1967	F1785	LEU	LEU	ILE	ILE	P472		
			K1968	F1883	ARG	ARG	SER	SER	Y473		
			I2059	L1789	ASN	ASN	LEU	LEU	M474		
			N2060	I1790	ARG	ARG	PRO	PRO	P485		
			A2061	S1791	ALA	ALA	THR	THR	L486		
			W2062	Y1792	GLN	GLN	PHE	PHE	Y487		
			S2063	Y1792	ASN	ASN	GLN	GLN	A401		
			P2067	E1801	G1725	G1725	PRO	PRO	P402		
			N2079	P1802	E1726	E1726	LYS	LYS	S406		
			I2071	R1803	K1731	K1731	GLU	GLU	Y407		
			K2072	H1804	K1732	K1732	GLY	GLY	K408		
			L2076	V1807	V1733	V1733	ASP	ASP	S409		
			M2079	T1812	V1734	V1734	MET	MET	Q410		
			I2080	R1813	F1735	F1735	TYR	TYR	Y411		
			I2081	T1814	R1736	R1736	GLU	GLU	L412		
			I2084	Y1815	E1737	E1737	ASP	ASP	M413		
			K2085	F1816	F1738	F1738	SER	SER	N414		
			T2086	V1819	G1741	G1741	ILE	ILE	R418		
			Q2087	H1821	S1742	S1742	THR	THR	I419		
			G2088	Q1820	F1743	F1743	GLU	GLU	D420		
			A2089	M1823	T1744	T1744	THR	THR	R421		
			K2092	T1826	Q1746	Q1746	GLY	GLY	L504		
			F2093	T1827	S1747	S1747	LEU	LEU	P505		
			S2094	L1912	F1748	F1748	SER	SER	K425		
			S2095	K1913	R1749	R1749	ASP	ASP	I508		
			T2012	E1914	F1827	F1827	PHE	PHE	F509		
			L2015	Y1915	D1828	D1828	ASP	ASP	K510		
			I2098	Y1916	E1829	E1829	ILE	ILE	Y511		
				Y1917	F1830	F1830	TYR	TYR	K512		
				R1917	D1831	D1831	GLY	GLY	W513		

- Molecule 2: 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

Chain C:  80% 20%

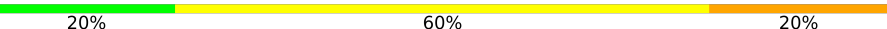
NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 2: 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

Chain E:  20% 60% 20%

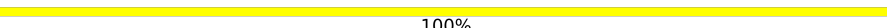
NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 2: 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

Chain F:  20% 60% 20%

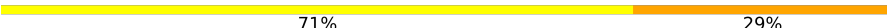
NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain D:  100%

NAG1
NAG2
BMA3

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

Chain G:  71% 29%

NAG1
NAG2
BMA3
MAN4
NAG5
MAN6
FUC7

- Molecule 5: alpha-D-mannopyranose-(1-2)-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

Chain H:  50% 50%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.00Å 135.86Å 196.11Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	49.03 – 3.20 49.03 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.03-3.20) 99.8 (49.03-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.206 , 0.287 (Not available) , 0.265	Depositor DCC
R_{free} test set	3077 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20622	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: CA, FUC, MAN, ZN, BMA, CU1, NAG

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	0.48	4/10434 (0.0%)	0.85	8/14149 (0.1%)
1	B	0.44	2/10367 (0.0%)	0.74	8/14053 (0.1%)
All	All	0.46	6/20801 (0.0%)	0.80	16/28202 (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
1	A	0	11
1	B	0	6
All	All	0	17

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	GLN	CD-NE2	8.04	1.50	1.33
1	B	2104	MET	SD-CE	-7.84	1.59	1.79
1	B	2150	ARG	CZ-NH2	-7.36	1.23	1.33
1	A	191	GLN	CD-OE1	-7.34	1.09	1.23
1	A	192	ASN	N-CA	-5.68	1.38	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CG-CD-OE1	29.55	179.90	120.80
1	A	191	GLN	OE1-CD-NE2	-23.94	98.66	122.60
1	A	191	GLN	CG-CD-NE2	-23.31	81.43	116.40
1	A	191	GLN	CA-CB-CG	20.70	155.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CB-CG-CD	-13.94	88.89	112.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	GLU	Peptide
1	A	39	LEU	Peptide
1	A	404	ASP	Peptide
1	A	473	TYR	Peptide
1	A	570	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10147	0	9905	454	2
1	B	10084	0	9837	530	1
2	C	61	0	52	3	0
2	E	61	0	52	2	0
2	F	61	0	52	0	2
3	D	39	0	34	0	0
4	G	85	0	73	2	0
5	H	72	0	61	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	5	0	0	0	0
9	B	1	0	0	0	0
All	All	20622	0	20066	981	3

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 24.

The worst 5 of 981 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:2104:MET:HE2	1:B:2150:ARG:HH21	1.08	1.17
1:B:2104:MET:CE	1:B:2150:ARG:HH21	1.60	1.12
1:B:44:SER:O	1:B:46:LEU:HD12	1.66	0.95
1:A:1728:PRO:HG3	1:A:1897:ARG:HH21	1.29	0.94
1:B:1776:LYS:HG3	1:B:1812:THR:HG22	1.49	0.92

All (3) 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)
1:A:504:LEU:O	2:F:4:MAN:O6[1_455]	1.98	0.22
1:A:469:ALA:O	2:F:4:MAN:O2[1_455]	2.04	0.16
1:B:326:ARG:NH2	1:B:2094:SER:OG[2_457]	2.11	0.09

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	A	1242/1467 (85%)	966 (78%)	174 (14%)	102 (8%)	0	4
1	B	1231/1467 (84%)	955 (78%)	182 (15%)	94 (8%)	1	5
All	All	2473/2934 (84%)	1921 (78%)	356 (14%)	196 (8%)	1	5

5 of 196 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	36	PRO
1	A	39	LEU
1	A	40	PRO
1	A	44	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/1301 (5%)	65 (100%)	0	100	100
1	B	1088/1301 (84%)	1086 (100%)	2 (0%)	87	89
All	All	1153/2602 (44%)	1151 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	PRO
1	B	163	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1796	GLN
1	B	2225	ASN
1	B	1864	ASN
1	B	2231	GLN
1	B	2172	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

31 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	C	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	2.12	3 (17%)
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.46	0
2	BMA	C	3	2	11,11,12	1.37	3 (27%)	15,15,17	1.11	0
2	MAN	C	4	2	11,11,12	0.79	0	15,15,17	0.94	1 (6%)
2	MAN	C	5	2	11,11,12	1.43	3 (27%)	15,15,17	1.99	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.76	1 (7%)	17,19,21	1.44	3 (17%)
3	NAG	D	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.29	2 (11%)
3	BMA	D	3	3	11,11,12	1.45	2 (18%)	15,15,17	0.81	0
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	1.91	5 (29%)
2	BMA	E	3	2	11,11,12	1.93	4 (36%)	15,15,17	1.09	0
2	MAN	E	4	2	11,11,12	1.60	2 (18%)	15,15,17	1.30	1 (6%)
2	MAN	E	5	2	11,11,12	0.85	0	15,15,17	0.97	0
2	NAG	F	1	1,2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	F	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.69	0
2	BMA	F	3	2	11,11,12	1.64	3 (27%)	15,15,17	2.29	6 (40%)
2	MAN	F	4	2	11,11,12	2.04	3 (27%)	15,15,17	2.85	5 (33%)
2	MAN	F	5	2	11,11,12	0.60	0	15,15,17	2.09	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
4	NAG	G	2	4	14,14,15	0.59	0	17,19,21	1.50	3 (17%)
4	BMA	G	3	4	11,11,12	1.16	2 (18%)	15,15,17	1.12	2 (13%)
4	MAN	G	4	4	11,11,12	1.05	1 (9%)	15,15,17	1.65	2 (13%)
4	NAG	G	5	4	14,14,15	0.41	0	17,19,21	1.56	3 (17%)
4	MAN	G	6	4	11,11,12	1.03	1 (9%)	15,15,17	1.70	3 (20%)
4	FUC	G	7	4	10,10,11	1.14	1 (10%)	14,14,16	1.09	0
5	NAG	H	1	1,5	14,14,15	0.66	1 (7%)	17,19,21	0.79	0
5	NAG	H	2	5	14,14,15	0.60	0	17,19,21	0.68	0
5	BMA	H	3	5	11,11,12	1.07	0	15,15,17	1.37	2 (13%)
5	MAN	H	4	5	11,11,12	0.98	0	15,15,17	1.15	1 (6%)
5	MAN	H	5	5	11,11,12	1.24	1 (9%)	15,15,17	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	H	6	5	11,11,12	1.53	3 (27%)	15,15,17	0.99	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
2	NAG	C	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	6/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	1/1/1/1
2	MAN	E	5	2	-	2/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	0/1/1/1
2	MAN	F	5	2	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	6/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	NAG	G	5	4	-	0/6/23/26	0/1/1/1
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
4	FUC	G	7	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	2/2/19/22	0/1/1/1
5	MAN	H	6	5	-	1/2/19/22	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	MAN	C4-C5	-4.38	1.43	1.53
2	E	4	MAN	O5-C5	4.08	1.51	1.43
2	F	4	MAN	O5-C5	3.76	1.50	1.43
2	E	3	BMA	C1-C2	3.65	1.60	1.52
2	E	3	BMA	C2-C3	3.52	1.57	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-O5-C5	7.26	121.92	112.19
2	F	5	MAN	C1-O5-C5	7.00	121.56	112.19
2	C	5	MAN	C1-O5-C5	6.27	120.59	112.19
2	C	1	NAG	C1-O5-C5	6.06	120.31	112.19
2	F	4	MAN	C2-C3-C4	5.99	121.39	110.86

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
2	E	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	MAN	C1-C2-C3-C4-C5-O5
2	E	4	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 11 short contacts:

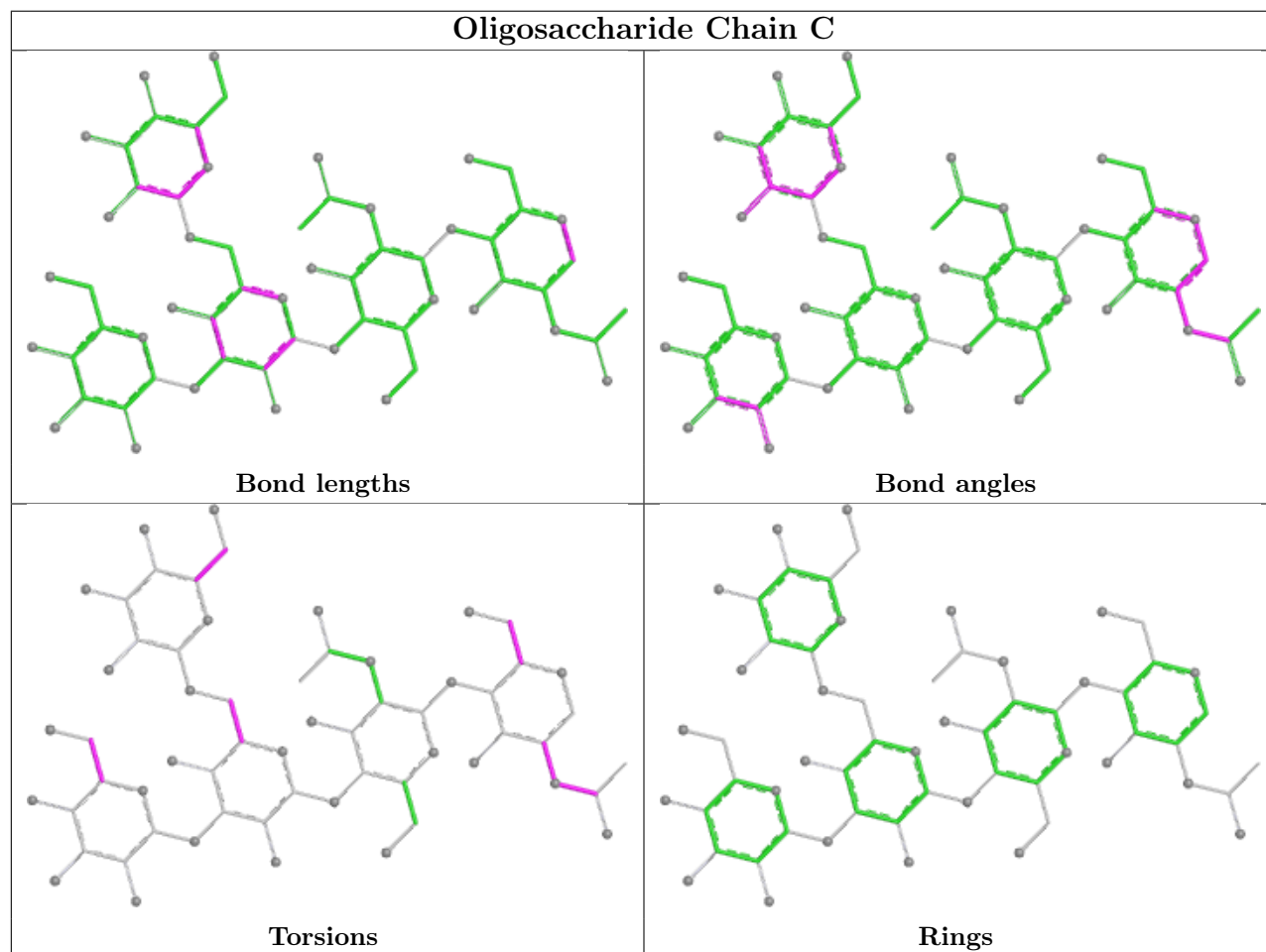
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
2	E	1	NAG	1	0
2	C	2	NAG	2	0
2	C	1	NAG	1	0
5	H	4	MAN	1	0
5	H	1	NAG	1	0
5	H	5	MAN	1	0

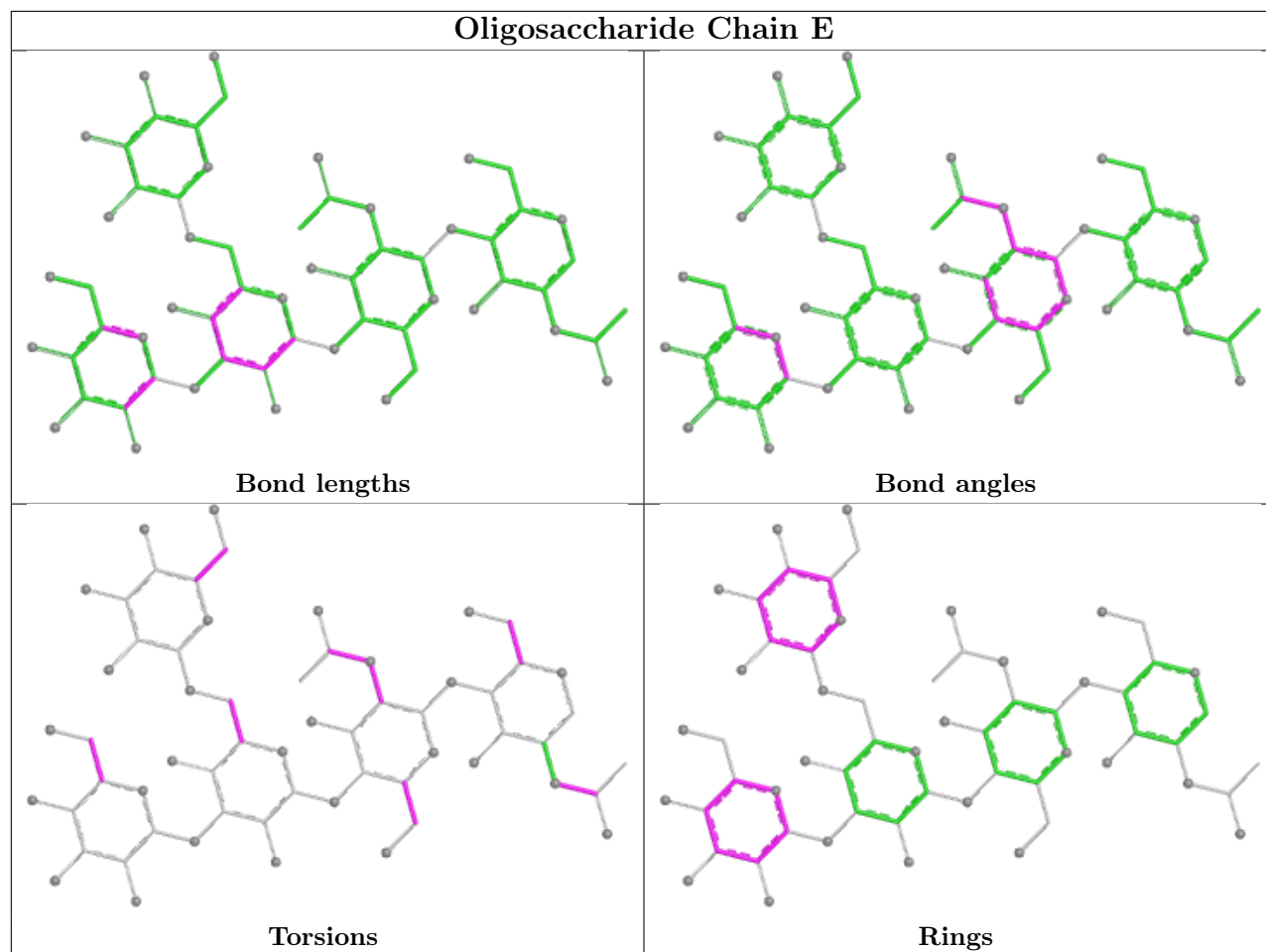
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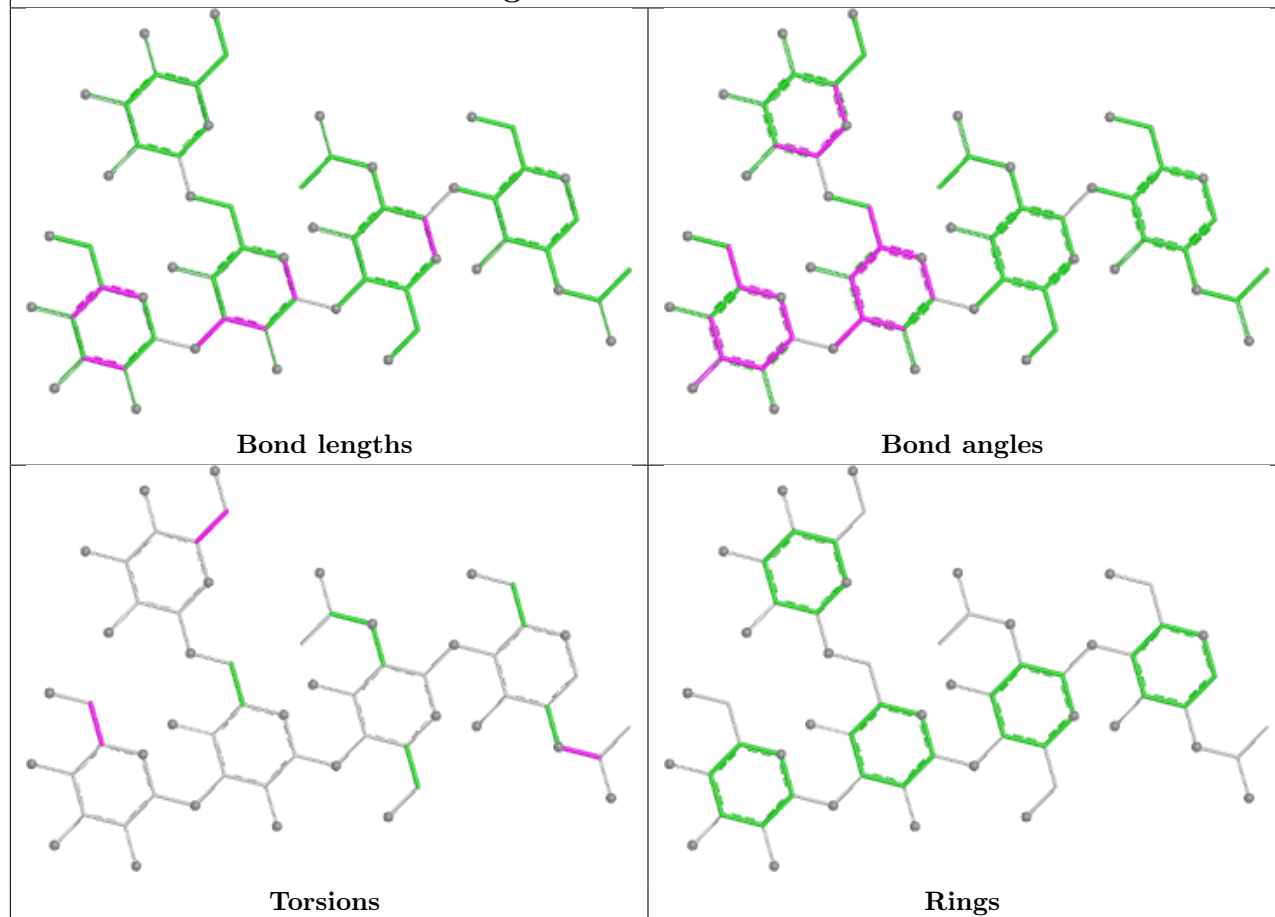
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
4	G	1	NAG	1	0
2	F	4	MAN	0	2
5	H	2	NAG	1	0

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

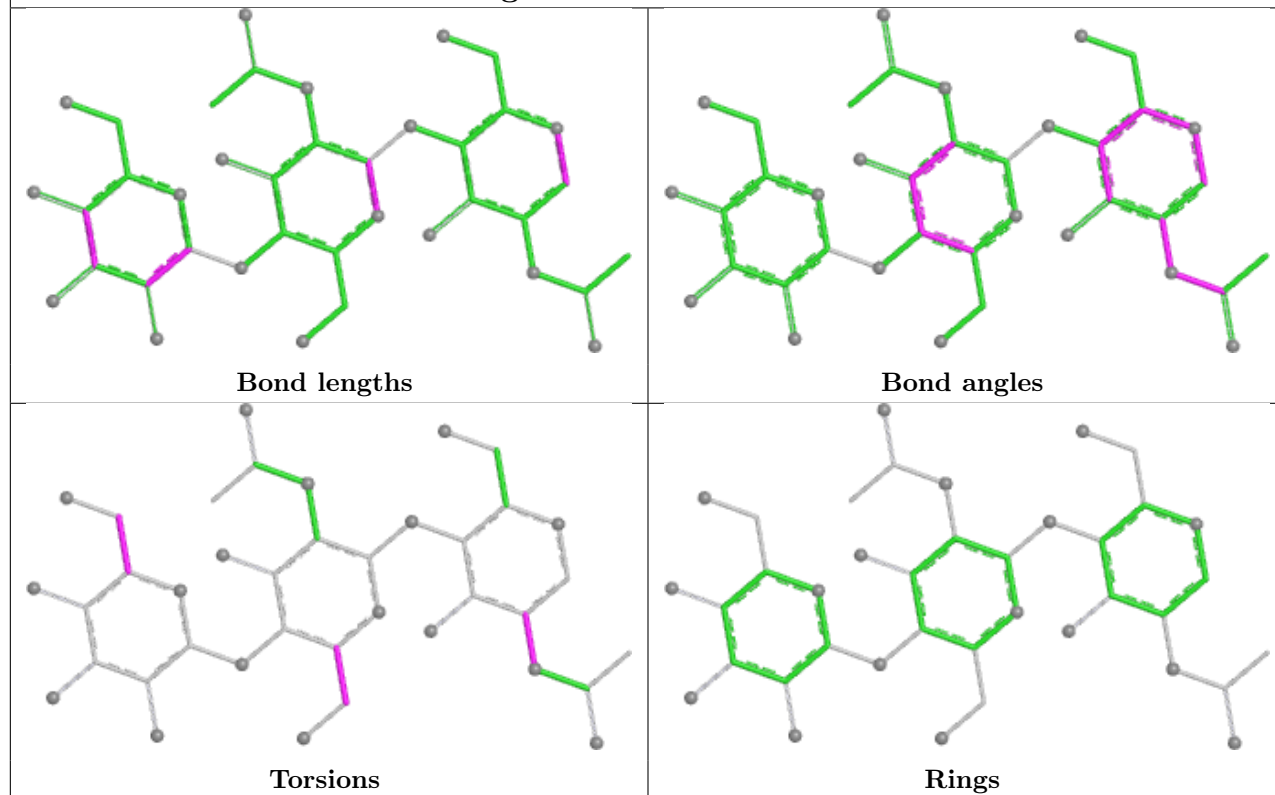


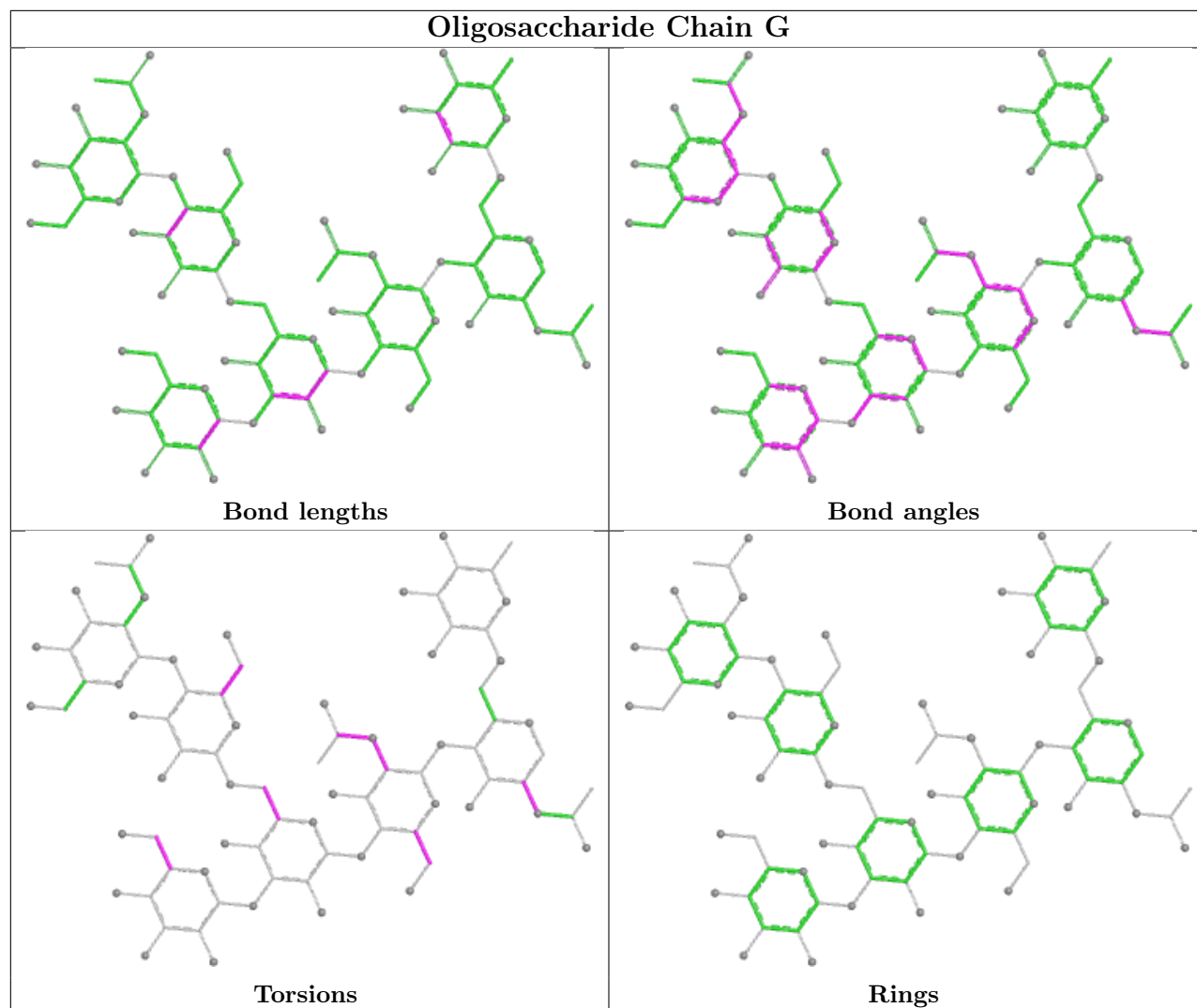


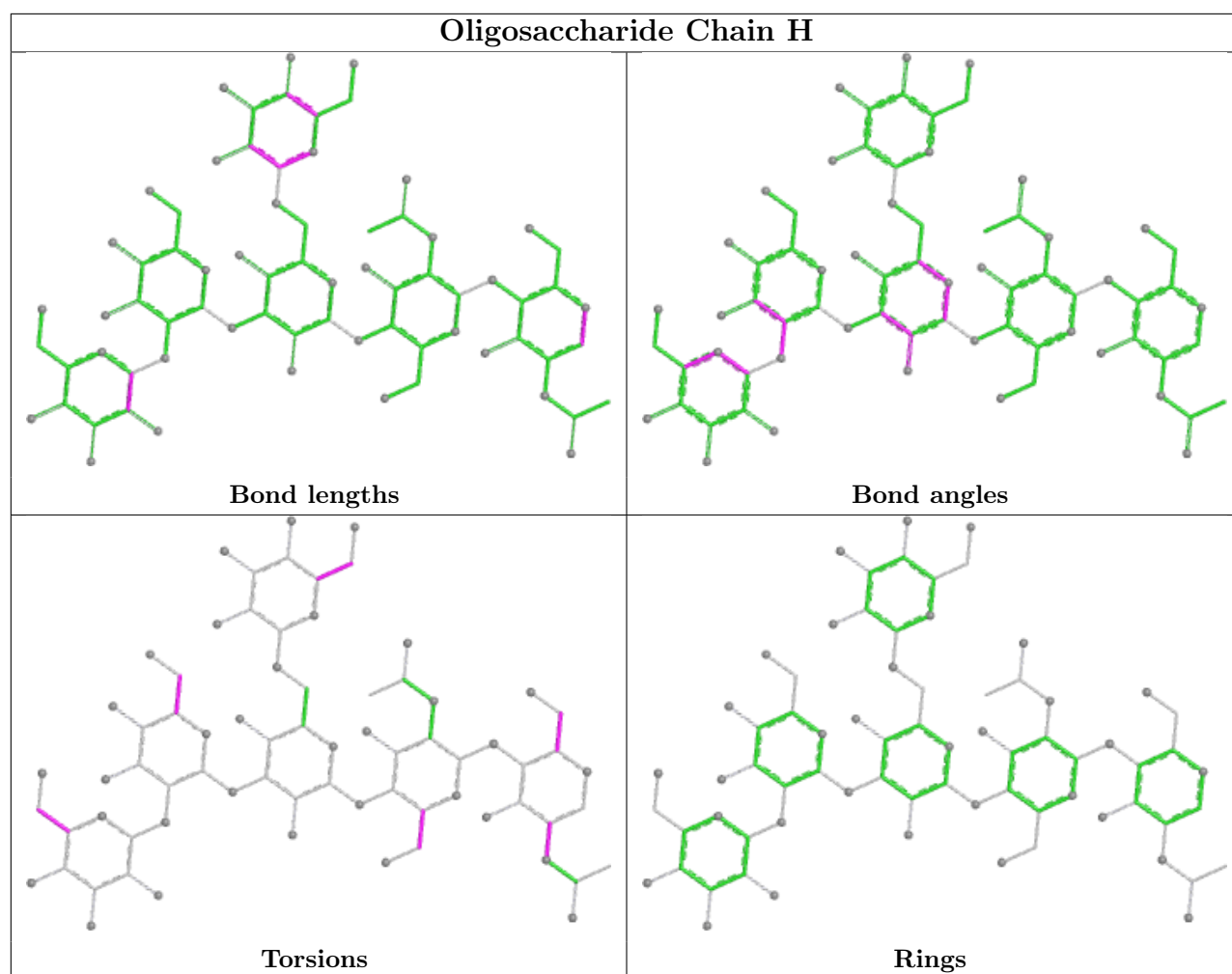
Oligosaccharide Chain F



Oligosaccharide Chain D







5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1256/1467 (85%)	-0.19	18 (1%) 73 54	30, 48, 88, 273	0
1	B	1247/1467 (85%)	0.03	21 (1%) 69 49	30, 58, 130, 157	0
All	All	2503/2934 (85%)	-0.08	39 (1%) 70 51	30, 52, 119, 273	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2319	LEU	5.1
1	A	505	PRO	4.8
1	A	31	PHE	4.5
1	A	27	VAL	4.3
1	B	2122	THR	4.2

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
3	NAG	D	2	14/15	0.17	0.16	114,145,152,154	0
2	MAN	F	5	11/12	0.18	0.16	149,151,160,160	0
4	MAN	G	6	11/12	0.26	0.14	128,135,144,145	0
4	FUC	G	7	10/11	0.26	0.12	124,134,139,144	0
2	MAN	E	4	11/12	0.30	0.14	117,124,129,131	0

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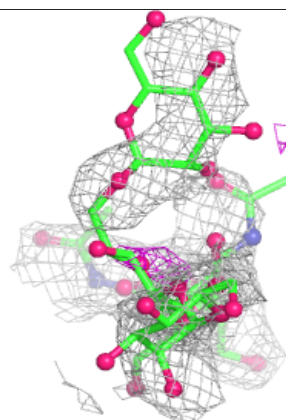
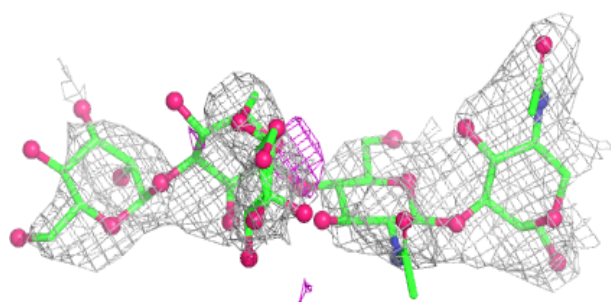
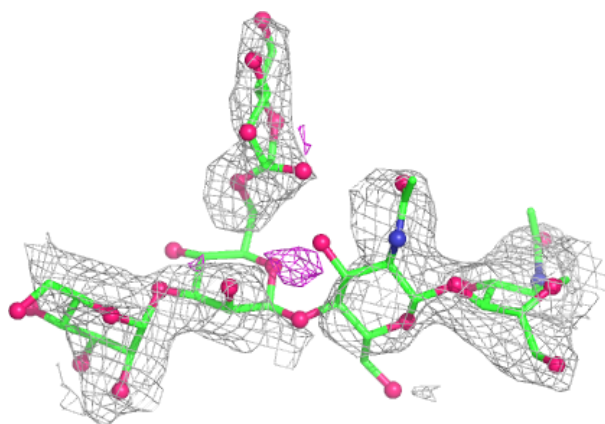
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	F	3	11/12	0.32	0.17	131,138,150,151	0
2	NAG	F	2	14/15	0.33	0.17	130,144,153,154	0
4	NAG	G	1	14/15	0.33	0.18	99,116,124,128	0
2	BMA	C	3	11/12	0.36	0.14	144,158,163,164	0
2	MAN	C	4	11/12	0.36	0.12	148,158,161,163	0
5	MAN	H	5	11/12	0.45	0.13	125,134,142,149	0
3	NAG	D	1	14/15	0.48	0.13	95,131,141,144	0
2	MAN	C	5	11/12	0.48	0.11	138,145,151,156	0
2	NAG	C	2	14/15	0.50	0.12	128,137,149,156	0
2	BMA	E	3	11/12	0.50	0.14	112,121,126,127	0
4	BMA	G	3	11/12	0.53	0.10	123,144,149,152	0
2	MAN	E	5	11/12	0.53	0.14	84,109,119,120	0
3	BMA	D	3	11/12	0.55	0.11	134,157,162,163	0
2	NAG	F	1	14/15	0.60	0.18	86,120,136,142	0
4	NAG	G	2	14/15	0.61	0.12	118,133,142,145	0
5	MAN	H	4	11/12	0.64	0.11	105,120,127,133	0
4	NAG	G	5	14/15	0.64	0.14	78,93,101,102	0
4	MAN	G	4	11/12	0.70	0.10	69,97,108,110	0
5	NAG	H	2	14/15	0.73	0.17	73,95,100,103	0
5	MAN	H	6	11/12	0.73	0.10	99,113,125,126	0
2	NAG	E	2	14/15	0.74	0.15	74,105,116,122	0
5	BMA	H	3	11/12	0.77	0.10	108,114,120,123	0
5	NAG	H	1	14/15	0.85	0.11	81,86,93,93	0
2	NAG	C	1	14/15	0.86	0.10	79,89,109,121	0
2	MAN	F	4	11/12	0.87	0.18	77,96,119,134	0
2	NAG	E	1	14/15	0.87	0.12	78,83,92,104	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.

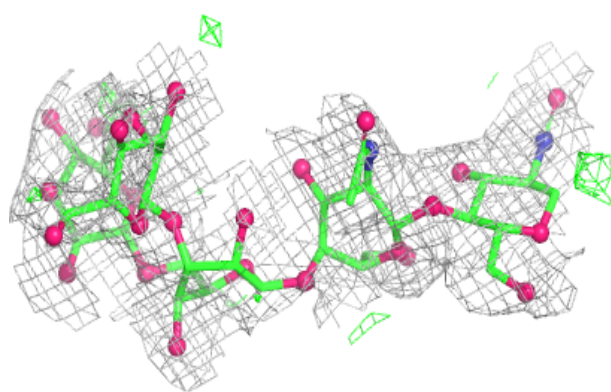
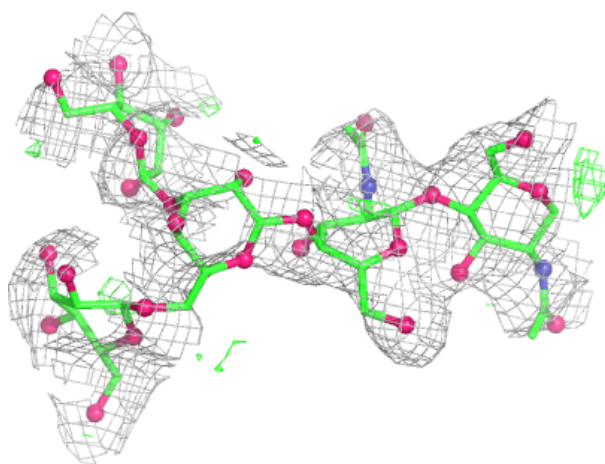
Electron density around Chain C:

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



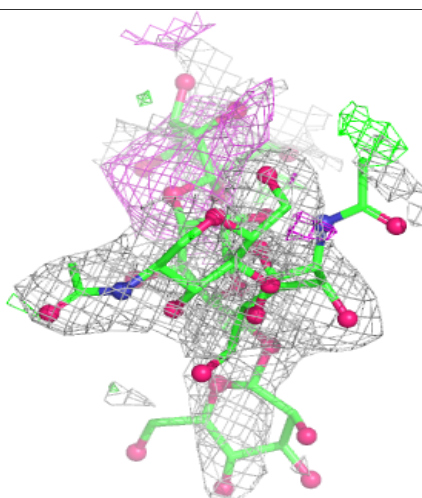
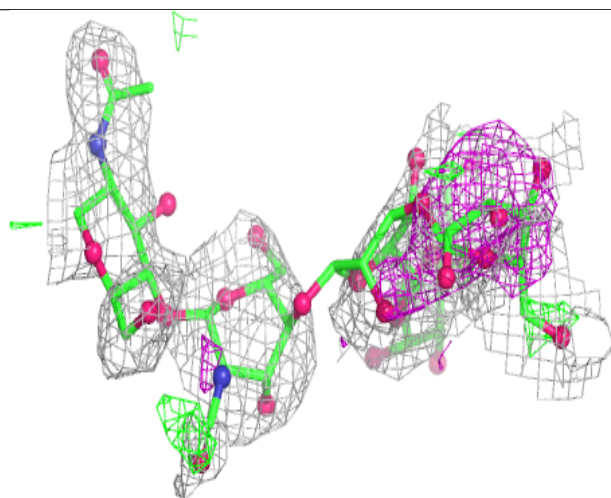
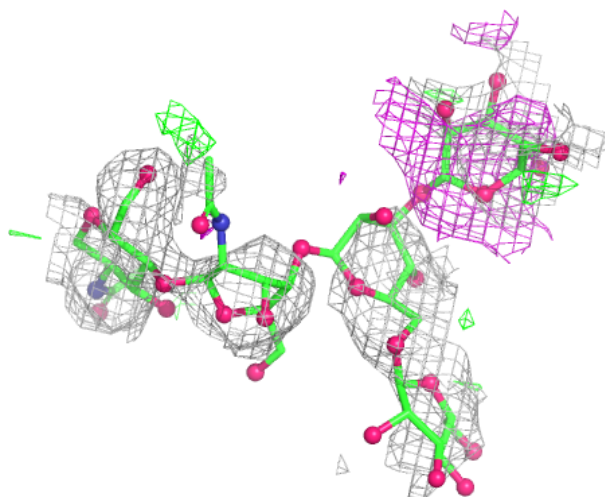
Electron density around Chain E:

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



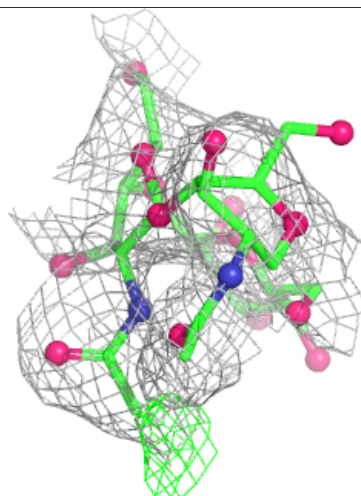
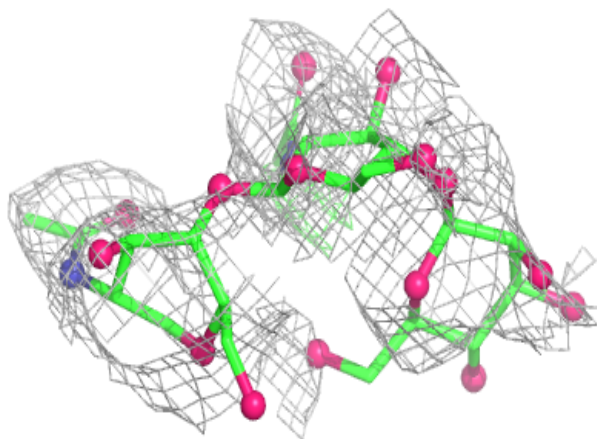
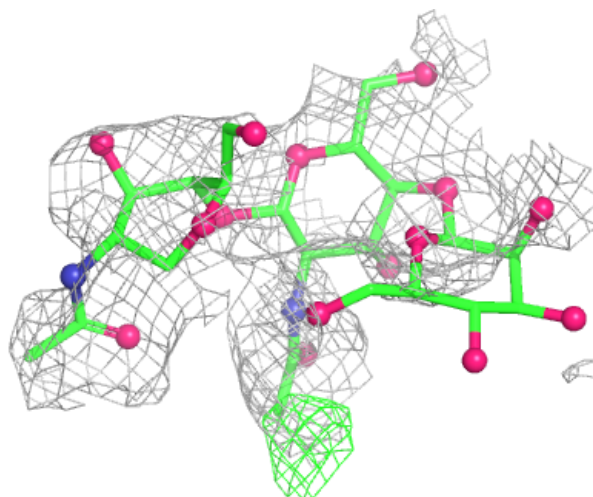
Electron density around Chain F:

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



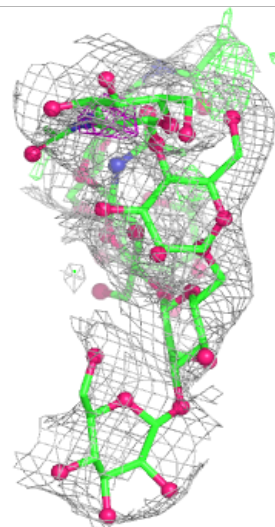
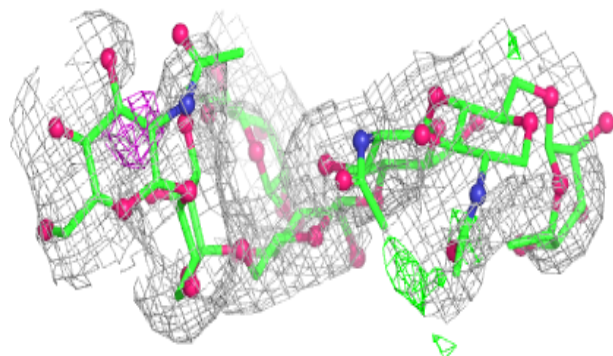
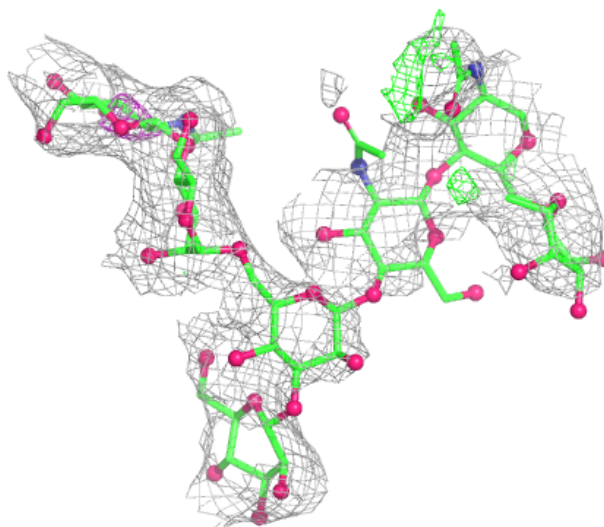
Electron density around Chain D:

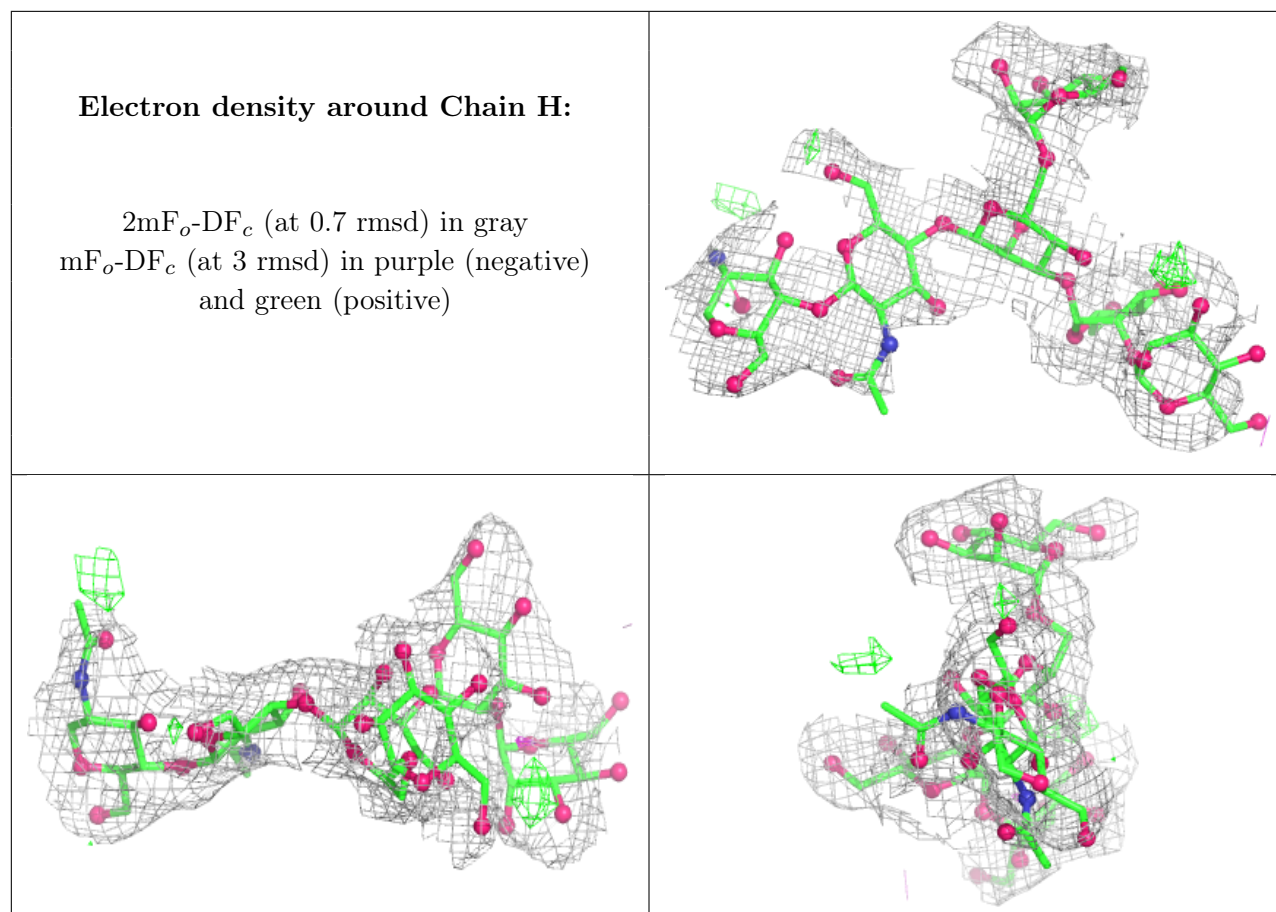
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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($\text{\AA}^2$)	Q<0.9
7	ZN	A	2415	1/1	0.97	0.04	46,46,46,46	0
6	CA	B	2419	1/1	0.99	0.06	59,59,59,59	0
6	CA	A	2414	1/1	0.99	0.06	40,40,40,40	0
7	ZN	B	2420	1/1	0.99	0.05	47,47,47,47	0
8	CU1	A	2416	1/1	0.99	0.07	40,40,40,40	0
8	CU1	B	2421	1/1	0.99	0.09	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.