



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:18 PM BST

PDB ID : 6MF0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

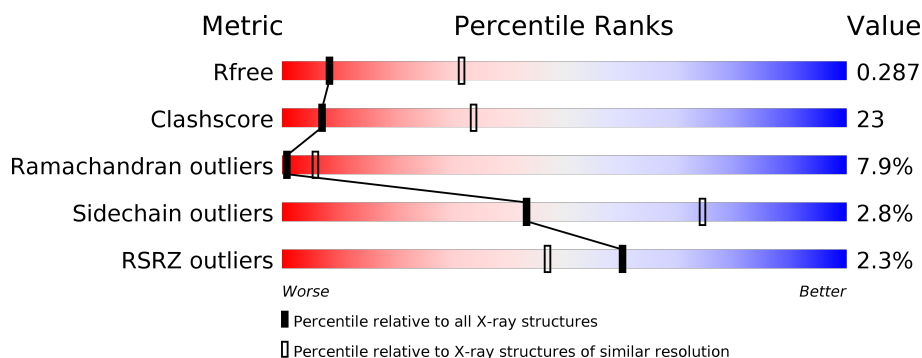
1 Overall quality at a glance

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>35%</div> <div>5%</div> <div>14%</div> </div> </div>
1	B	1467	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>38%</div> <div>5%</div> <div>15%</div> </div> </div>
2	C	5	<div> <div></div> <div>80%</div> <div>20%</div> </div>
2	E	5	<div> <div></div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
2	F	5	<div> <div></div> <div>20%</div> <div>60%</div> <div>20%</div> </div>
3	D	3	<div> <div></div> <div>100%</div> </div>

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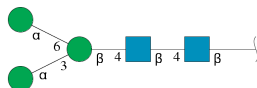
Mol	Chain	Length	Quality of chain
4	G	7	
5	H	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	2	-	-	-	X
2	BMA	C	3	-	-	-	X
2	MAN	C	4	-	-	-	X
2	MAN	C	5	-	-	-	X
2	BMA	F	3	-	-	-	X
2	MAN	F	4	-	-	-	X
2	MAN	F	5	-	-	-	X
3	BMA	D	3	-	-	-	X
4	FUC	G	7	-	-	-	X
5	MAN	H	5	-	-	-	X

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 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.

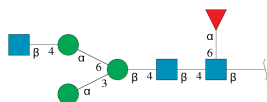


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total 61	C 34	N 2	O 25	0	0	0
2	E	5	Total 61	C 34	N 2	O 25	0	0	0
2	F	5	Total 61	C 34	N 2	O 25	0	0	0



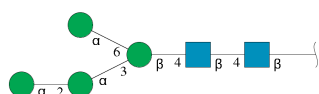
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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 (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

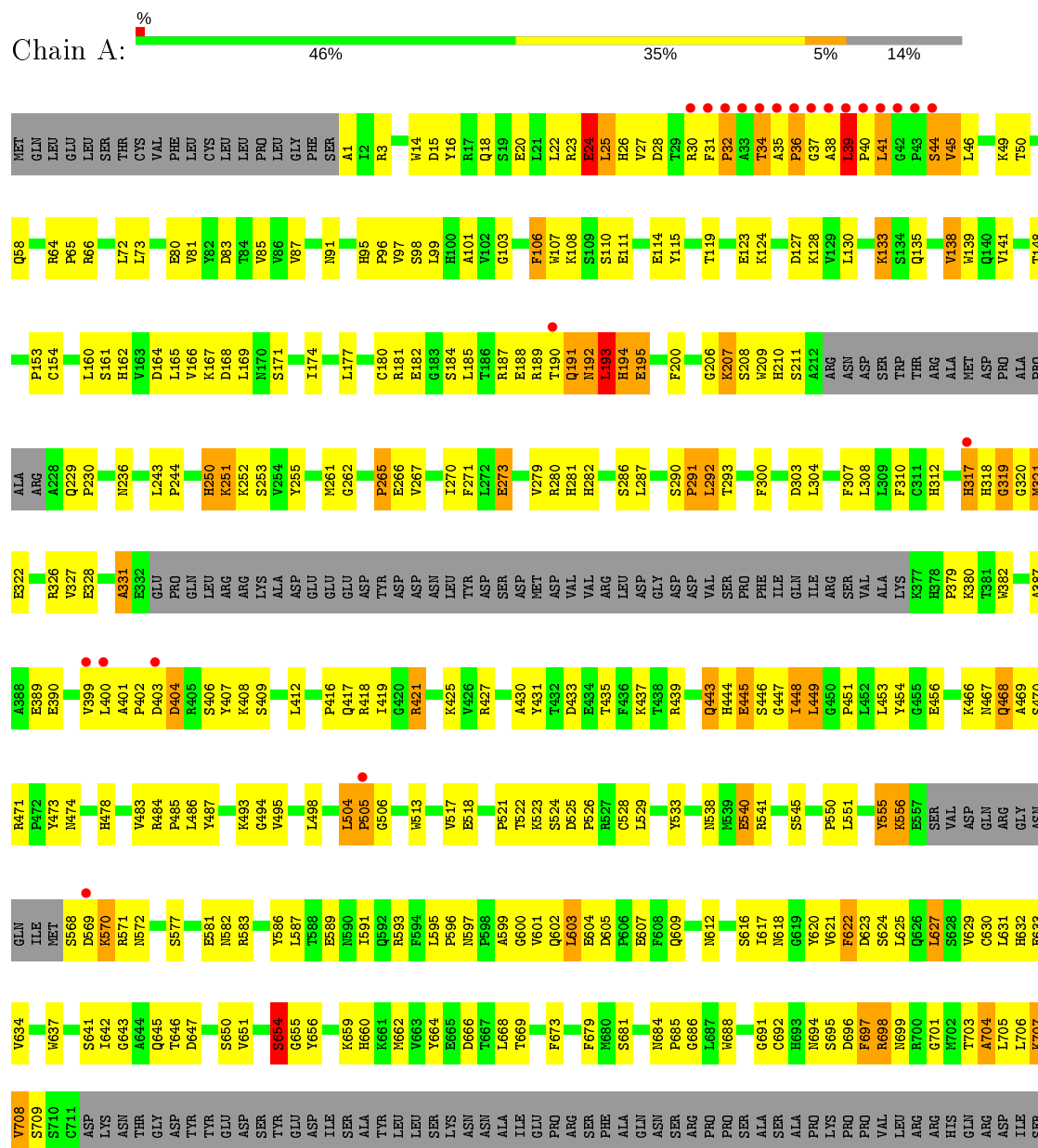
- Molecule 9 is water.

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

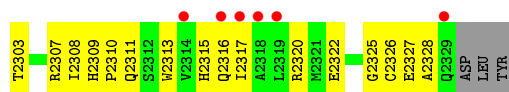
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



WORLDWIDE
PDB
PROTEIN DATA BANK

N2225	H2155	K2092	L2006	T1911	E1827	L1752	I1E	ASN	L668	E589	T514	T435	ASP
F2226	T2156	F2093	Q2007	L1912	D1828	M1753	TTR	ALA	L668	E589	V515	F436	GLY
E2227	S2157	K1913	A2008	K1913	E1829	H1754	GLU	ILE	F671	R593	E518	K437	ASP
E2228	I2158	S2094	G2009	E1914	F1830	H1755	ASP	PRO	F671	R594	E518	T438	VAL
E2229	R2159	S2095	M2010	N1915	C1832	L1756	GLU	ARG	G675	A598	G520	R439	SER
L2230	S2160	L2096	S2011	N1916	C1832	G1757	ASN	ARG	G675	A598	G520	P440	PRO
T2231	T2161	Y2097	T2012	R1917	K1833	L1758	GLN	PHE	M680	L603	T522	A441	PHE
D2233	L2162	I2098	L2015	F1918	A1834	L1759	ASP	ALA	S681	E507	K523	I442	ILE
F2234	R2163	S2099	L2015	H1919	W1835	G1760	PRO	GLN	M682	E507	K523	Q443	ILE
Q2235	M2164	Q2100	K2020	Y1837	Y1836	Y1762	ARG	ARG	M683	E507	K523	S446	GLN
K2239	E2165	I2102	K2020	G1923	Y1837	Y1762	ARG	ARG	M683	E507	K523	S446	GLN
T2244	C2169	I2103	G2026	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
T2245	D2170	M2104	K2027	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
Q2246	Y2105	S2106	A2028	M1926	D1946	A1765	GLN	PRO	G686	R612	G528	L449	VAL
G2247	T2107	L2107	A2028	D1928	D1946	A1765	GLN	PRO	G686	R612	G528	L449	VAL
V2248	S2175	L2108	I2032	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
K2249	L2178	G2109	Q2036	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
S2250	G2110	K2110	T2037	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
S2254	E2181	Q2112	T2038	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
S2254	S2182	Q2113	A2039	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
V2257	K2183	T2114	Y2043	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
K2258	A2184	Y2115	G2044	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
E2259	T2185	R2116	Q2045	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2260	S2186	G2117	Q2046	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
L2261	D2187	N2118	A2047	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
L2262	S2188	S2119	P2048	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
S2263	G2120	K2049	K2049	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
S2264	G2121	L2050	L2050	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
S2265	T2122	K2051	K2051	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
K2269	L2123	R2052	R2052	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
Q2270	M2124	L2053	L2053	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
K2271	F2126	H2054	H2054	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2274	T2197	V1965	V1965	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2275	N2198	K1966	K1966	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
Q2276	M2199	K1967	K1967	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
N2277	T2202	S2133	S2133	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
Q2278	W2203	G2134	G2134	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
K2279	S2204	I2135	I2135	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
V2280	P2205	H2137	H2137	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2283	R2209	N2140	N2140	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
Q2284	L2210	F2141	F2141	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
G2285	H2211	P2142	P2142	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
K2286	L2212	Q2143	Q2143	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2292	Q2213	I2144	I2144	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
V2293	G2214	I2145	I2145	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
V2294	S2215	A2146	A2146	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
N2295	R2216	R2147	R2147	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
D2298	L2217	I2149	I2149	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2299	R2220	R2150	R2150	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
F2300	P2221	L2151	L2151	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
L2301	Q2222	H2152	H2152	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
L2302	T2223	L2153	L2153	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG
	N2224	T2154	T2154	Y1924	V1841	R1764	PHE	ARG	N684	A610	P526	G447	ARG



- 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%



- 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%



- 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%



- 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%



- 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%



- 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:



HA01
HA02
HA03
HA04
HA05
HA06

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.00 Å 135.86 Å 196.11 Å 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) 99.9 (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 3.19 Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.206 , 0.287 0.206 , 0.287	Depositor DCC
R_{free} test set	3077 reflections (4.94%)	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)	0.29 , 47.2	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	0.91	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, BMA, NAG, CU1, CA, FUC, 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	0.54	5/10434 (0.0%)	0.78	8/14149 (0.1%)
1	B	0.49	1/10367 (0.0%)	0.72	7/14053 (0.0%)
All	All	0.51	6/20801 (0.0%)	0.75	15/28202 (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	B	2150	ARG	CZ-NH2	-7.05	1.23	1.33
1	A	191	GLN	CD-NE2	6.91	1.50	1.32
1	A	2174	CYS	CA-CB	-6.57	1.39	1.53
1	A	191	GLN	CD-OE1	-6.53	1.09	1.24
1	A	2016	VAL	CB-CG2	-5.65	1.41	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CG-CD-OE1	29.15	179.90	121.60
1	A	191	GLN	CA-CB-CG	19.14	155.50	113.40
1	A	191	GLN	CG-CD-NE2	-14.70	81.43	116.70
1	A	191	GLN	OE1-CD-NE2	-10.11	98.66	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CB-CG-CD	-8.73	88.89	111.60

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	424	2
1	B	10084	0	9837	506	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	927	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 23.

The worst 5 of 927 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:CE	1:B:2150:ARG:HH21	1.60	1.12
1:B:2104:MET:HE2	1:B:2150:ARG:HH21	1.04	1.10
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%)	1	5
1	B	1231/1467 (84%)	955 (78%)	182 (15%)	94 (8%)	1	7
All	All	2473/2934 (84%)	1921 (78%)	356 (14%)	196 (8%)	1	6

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 ⓘ

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	1110/1301 (85%)	1074 (97%)	36 (3%)	39	71
1	B	1104/1301 (85%)	1079 (98%)	25 (2%)	50	78
All	All	2214/2602 (85%)	2153 (97%)	61 (3%)	43	74

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2055	TYR
1	A	2295	ASN
1	B	1983	PHE
1	A	2110	LYS
1	A	2157	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2246	GLN
1	B	26	HIS
1	B	318	HIS
1	A	2082	HIS
1	B	233	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 ⓘ

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	1.07	1 (7%)	17,19,21	2.05	3 (17%)
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.44	0
2	BMA	C	3	2	11,11,12	1.38	3 (27%)	15,15,17	1.21	0
2	MAN	C	4	2	11,11,12	0.81	0	15,15,17	1.00	1 (6%)
2	MAN	C	5	2	11,11,12	1.47	3 (27%)	15,15,17	2.08	4 (26%)
3	NAG	D	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	1.41	3 (17%)
3	NAG	D	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.29	2 (11%)
3	BMA	D	3	3	11,11,12	1.49	2 (18%)	15,15,17	0.91	0
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	0.67	0
2	NAG	E	2	2	14,14,15	0.68	0	17,19,21	1.85	5 (29%)
2	BMA	E	3	2	11,11,12	1.98	4 (36%)	15,15,17	1.27	1 (6%)
2	MAN	E	4	2	11,11,12	1.59	2 (18%)	15,15,17	1.36	2 (13%)
2	MAN	E	5	2	11,11,12	0.87	0	15,15,17	1.05	0
2	NAG	F	1	1,2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	F	2	2	14,14,15	0.73	1 (7%)	17,19,21	0.68	0
2	BMA	F	3	2	11,11,12	1.69	3 (27%)	15,15,17	2.41	8 (53%)
2	MAN	F	4	2	11,11,12	2.04	4 (36%)	15,15,17	2.98	5 (33%)
2	MAN	F	5	2	11,11,12	0.62	0	15,15,17	2.20	3 (20%)
4	NAG	G	1	1,4	14,14,15	0.55	0	17,19,21	1.07	1 (5%)
4	NAG	G	2	4	14,14,15	0.55	0	17,19,21	1.42	3 (17%)
4	BMA	G	3	4	11,11,12	1.20	2 (18%)	15,15,17	1.17	2 (13%)
4	MAN	G	4	4	11,11,12	1.09	1 (9%)	15,15,17	1.65	2 (13%)
4	NAG	G	5	4	14,14,15	0.41	0	17,19,21	1.50	3 (17%)
4	MAN	G	6	4	11,11,12	1.04	1 (9%)	15,15,17	1.81	4 (26%)
4	FUC	G	7	4	10,10,11	1.17	1 (10%)	14,14,16	1.20	1 (7%)
5	NAG	H	1	1,5	14,14,15	0.68	1 (7%)	17,19,21	0.76	0
5	NAG	H	2	5	14,14,15	0.61	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	H	3	5	11,11,12	1.09	0	15,15,17	1.41	2 (13%)
5	MAN	H	4	5	11,11,12	0.99	0	15,15,17	1.26	1 (6%)
5	MAN	H	5	5	11,11,12	1.28	1 (9%)	15,15,17	1.17	1 (6%)
5	MAN	H	6	5	11,11,12	1.57	3 (27%)	15,15,17	1.04	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	-	4/6/23/26	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	-	5/6/23/26	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	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	MAN	C4-C5	-4.45	1.43	1.53
2	E	4	MAN	O5-C5	3.91	1.51	1.43
2	E	3	BMA	C1-C2	3.83	1.60	1.52
2	E	3	BMA	C2-C3	3.64	1.57	1.52
2	C	1	NAG	O5-C1	3.62	1.49	1.43

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-O5-C5	7.18	121.92	112.19
2	F	5	MAN	C1-O5-C5	6.92	121.56	112.19
2	C	5	MAN	C1-O5-C5	6.20	120.59	112.19
2	F	4	MAN	C2-C3-C4	6.07	121.39	110.89
2	C	1	NAG	C1-O5-C5	5.99	120.31	112.19

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	F	4	MAN	O5-C5-C6-O6

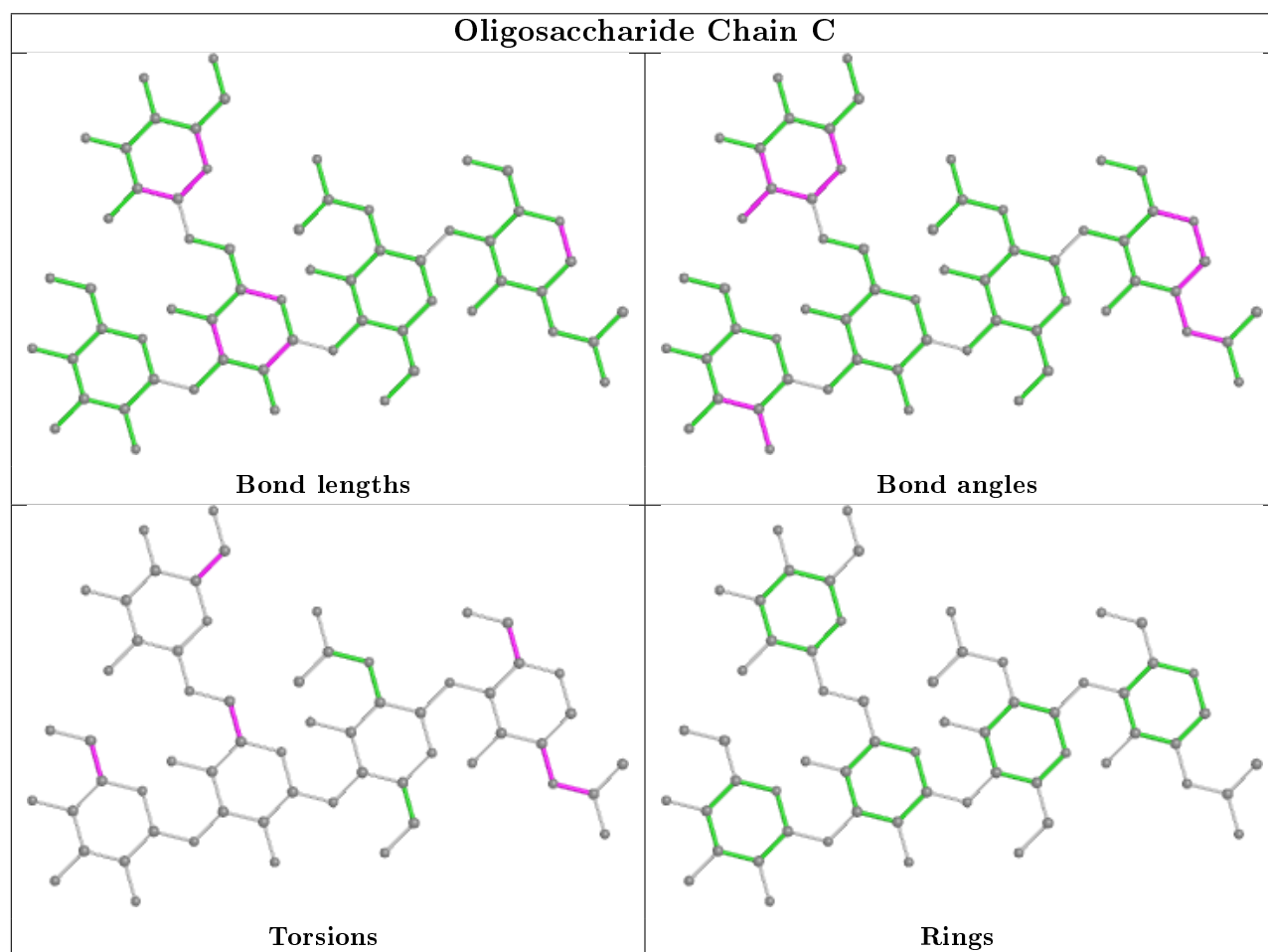
All (2) ring outliers are listed below:

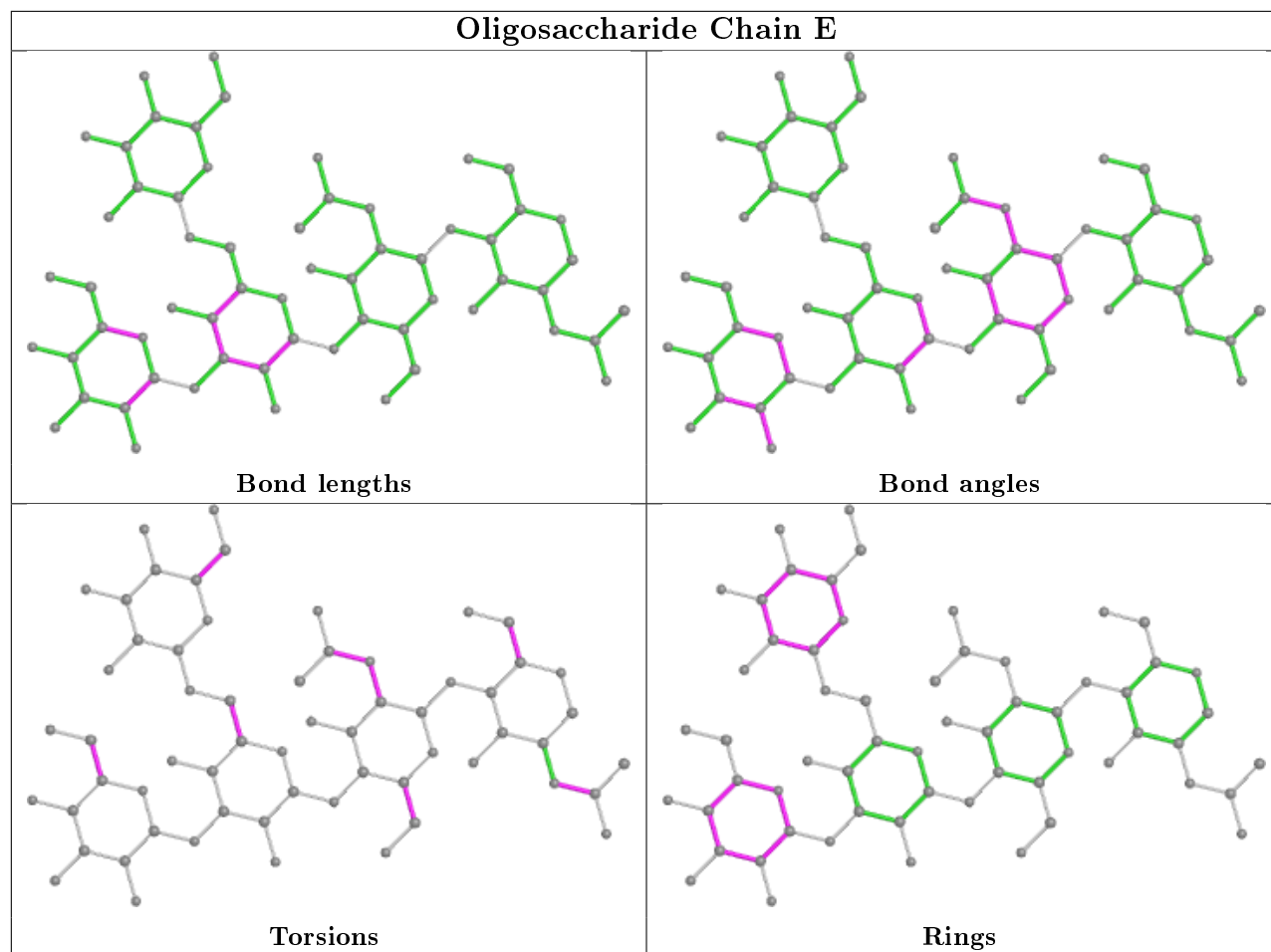
Mol	Chain	Res	Type	Atoms
2	E	5	MAN	C1-C2-C3-C4-C5-O5
2	E	4	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 11 short contacts:

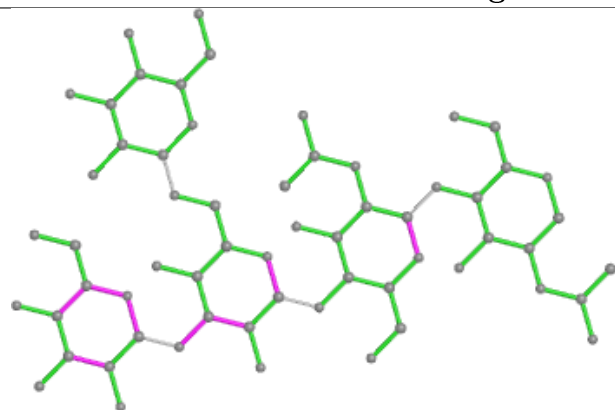
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	C	1	NAG	1	0
5	H	1	NAG	1	0
4	G	2	NAG	2	0
2	F	4	MAN	0	2
5	H	4	MAN	1	0
2	E	1	NAG	1	0
2	C	2	NAG	2	0
5	H	5	MAN	1	0
4	G	1	NAG	1	0
5	H	2	NAG	1	0

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

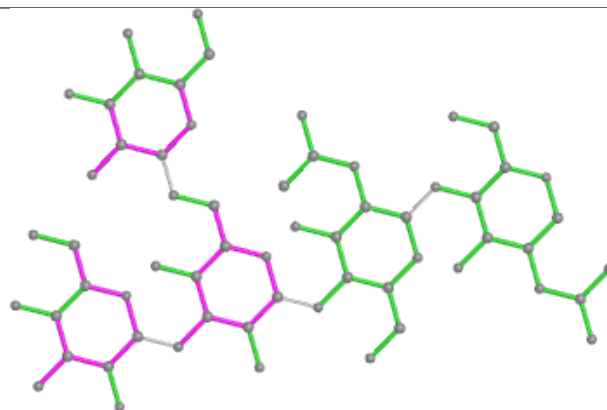




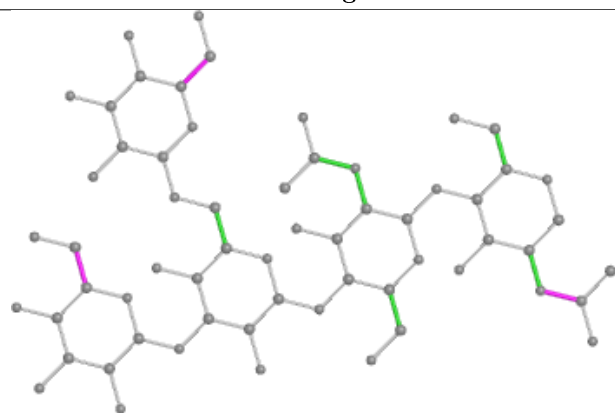
Oligosaccharide Chain F



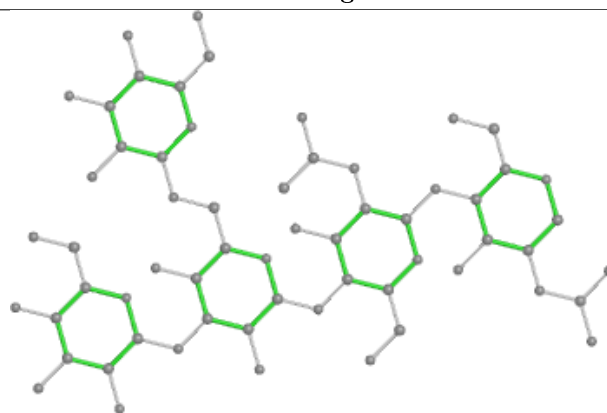
Bond lengths



Bond angles

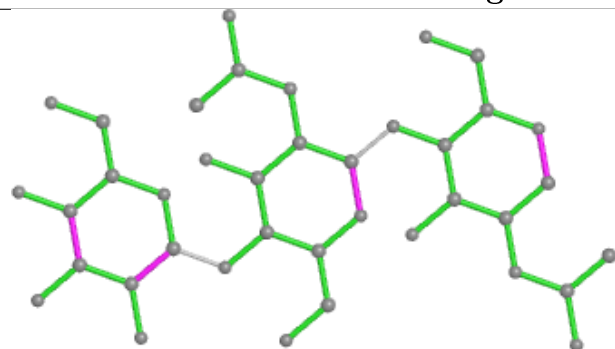


Torsions

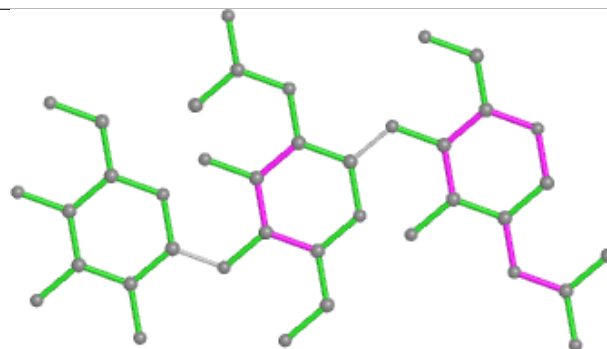


Rings

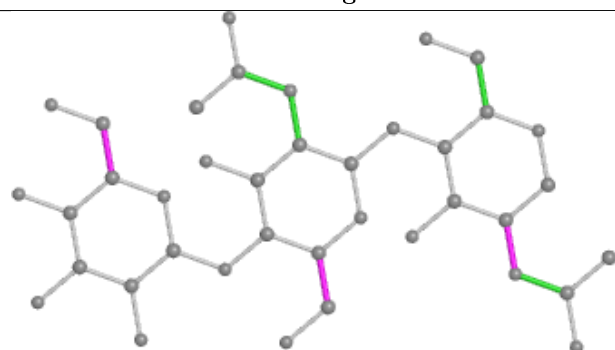
Oligosaccharide Chain D



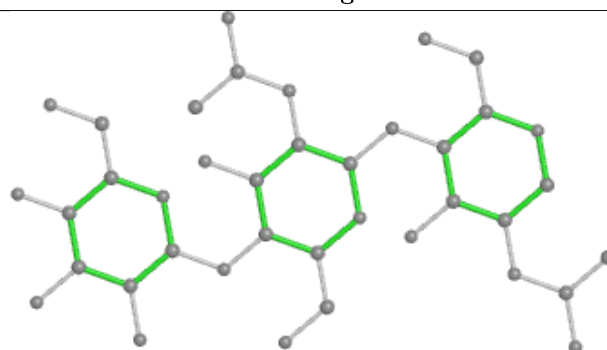
Bond lengths



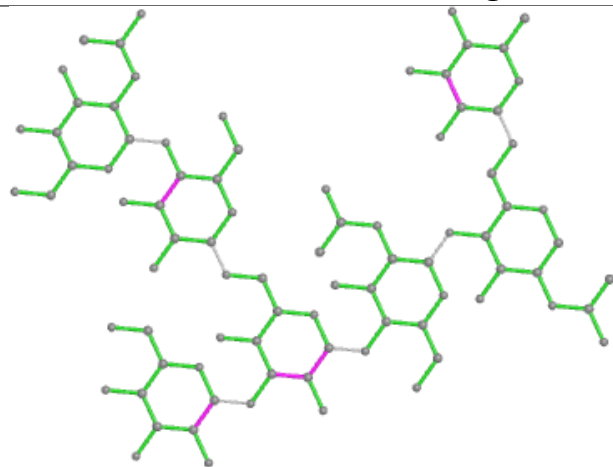
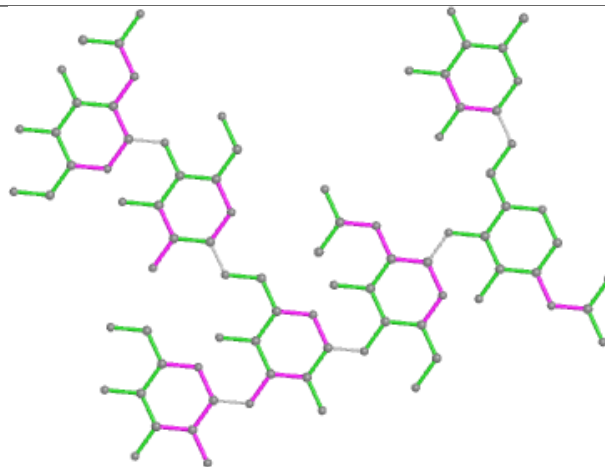
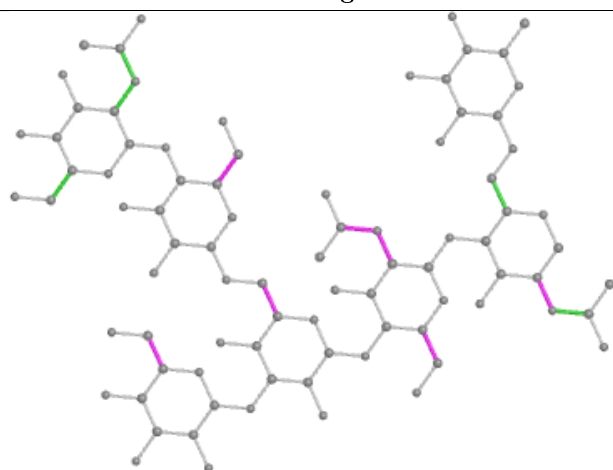
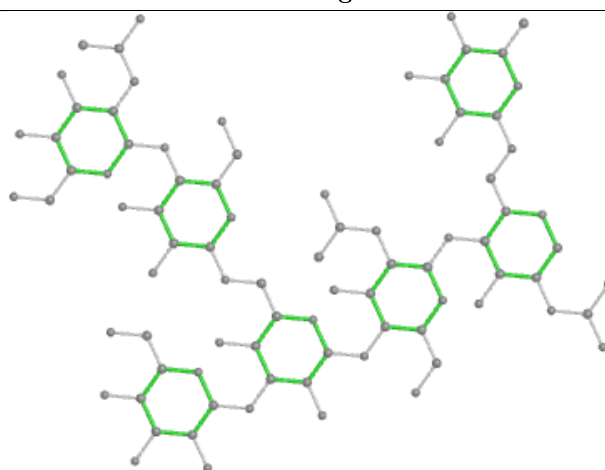
Bond angles

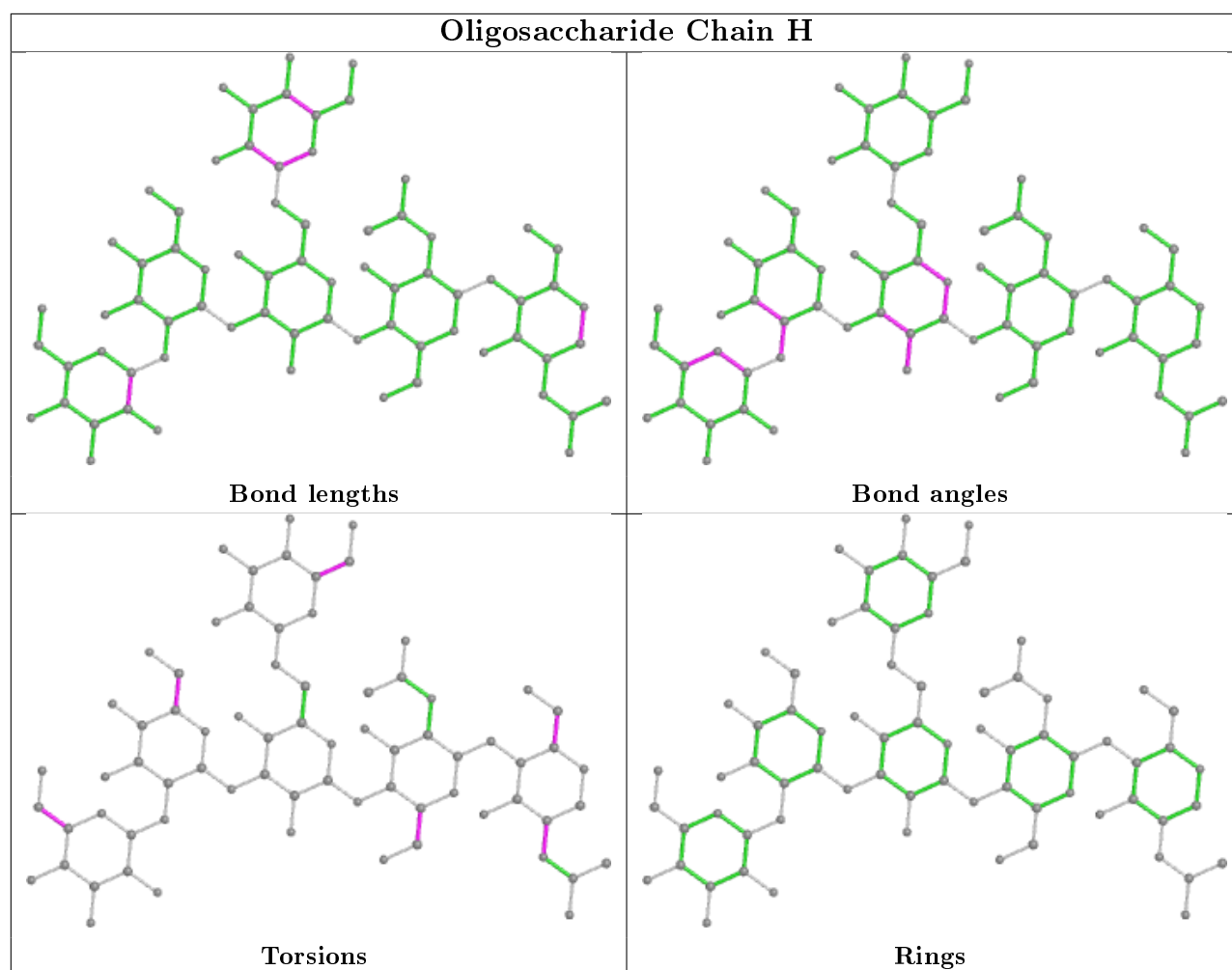


Torsions



Rings

Oligosaccharide Chain G**Bond lengths****Bond angles****Torsions****Rings**



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%)	-0.29	22 (1%) 68 55	30, 48, 88, 273	0
1	B	1247/1467 (85%)	-0.13	35 (2%) 53 37	30, 58, 130, 157	0
All	All	2503/2934 (85%)	-0.21	57 (2%) 60 47	30, 52, 119, 273	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	THR	9.4
1	A	37	GLY	9.1
1	A	40	PRO	8.6
1	A	33	ALA	7.9
1	B	2318	ALA	6.3

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	MAN	F	5	11/12	0.49	0.59	149,151,160,160	0
2	MAN	E	4	11/12	0.52	0.33	117,124,129,131	0
5	MAN	H	5	11/12	0.57	0.42	125,134,142,149	0
2	BMA	F	3	11/12	0.59	0.60	131,138,150,151	0

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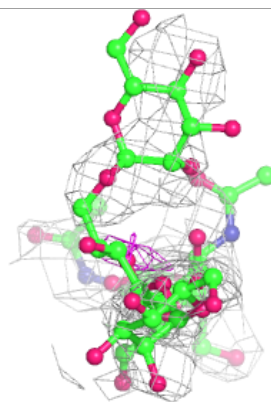
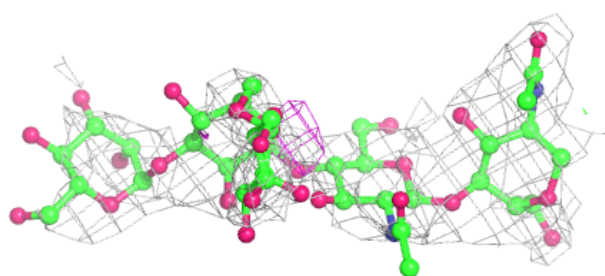
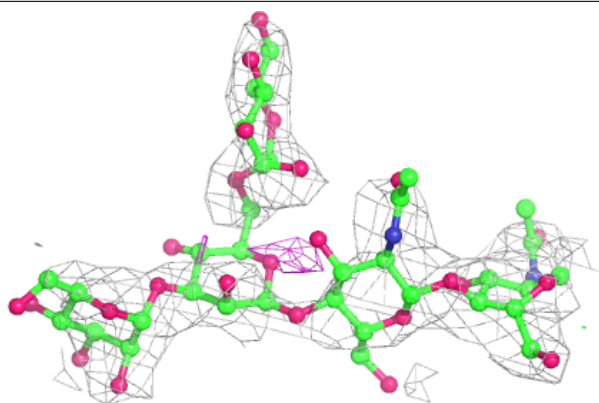
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	C	3	11/12	0.60	0.61	144,158,163,164	0
4	NAG	G	2	14/15	0.61	0.39	118,133,142,145	0
2	NAG	F	2	14/15	0.61	0.37	130,144,153,154	0
3	BMA	D	3	11/12	0.62	0.56	134,157,162,163	0
5	MAN	H	6	11/12	0.63	0.30	99,113,125,126	0
2	NAG	C	2	14/15	0.64	0.47	128,137,149,156	0
2	MAN	C	4	11/12	0.64	0.56	148,158,161,163	0
4	NAG	G	5	14/15	0.67	0.32	78,93,101,102	0
2	MAN	C	5	11/12	0.70	0.51	138,145,151,156	0
2	MAN	F	4	11/12	0.71	0.43	77,96,119,134	0
2	NAG	F	1	14/15	0.72	0.33	86,120,136,142	0
3	NAG	D	2	14/15	0.74	0.38	114,145,152,154	0
4	BMA	G	3	11/12	0.75	0.39	123,144,149,152	0
5	NAG	H	2	14/15	0.75	0.28	73,95,100,103	0
4	MAN	G	6	11/12	0.77	0.36	128,135,144,145	0
4	NAG	G	1	14/15	0.78	0.23	99,116,124,128	0
2	NAG	E	2	14/15	0.79	0.28	74,105,116,122	0
2	BMA	E	3	11/12	0.79	0.24	112,121,126,127	0
4	MAN	G	4	11/12	0.80	0.22	69,97,108,110	0
4	FUC	G	7	10/11	0.80	0.41	124,134,139,144	0
3	NAG	D	1	14/15	0.82	0.38	95,131,141,144	0
5	MAN	H	4	11/12	0.84	0.18	105,120,127,133	0
2	MAN	E	5	11/12	0.84	0.16	84,109,119,120	0
5	BMA	H	3	11/12	0.86	0.18	108,114,120,123	0
2	NAG	C	1	14/15	0.88	0.28	79,89,109,121	0
2	NAG	E	1	14/15	0.89	0.18	78,83,92,104	0
5	NAG	H	1	14/15	0.91	0.18	81,86,93,93	0

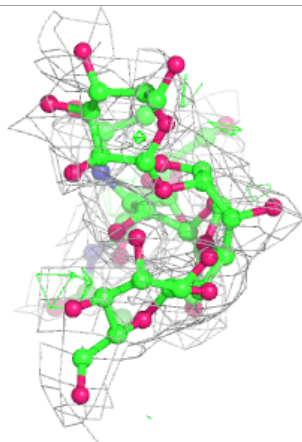
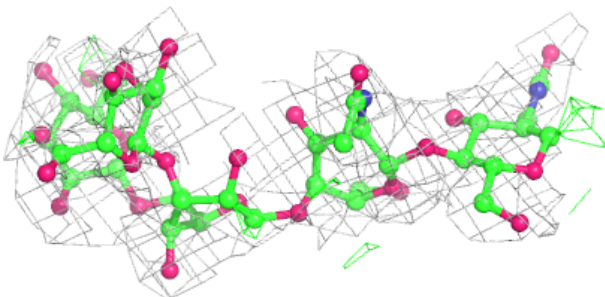
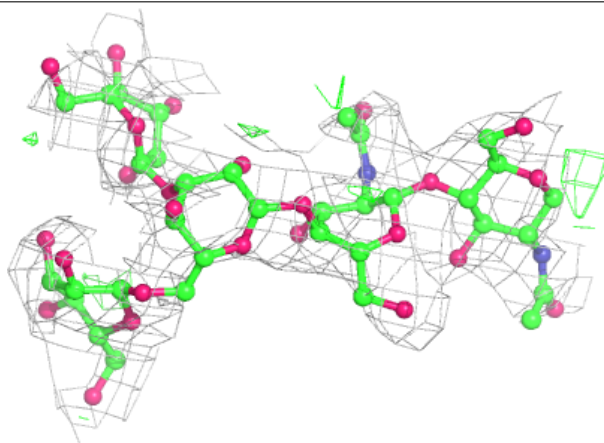
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

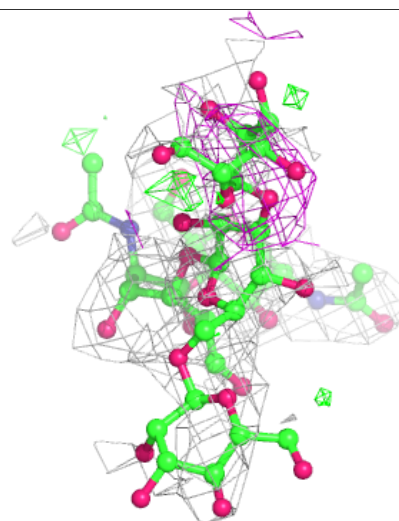
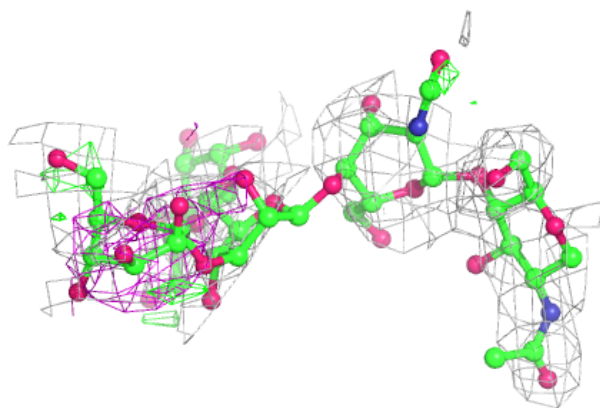
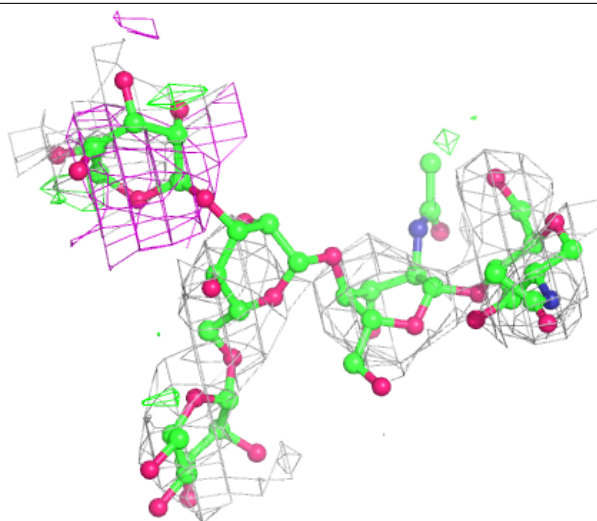
**Electron density around Chain E:**

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



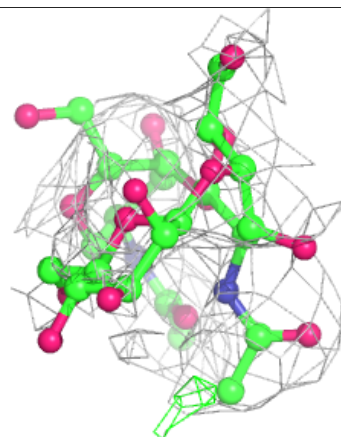
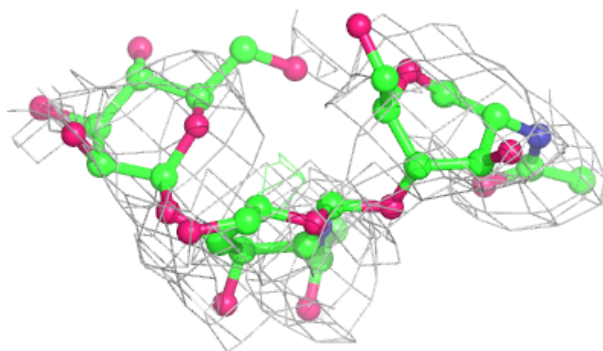
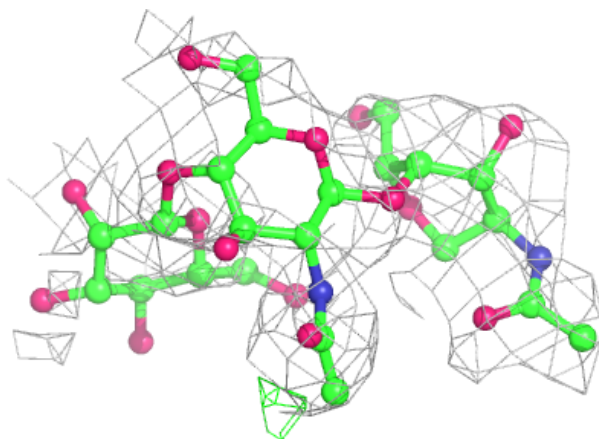
Electron density around Chain F:

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



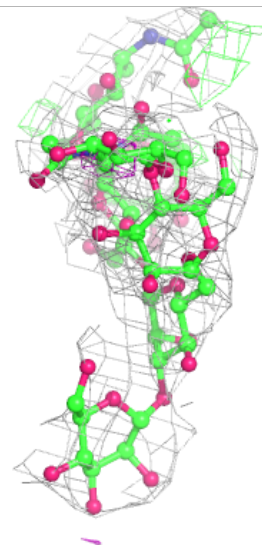
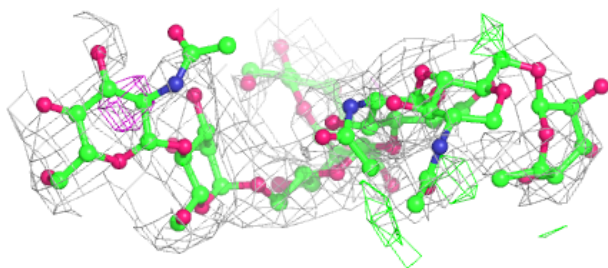
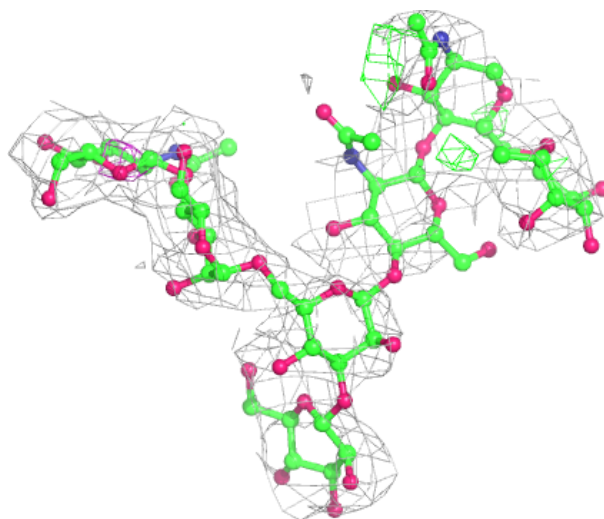
Electron density around Chain D:

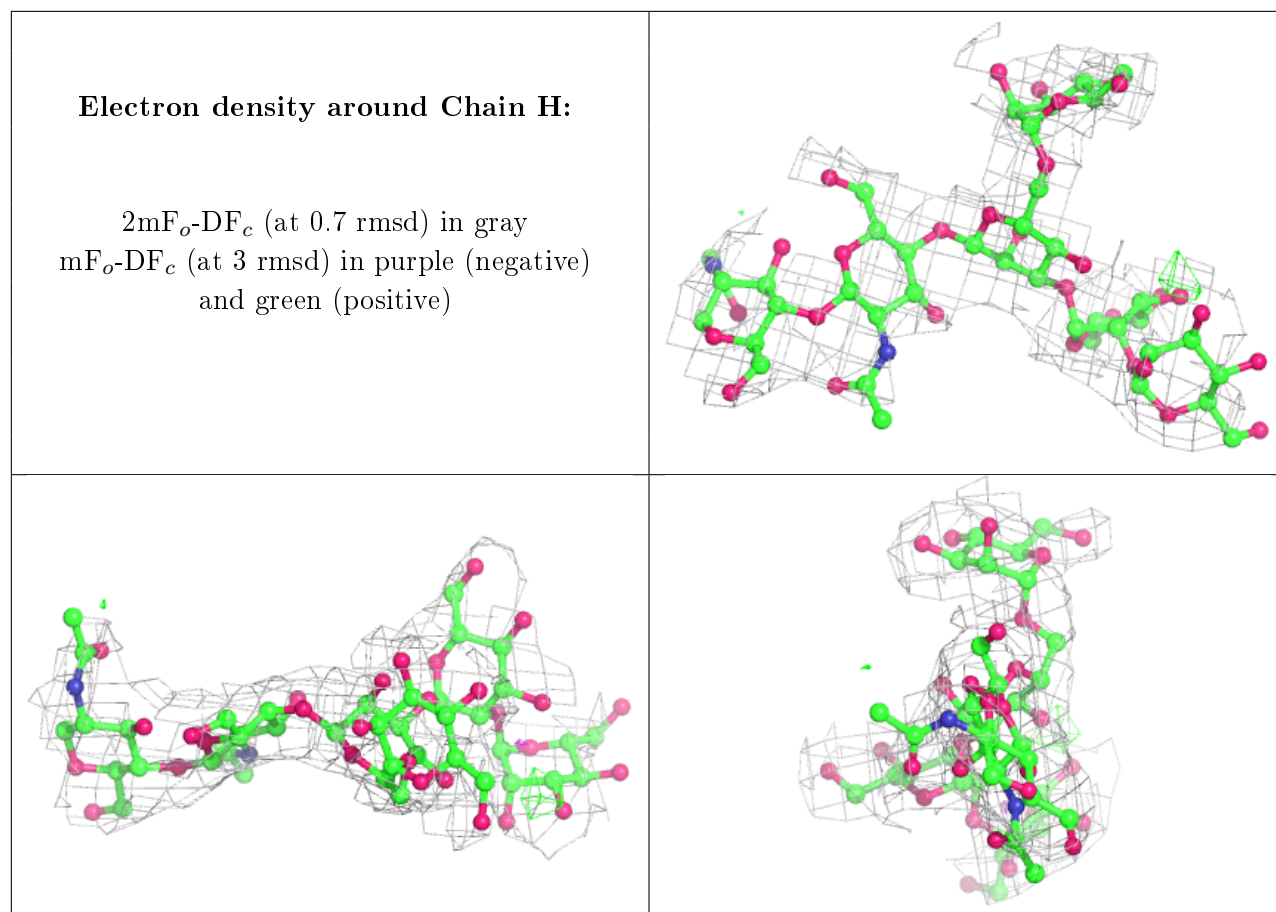
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å ²)	Q<0.9
7	ZN	A	2415	1/1	0.97	0.15	46,46,46,46	0
6	CA	B	2419	1/1	0.98	0.20	59,59,59,59	0
8	CU1	B	2421	1/1	0.99	0.22	48,48,48,48	0
8	CU1	A	2416	1/1	0.99	0.20	40,40,40,40	0
6	CA	A	2414	1/1	0.99	0.20	40,40,40,40	0
7	ZN	B	2420	1/1	1.00	0.19	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.