WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 04:27 AM EDT

PDB ID	:	3CDZ
Title	:	Crystal structure of human factor VIII
Authors	:	Ngo, J.C.; Huang, M.; Roth, D.A.; Furie, B.C.; Furie, B.
Deposited on	:	2008-02-27
Resolution	:	3.98 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

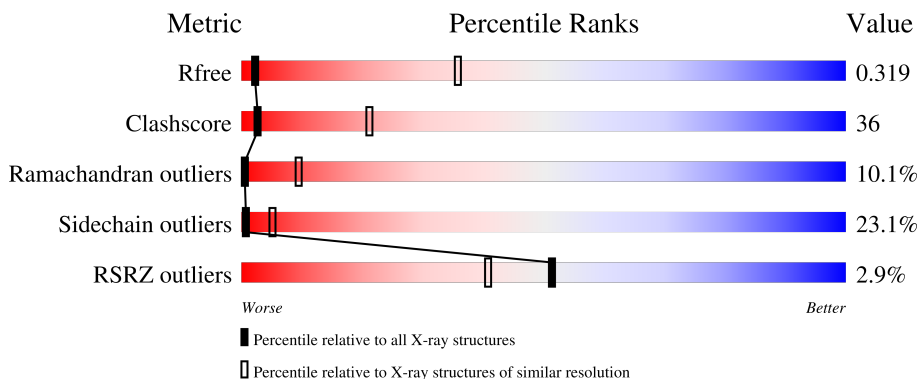|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.98 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	Percentile Ranks	Value
Rfree		0.319
Clashscore		36
Ramachandran outliers		10.1%
Sidechain outliers		23.1%
RSRZ outliers		2.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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 <=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	754	2% / 27% / 38% / 15% / • / 16%
2	B	684	3% / 36% / 41% / 14% / • / 8%
3	C	2	50% / 50%
4	D	4	75% / 25%

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
4	MAN	D	2	X	-	-	-
4	MAN	D	4	X	-	-	-
7	NAG	B	2333	X	-	-	-
7	NAG	B	2334	X	-	-	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 10317 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total 5086	C 3278	N 855	O 928	S 25	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	SER	-	SEE REMARK 999	UNP P00451
A	742	PHE	-	SEE REMARK 999	UNP P00451
A	743	SER	-	SEE REMARK 999	UNP P00451
A	744	GLN	-	SEE REMARK 999	UNP P00451
A	745	ASN	-	SEE REMARK 999	UNP P00451
A	746	PRO	-	SEE REMARK 999	UNP P00451
A	747	PRO	-	SEE REMARK 999	UNP P00451
A	748	VAL	-	SEE REMARK 999	UNP P00451
A	749	LEU	-	SEE REMARK 999	UNP P00451
A	750	LYS	-	SEE REMARK 999	UNP P00451
A	751	ARG	-	SEE REMARK 999	UNP P00451
A	752	HIS	-	SEE REMARK 999	UNP P00451
A	753	GLN	-	SEE REMARK 999	UNP P00451
A	754	ARG	-	SEE REMARK 999	UNP P00451

- Molecule 2 is a protein called Coagulation factor VIII light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	631	Total 5125	C 3288	N 881	O 924	S 32	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1880	LEU	PHE	variant	UNP P00451

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
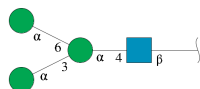
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O1
HO

O5
O

C1(R) C5(R)

C6

C2(R) C4(S)
C3(R)

N2
HN

OH
O4

C7

OH
O3

C8

O
O7

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	B	1	Total 14	C 8	N 1	O 5	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 =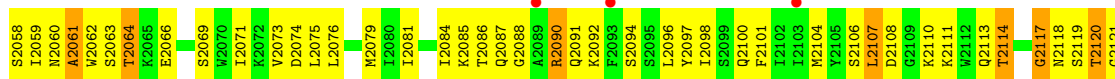 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Coagulation factor VIII heavy chain

V663 Y664 E665 D666 T667 L668 T669 L670 F671 P672 F673 S674 G675 E676 T677 V678 F679 M680 S681 M682 E683 N684 P685 G686 L687 W688 I689 L690 G691 N694 S695 D696 F697 R698 N699 A704 L705 L706 K707 V708 S709 S710 C711 D712 K713 ASN THR GLY ASP TYR TYR GLU ASP SER TYR GLU ASP ILE

SER ALA TYR LEU SER ASN ILE GLU PRO SER PHE SER GLN ASN PRO VAL LEU LYS ARG HIS GLN ARG

• Molecule 2: Coagulation factor VIII light chain

Chain B:

3%

36%   41%   14%   •   8%

GLU ILE THR ARG THR THR LEU GLN SER ASP GLN GLU GLU ILE ASP TYR ASP ASP THR ILE SER VAL GLU MET LYS LYS GLU ASP PHE ASP ILE TYR ASP ASP GLU ASN GLN SER PRO ARG SER F1691 Q1692 K1693 K1694 T1695 R1696 H1697 Y1698 F1699 V1703 E1704 R1705 L1706 W1707 D1708 Y1709 G1710

M1711 S1712 S1713 SER PRO HIS VAL LEU ARG ASN ARG ALA GLN SER G1725 S1726 V1727 P1728 Q1729 F1730 K1731 K1732 V1733 V1734 F1735 Q1736 E1737 F1738 T1739 S1742 F1743 T1744 Q1745 P1746 L1747 Y1748 L1752 N1753 E1754 H1755 L1756 L1757 L1758 L1759 G1760 P1761 Y1762 I1763 V1767 E1768 D1769 N1770 I1771 M1772 V1773 T1774

N1777 Q1778 A1779 S1780 R1781 P1782 Y1783 S1784 F1785 Y1786 S1787 S1788 L1789 I1790 S1791 Y1792 E1793 E1794 R1797 Q1798 G1799 A1800 E1801 P1802 R1803 V1807 K1808 P1809 K1813 T1814 Y1815 F1816 Q1820 H1821 H1822 M1823 T1826 K1827 D1828 E1829 F1830 D1831 C1832 K1833 A1834 W1835 A1836 Y1837 F1838 S1839 I1843 E1844 K1845 D1846

V1847 H1848 S1849 G1850 L1851 I1852 G1853 P1854 V1857 T1860 N1861 M1864 P1865 A1866 H1867 G1868 R1869 Q1870 V1871 T1872 V1873 Q1874 E1875 F1876 A1877 L1878 F1879 L1880 F1883 D1884 E1885 T1886 K1887 S1888 W1889 Y1890 F1891 T1892 E1893 R1897 N1898 C1899 R1900 A1901 P1902 C1903 N1904 I1905 Q1906 M1907 E1908 D1909 P1910 T1911 F1912

K1913 E1914 N1915 Y1916 R1917 F1918 I1921 N1922 G1923 Y1924 I1925 M1926 D1927 T1928 L1929 P1930 G1931 L1932 V1933 M1934 A1935 Q1936 D1937 Q1938 R1939 I1940 R1941 W1942 Y1943 L1944 L1945 S1946 S1949 N1950 E1951 N1952 I1953 I1956 H1957 F1958 S1959 G1960 H1961 V1962 F1963 T1964 V1965 R1966 K1967 K1968 E1969 E1970 Y1971 K1972 M1973 A1974 L1975

Y1976 N1977 L1978 Y1979 F1983 E1984 T1985 V1986 S1991 I1995 W1996 R1997 V1998 L2001 I2002 G2003 L2006 M2010 S2011 T2012 L2013 F2014 L2015 P2024 L2025 G2026 M2027 H2031 I2032 R2033 D2034 F2035 G2036 I2037 T2038 A2039 S2040 G2041 G2042 Y2043 G2044 Q2045 W2046 A2047 P2048 K2049 L2050 A2051 R2052 Y2055

S2058 I2059 N2060 A2061 W2062 S2063 T2064 K2065 E2066 S2069 W2070 I2071 K2072 V2073 D2074 L2075 L2076 M2079 I2080 I2081 I2084 K2085 T2086 G2087 G2088 A2089 R2090 Q2091 K2092 S2094 S2095 L2096 Y2097 I2098 Q2100 F2101 I2102 I2103 M2104 Y2105 S2106 L2107 D2108 G2109 K2110 K2111 W2112 Q2113 T2114 G2117 N2118 S2119 T2120 G2121

T2122 F2126 F2127 G2128 N2129 V2130 D2131 S2132 I2135 K2136 H2137 F2140 N2141 P2142 P2143 I2144 I2145 I2149 R2150 T2154 H2155 Y2156 S2157 I2158 R2159 S2160 T2161 I2162 R2163 M2164 E2165 L2166 M2167 L2171 N2172 C2174 S2175 P2176 P2177 I2178 G2179 M2180 Q2189 I2190 T2191 A2192 S2193 M2199 F2200 P2205

S2206 K2207 A2208 R2209 L2210 H2211 L2212 A2218 V2223 N2224 N2225 P2226 K2227 E2228 Q2231 V2232 D2233 F2234 Q2235 K2236 T2237 M2238 G2242 V2243 T2244 V2248 K2249 S2250 L2251 L2252 M2255 Y2256 F2260 L2261 I2262 S2263 S2264 S2265 Q2266 Q2270 W2271 T2272 D2273 F2274 P2275 Q2276 N2277 K2281 V2282 Q2283 Q2284

Q2287 T2291 P2292 V2293 V2294 N2295 S2296 L2297 D2298 P2299 P2300 P2301 L2302 T2303 R2304 Y2305 L2306 R2307 I2308 H2309 P2310 Q2311 S2312 W2313 V2314 H2315 A2318 E2322 C2326 E2327 A2328 Q2329 D2330 L2331 Y2332

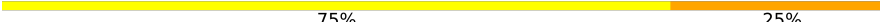• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain C:

50%   50%

NAG1 NAG2

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyran
ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

75%   25%

NAG1 MAN2 MAN3 MAN4

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.11Å 134.11Å 349.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.98 49.66 – 3.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.98) 98.6 (49.66-3.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.256 , 0.327 0.251 , 0.319	Depositor DCC
R_{free} test set	1399 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	151.1	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 203.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10317	wwPDB-VP
Average B, all atoms (Å^2)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CU, CA, MAN, 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	0.74	8/5230 (0.2%)	0.94	8/7098 (0.1%)
2	B	0.62	2/5270 (0.0%)	0.77	6/7136 (0.1%)
All	All	0.68	10/10500 (0.1%)	0.86	14/14234 (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	7
2	B	0	6
All	All	0	13

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	ARG	CZ-NH1	13.13	1.50	1.33
2	B	1904	ASN	CG-OD1	9.72	1.45	1.24
1	A	121	ARG	NE-CZ	8.65	1.44	1.33
2	B	1904	ASN	CG-ND2	8.33	1.53	1.32
1	A	107	LYS	CG-CD	6.53	1.74	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-24.01	108.29	120.30
1	A	121	ARG	NE-CZ-NH1	23.51	132.06	120.30
2	B	1945	LEU	CA-CB-CG	7.79	133.22	115.30
1	A	277	LEU	CA-CB-CG	7.46	132.46	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2050	LEU	CA-CB-CG	6.82	130.98	115.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Peptide
1	A	278	VAL	Peptide
1	A	281	HIS	Peptide
1	A	282	ARG	Peptide
1	A	56	ASP	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	5086	0	4971	402	0
2	B	5125	0	4994	354	0
3	C	28	0	25	1	0
4	D	47	0	40	2	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	B	28	0	26	0	0
All	All	10317	0	10056	737	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 36.

The worst 5 of 737 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:A:107:LYS:CG	1:A:107:LYS:CD	1.74	1.58
1:A:378:HIS:HB3	1:A:379:PRO:CD	1.71	1.19
2:B:1963:PHE:CD2	2:B:1986:VAL:HG21	1.77	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:CB	1:A:421:ARG:HG2	1.76	1.15
1:A:572:ASN:HB3	1:A:637:TRP:CZ3	1.82	1.15

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	622/754 (82%)	430 (69%)	130 (21%)	62 (10%)	0	9
2	B	627/684 (92%)	437 (70%)	126 (20%)	64 (10%)	0	9
All	All	1249/1438 (87%)	867 (69%)	256 (20%)	126 (10%)	0	9

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	A	133	SER
1	A	181	GLU
1	A	227	ALA
1	A	232	HIS

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	559/674 (83%)	414 (74%)	145 (26%)	0	4
2	B	560/612 (92%)	446 (80%)	114 (20%)	1	7
All	All	1119/1286 (87%)	860 (77%)	259 (23%)	1	5

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2132	SER
2	B	2163	ARG
1	A	497	HIS
1	A	484	ARG
2	B	2178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1820	GLN
2	B	1864	ASN
2	B	2266	GLN
2	B	1861	ASN
2	B	1867	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 ⓘ

6 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
3	NAG	C	1	3,1	14,14,15	0.87	0	17,19,21	1.08	1 (5%)
3	NAG	C	2	3	14,14,15	2.88	3 (21%)	17,19,21	1.74	2 (11%)
4	NAG	D	1	4	14,14,15	0.95	0	17,19,21	1.63	6 (35%)
4	MAN	D	2	4	11,11,12	0.65	0	15,15,17	1.64	2 (13%)
4	MAN	D	3	4	11,11,12	0.70	0	15,15,17	1.99	2 (13%)
4	MAN	D	4	4	11,11,12	0.80	0	15,15,17	1.70	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4	-	5/6/23/26	0/1/1/1
4	MAN	D	2	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	1/1/4/5	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O7-C7	8.00	1.41	1.23
3	C	2	NAG	C8-C7	-6.01	1.38	1.50
3	C	2	NAG	C1-C2	2.69	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3	MAN	C1-O5-C5	6.47	120.96	112.19
3	C	2	NAG	C4-C3-C2	5.16	118.58	111.02
4	D	2	MAN	C1-O5-C5	4.51	118.30	112.19
4	D	4	MAN	C1-C2-C3	3.86	114.42	109.67
4	D	4	MAN	C2-C3-C4	3.79	117.45	110.89

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	2	MAN	C1
4	D	4	MAN	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C3-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
4	D	1	NAG	2	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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths | Bond angles

Torsions | Rings
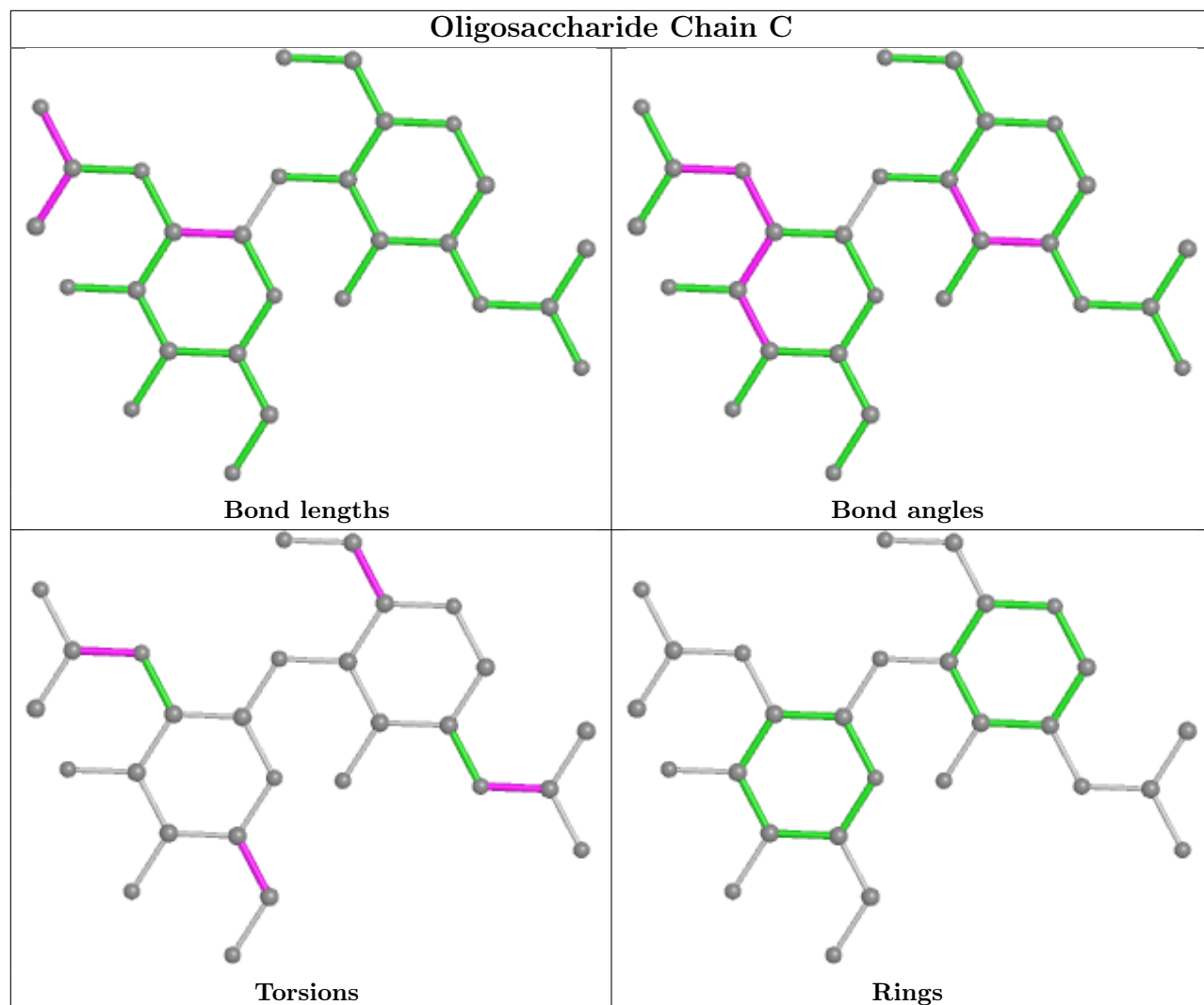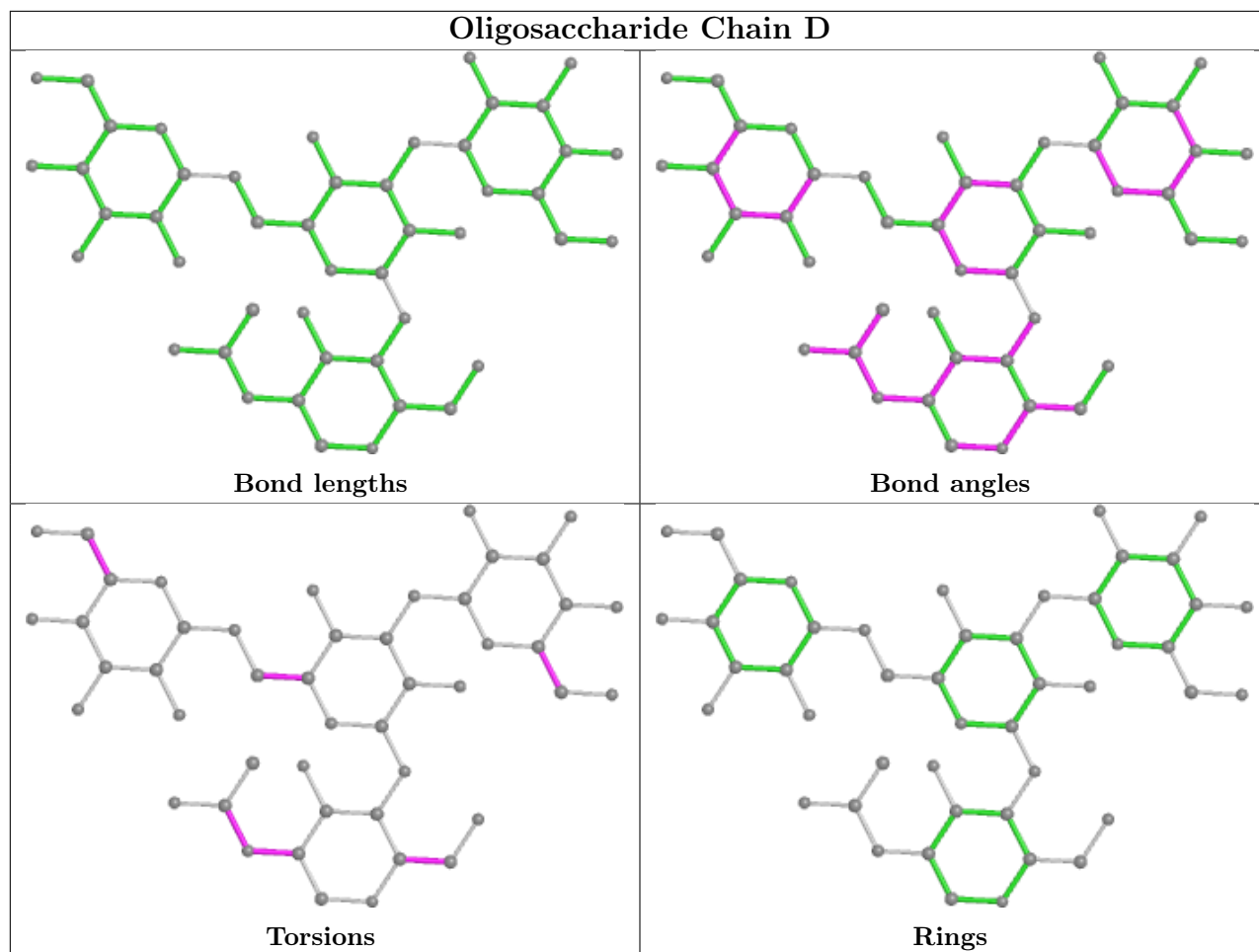
5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
7	NAG	B	2334	2	14,14,15	0.84	0	17,19,21	1.25	2 (11%)
7	NAG	B	2333	2	14,14,15	0.76	0	17,19,21	2.03	5 (29%)

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
7	NAG	B	2334	2	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	B	2333	2	1/1/5/7	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2333	NAG	C1-O5-C5	5.06	119.05	112.19
7	B	2333	NAG	C3-C4-C5	4.43	118.14	110.24
7	B	2334	NAG	C1-O5-C5	2.99	116.25	112.19
7	B	2333	NAG	C2-N2-C7	2.54	126.52	122.90
7	B	2334	NAG	C2-N2-C7	2.47	126.42	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	2333	NAG	C1
7	B	2334	NAG	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2333	NAG	C8-C7-N2-C2
7	B	2333	NAG	O7-C7-N2-C2
7	B	2334	NAG	C8-C7-N2-C2
7	B	2334	NAG	O7-C7-N2-C2
7	B	2334	NAG	O5-C5-C6-O6

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 (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	630/754 (83%)	0.14	18 (2%)	51	41	182, 196, 215, 239	0
2	B	631/684 (92%)	0.11	18 (2%)	51	41	181, 198, 214, 231	1 (0%)
All	All	1261/1438 (87%)	0.13	36 (2%)	51	41	181, 197, 215, 239	1 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1901	ALA	4.2
2	B	1902	PRO	4.0
1	A	333	PRO	3.9
2	B	2038	THR	3.3
2	B	2093	PHE	2.9

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
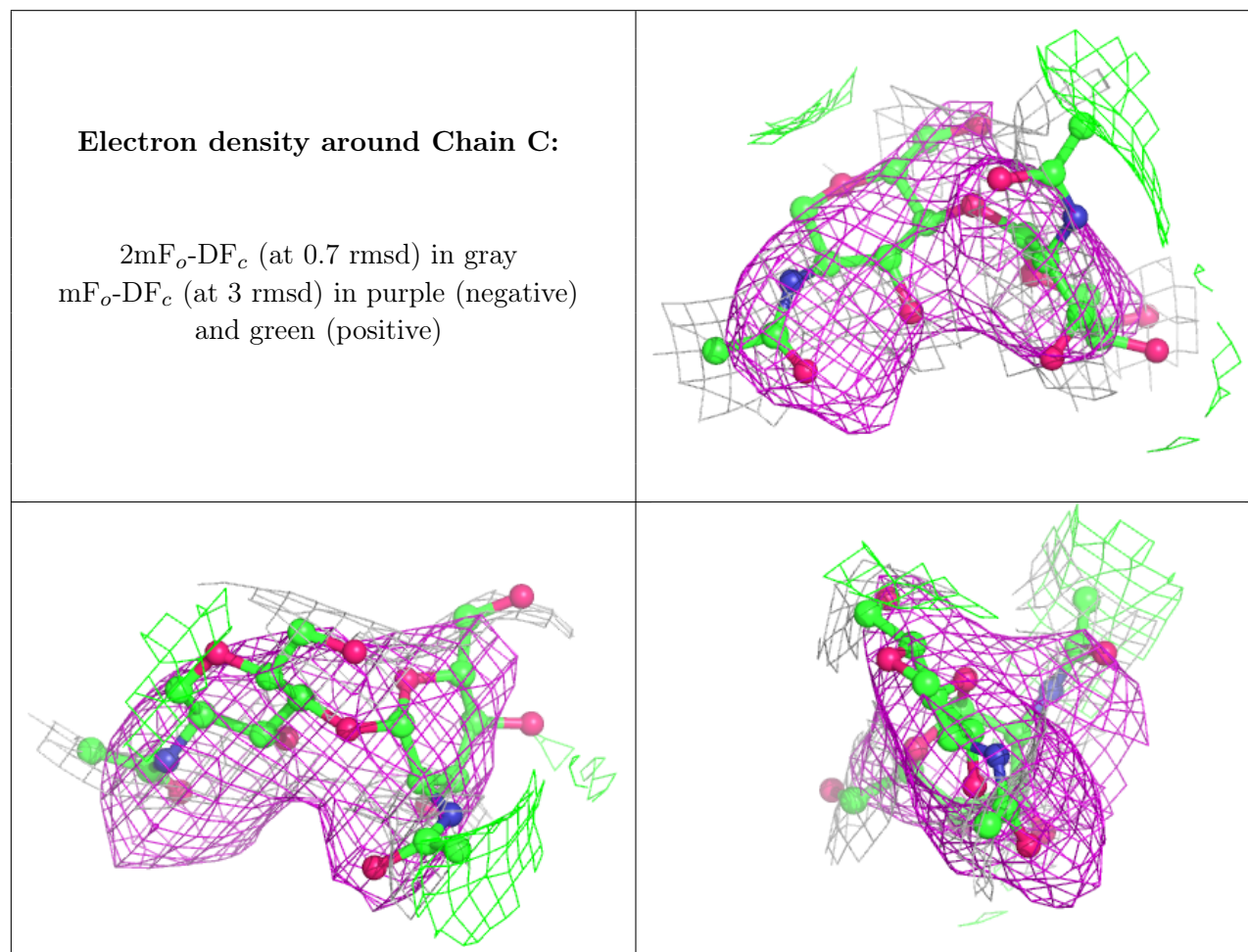
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	D	2	11/12	0.40	0.26	257,259,260,261	0
4	MAN	D	3	11/12	0.56	0.28	258,261,261,261	0
3	NAG	C	2	14/15	0.58	0.40	227,229,230,231	0
4	MAN	D	4	11/12	0.68	0.27	254,255,256,256	0
3	NAG	C	1	14/15	0.72	0.34	210,216,218,222	0

Continued on next page...

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
4	NAG	D	1	14/15	0.77	0.30	257,257,257,258	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:

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

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
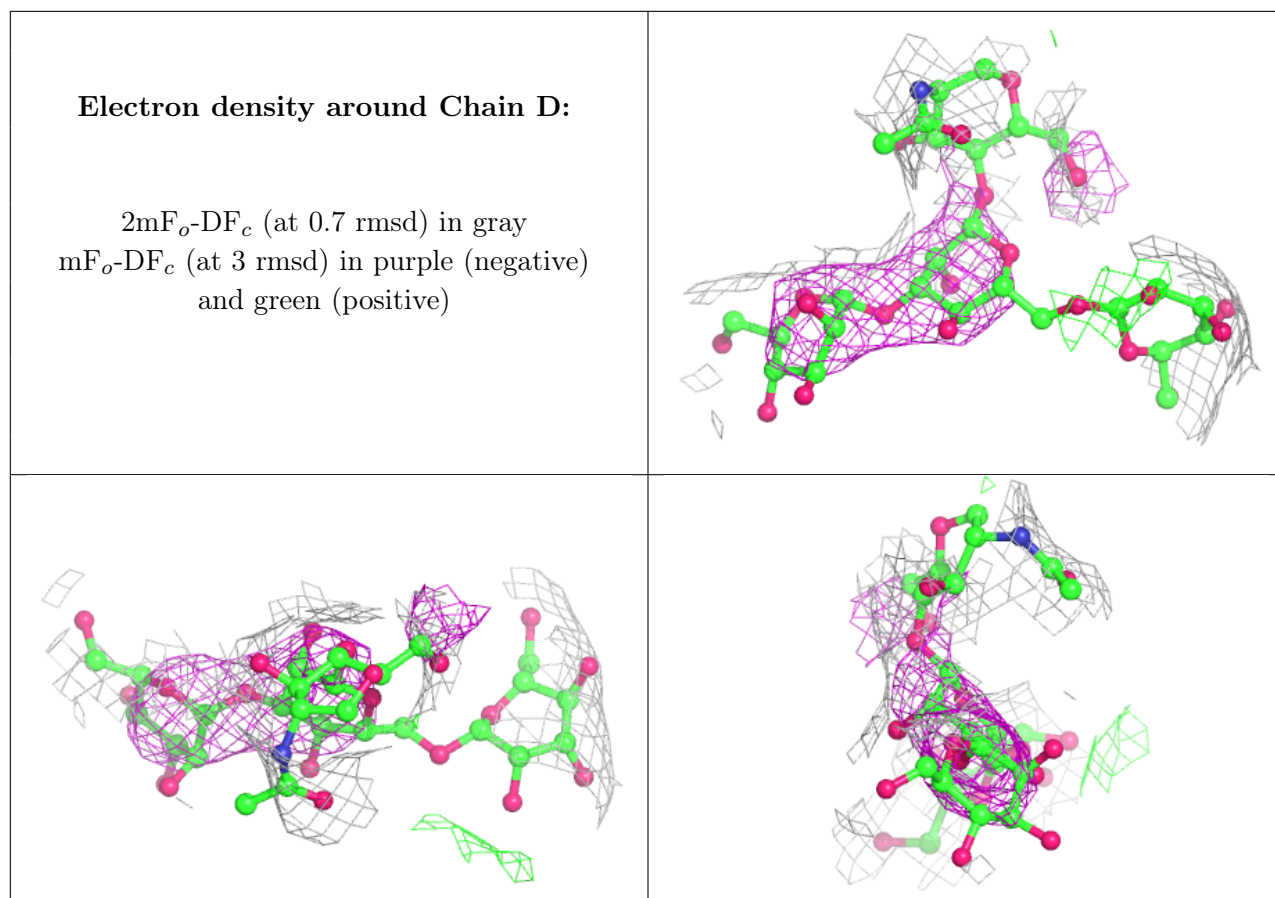
6.4 Ligands (i)

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	NAG	B	2333	14/15	0.86	0.49	210,213,214,214	0
7	NAG	B	2334	14/15	0.90	0.20	191,194,196,197	0
6	CA	A	758	1/1	0.91	0.13	172,172,172,172	0
5	CU	B	1	1/1	0.95	0.18	174,174,174,174	0
5	CU	A	757	1/1	1.00	0.16	171,171,171,171	0

6.5 Other polymers (i)

There are no such residues in this entry.