



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 05:12 pm GMT

PDB ID : 2X61  
Title : Crystal structure of the sialyltransferase CST-II in complex with trisaccharide acceptor and CMP  
Authors : Lee, H.J.; Lairson, L.L.; Rich, J.R.; Wakarchuk, W.W.; Withers, S.G.; Strynadka, N.C.J.  
Deposited on : 2010-02-16  
Resolution : 1.95 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

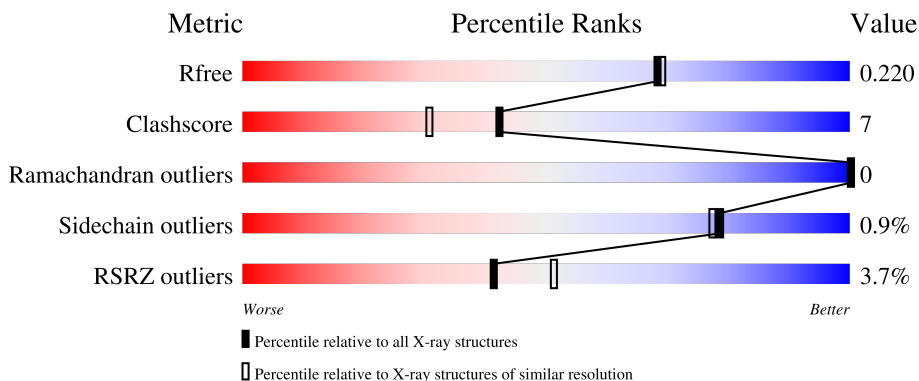
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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	258	 3% 87% 7% 5%
1	B	258	 4% 87% 7% 6%
2	C	3	 33% 67%
2	D	3	 100%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	SIA	C	3	X	-	-	-
2	SIA	D	3	X	-	-	-
4	MPD	A	1263	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4512 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.

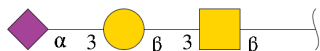
- Molecule 1 is a protein called ALPHA-2,3-/2,8-SIALYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	Total 2057	C 1353	N 321	O 375	S 8	0	2	0
1	B	243	Total 2030	C 1334	N 317	O 371	S 8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	SER	ILE	engineered mutation	UNP Q9LAK3
A	222	GLY	GLU	engineered mutation	UNP Q9LAK3
B	53	SER	ILE	engineered mutation	UNP Q9LAK3
B	222	GLY	GLU	engineered mutation	UNP Q9LAK3

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose.



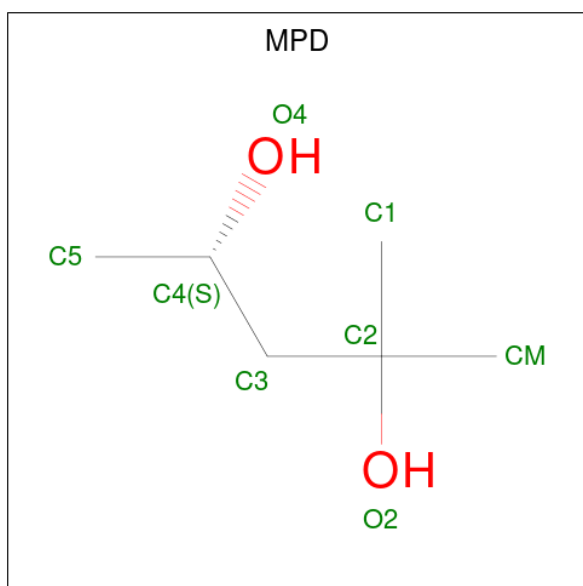
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	Total 46	C 25	N 2	O 19	0	0	0
2	D	3	Total 46	C 25	N 2	O 19	0	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



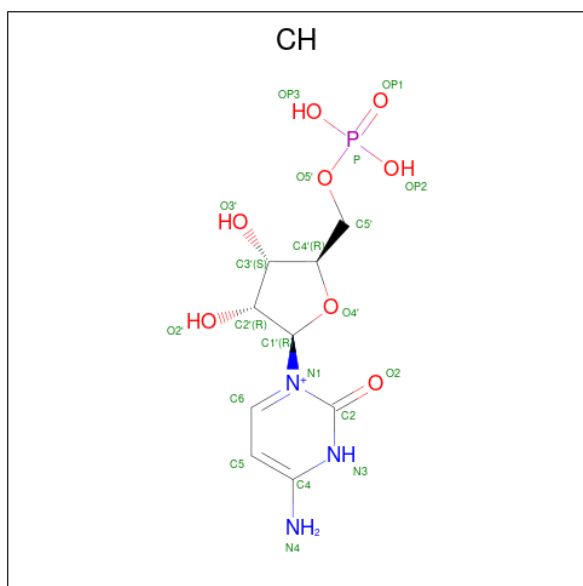
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is N3-PROTONATED CYTIDINE-5'-MONOPHOSPHATE (three-letter code: CH) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>3</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
5	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

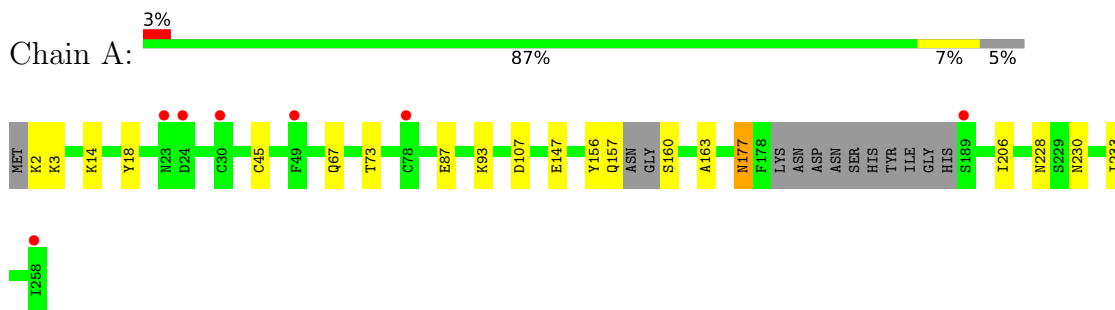
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	162	Total O 162 162	0	0
7	B	101	Total O 101 101	0	0

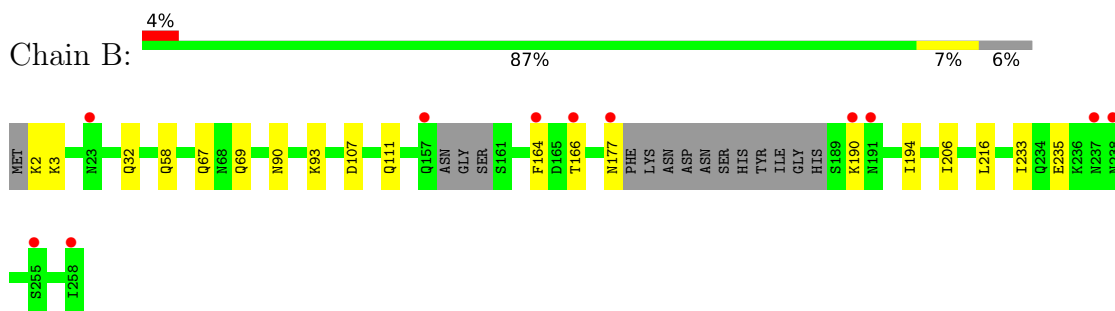
### 3 Residue-property plots [i](#)

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: ALPHA-2,3-/2,8-SIALYLTRANSFERASE



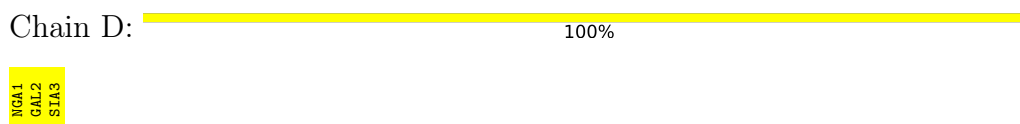
- Molecule 1: ALPHA-2,3-/2,8-SIALYLTRANSFERASE



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.67Å 117.67Å 46.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 36.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.95) 99.6 (36.53-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.164 , 0.198 0.183 , 0.220	Depositor DCC
$R_{free}$ test set	2368 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.839	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: SIA, GAL, NGA, CH, EDO, ACT, MPD

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	0.44	0/2119	0.51	0/2856
1	B	0.40	0/2084	0.48	0/2809
All	All	0.42	0/4203	0.50	0/5665

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2057	0	2002	23	0
1	B	2030	0	1976	22	0
2	C	46	0	39	2	0
2	D	46	0	39	0	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	8	0	14	9	0
5	A	21	0	13	0	0
5	B	21	0	13	5	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	162	0	0	13	0
7	B	101	0	0	4	0
All	All	4512	0	4117	58	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 7.

All (58) 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)
4:A:1263:MPD:H12	4:A:1263:MPD:C5	1.55	1.27
1:A:93:LYS:HE2	7:A:2065:HOH:O	1.38	1.22
1:A:2:LYS:HG2	1:A:3:LYS:H	1.09	1.17
4:A:1263:MPD:H53	4:A:1263:MPD:C1	1.77	1.13
5:B:1262:CH:H5'	5:B:1262:CH:H6	1.22	1.12
1:A:93:LYS:CE	7:A:2065:HOH:O	1.98	1.06
5:B:1262:CH:H6	5:B:1262:CH:C5'	1.88	1.04
1:B:2:LYS:HG2	1:B:3:LYS:N	1.69	1.01
1:A:107:ASP:OD1	7:A:2082:HOH:O	1.78	1.01
4:A:1263:MPD:H4	7:A:2078:HOH:O	1.58	1.00
1:B:2:LYS:HG2	1:B:3:LYS:H	0.87	1.00
1:B:2:LYS:CG	1:B:3:LYS:H	1.79	0.90
1:A:2:LYS:HG2	1:A:3:LYS:N	1.87	0.89
5:B:1262:CH:H5'	5:B:1262:CH:C6	2.02	0.89
1:A:160:SER:CB	1:B:67:GLN:OE1	2.24	0.86
4:A:1263:MPD:H12	4:A:1263:MPD:H53	0.87	0.84
1:A:3:LYS:NZ	1:A:147:GLU:OE1	2.10	0.84
4:A:1263:MPD:C5	4:A:1263:MPD:C1	2.35	0.83
1:A:160:SER:HB2	1:B:67:GLN:OE1	1.79	0.81
1:B:107:ASP:OD1	7:B:2054:HOH:O	1.98	0.80
1:B:164:PHE:HE2	1:B:166:THR:CG2	2.08	0.66
2:C:1:NGA:H83	2:C:3:SIA:H92	1.76	0.66
1:B:233:ILE:HD12	1:B:233:ILE:N	2.12	0.65
1:B:164:PHE:HE2	1:B:166:THR:HG22	1.62	0.65
4:A:1263:MPD:H12	4:A:1263:MPD:H52	1.71	0.63
1:A:14:LYS:NZ	1:B:69:GLN:OE1	2.26	0.63
1:B:177:ASN:OD1	1:B:177:ASN:C	2.35	0.62
1:A:2:LYS:CG	1:A:3:LYS:H	1.98	0.62
1:A:18:TYR:CE2	1:A:233:ILE:HD11	2.34	0.62
1:B:166:THR:HG21	7:B:2008:HOH:O	1.98	0.61
4:A:1263:MPD:C4	7:A:2078:HOH:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:HG3	7:A:2104:HOH:O	2.02	0.59
1:B:90:ASN:OD1	7:B:2039:HOH:O	2.16	0.58
1:B:164:PHE:CE2	1:B:166:THR:CG2	2.86	0.57
1:A:14:LYS:HE3	1:A:163:ALA:O	2.05	0.57
5:B:1262:CH:H6	5:B:1262:CH:H5''	1.85	0.56
1:A:230:ASN:ND2	7:A:2135:HOH:O	2.38	0.54
1:A:87:GLU:CG	7:A:2057:HOH:O	2.56	0.53
1:A:177:ASN:ND2	1:A:177:ASN:H	2.06	0.53
1:A:87:GLU:HG3	7:A:2057:HOH:O	2.08	0.52
1:B:164:PHE:CE2	1:B:166:THR:HG22	2.45	0.52
1:A:93:LYS:NZ	7:A:2065:HOH:O	2.32	0.52
2:C:1:NGA:H83	2:C:3:SIA:C9	2.39	0.52
1:B:32:GLN:HE21	1:B:58:GLN:HE22	1.57	0.52
1:B:2:LYS:CG	1:B:3:LYS:N	2.51	0.51
5:B:1262:CH:C5'	5:B:1262:CH:C6	2.73	0.49
1:A:156:TYR:O	1:A:157:GLN:HB2	2.12	0.49
4:A:1263:MPD:H32	7:A:2078:HOH:O	2.14	0.48
1:A:228:ASN:OD1	7:A:2134:HOH:O	2.20	0.47
1:A:45:CYS:O	1:A:73:THR:HA	2.15	0.47
1:B:233:ILE:HD12	1:B:233:ILE:H	1.80	0.46
1:B:206:ILE:HD12	1:B:206:ILE:C	2.36	0.46
1:A:67:GLN:NE2	7:A:2042:HOH:O	2.47	0.45
1:A:206:ILE:C	1:A:206:ILE:HD12	2.39	0.43
1:B:233:ILE:N	1:B:233:ILE:CD1	2.81	0.42
4:A:1263:MPD:H52	4:A:1263:MPD:O2	2.19	0.42
1:B:190:LYS:O	1:B:194:ILE:HG13	2.20	0.41
1:B:93:LYS:HD3	7:B:2039:HOH:O	2.21	0.41

There are no symmetry-related clashes.

## 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	241/258 (93%)	239 (99%)	2 (1%)	0	100	100
1	B	237/258 (92%)	233 (98%)	4 (2%)	0	100	100
All	All	478/516 (93%)	472 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	224/233 (96%)	223 (100%)	1 (0%)	91	90
1	B	220/233 (94%)	217 (99%)	3 (1%)	67	62
All	All	444/466 (95%)	440 (99%)	4 (1%)	78	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	B	111	GLN
1	B	216	LEU
1	B	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	83	GLN
1	A	157	GLN
1	A	177	ASN
1	A	214	ASN
1	A	228	ASN
1	A	230	ASN
1	B	9	ASN
1	B	32	GLN

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Mol	Chain	Res	Type
1	B	191	ASN
1	B	214	ASN
1	B	219	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](#)

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
2	NGA	C	1	2	15,15,15	1.43	1 (6%)	21,21,21	1.05	2 (9%)
2	GAL	C	2	2	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
2	SIA	C	3	2	20,20,21	1.21	2 (10%)	24,28,31	1.05	1 (4%)
2	NGA	D	1	2	15,15,15	1.34	1 (6%)	21,21,21	1.11	3 (14%)
2	GAL	D	2	2	11,11,12	0.58	0	15,15,17	1.31	2 (13%)
2	SIA	D	3	2	20,20,21	1.49	3 (15%)	24,28,31	0.93	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	NGA	C	1	2	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	SIA	C	3	2	1/1/8/9	5/18/34/38	0/1/1/1
2	NGA	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	1/2/19/22	0/1/1/1
2	SIA	D	3	2	1/1/8/9	5/18/34/38	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NGA	O6-C6	-4.48	1.23	1.42
2	C	1	NGA	O6-C6	-4.45	1.23	1.42
2	D	3	SIA	C2-C1	4.32	1.56	1.52
2	C	3	SIA	C2-C1	3.54	1.55	1.52
2	D	3	SIA	O6-C2	2.41	1.47	1.43
2	D	3	SIA	C3-C2	2.22	1.56	1.52
2	C	3	SIA	C3-C2	2.18	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	C2-C3-C4	-3.08	105.56	110.89
2	C	1	NGA	O6-C6-C5	2.71	120.58	111.29
2	D	2	GAL	O5-C5-C6	-2.69	102.98	107.20
2	D	1	NGA	O6-C6-C5	2.62	120.28	111.29
2	C	1	NGA	C1-O5-C5	-2.45	109.04	113.66
2	D	1	NGA	C6-C5-C4	-2.38	107.43	113.00
2	C	3	SIA	O9-C9-C8	-2.19	106.31	111.07
2	C	2	GAL	O5-C5-C6	-2.10	103.92	107.20
2	D	1	NGA	O5-C5-C4	2.06	113.44	109.69

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	SIA	C8
2	D	3	SIA	C8

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	SIA	C6-C7-C8-O8
2	C	3	SIA	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	C	3	SIA	O7-C7-C8-O8
2	D	3	SIA	O7-C7-C8-C9
2	D	1	NGA	O5-C5-C6-O6
2	D	3	SIA	O7-C7-C8-O8
2	D	3	SIA	C6-C7-C8-O8
2	C	3	SIA	C6-C7-C8-C9
2	C	1	NGA	O5-C5-C6-O6
2	D	1	NGA	C4-C5-C6-O6
2	D	3	SIA	C6-C7-C8-C9
2	D	3	SIA	O8-C8-C9-O9
2	D	2	GAL	O5-C5-C6-O6
2	C	2	GAL	O5-C5-C6-O6
2	C	1	NGA	C4-C5-C6-O6
2	C	3	SIA	C7-C8-C9-O9

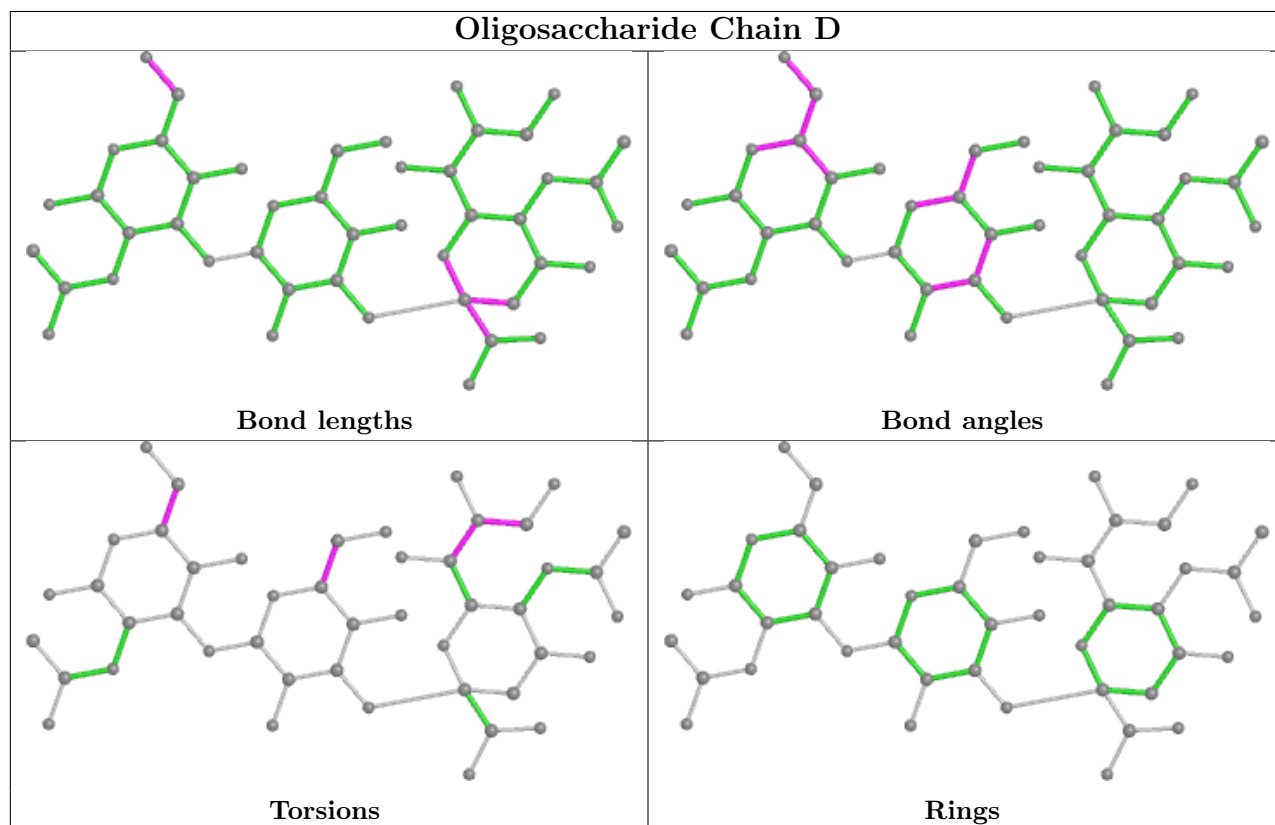
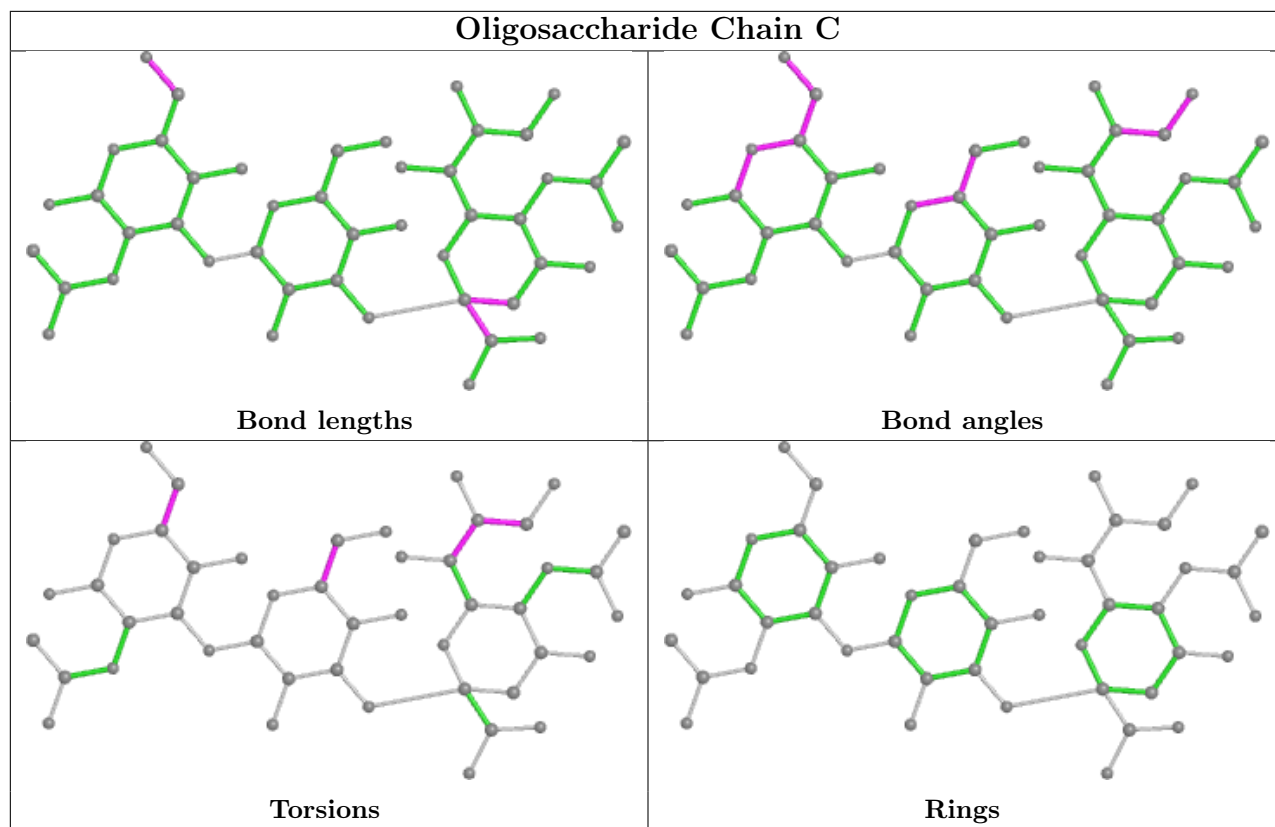
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	SIA	2	0
2	C	1	NGA	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.





## 5.6 Ligand geometry

8 ligands 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	ACT	B	1264	-	3,3,3	0.77	0	3,3,3	1.38	0
5	CH	A	1264	-	20,22,22	1.04	1 (5%)	27,33,33	1.33	5 (18%)
6	EDO	B	1263	-	3,3,3	0.45	0	2,2,2	0.36	0
6	EDO	A	1266	-	3,3,3	0.48	0	2,2,2	0.27	0
3	ACT	A	1262	-	3,3,3	0.76	0	3,3,3	1.42	0
5	CH	B	1262	-	20,22,22	1.17	3 (15%)	27,33,33	1.83	8 (29%)
4	MPD	A	1263	-	7,7,7	0.39	0	9,10,10	0.33	0
3	ACT	A	1265	-	3,3,3	0.74	0	3,3,3	1.32	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
5	CH	A	1264	-	-	2/8/26/26	0/2/2/2
6	EDO	B	1263	-	-	1/1/1/1	-
6	EDO	A	1266	-	-	1/1/1/1	-
5	CH	B	1262	-	-	4/8/26/26	0/2/2/2
4	MPD	A	1263	-	-	2/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1262	CH	C4-N3	2.74	1.40	1.37
5	B	1262	CH	O5'-C5'	-2.45	1.35	1.44
5	B	1262	CH	C6-N1	2.39	1.41	1.36
5	A	1264	CH	C4-N3	2.35	1.40	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1262	CH	O4'-C4'-C5'	-5.13	92.49	109.37
5	A	1264	CH	C5-C4-N3	3.80	120.21	118.04
5	A	1264	CH	C4'-O4'-C1'	-3.43	106.59	109.85
5	B	1262	CH	C5-C4-N3	3.38	119.97	118.04
5	B	1262	CH	C5'-C4'-C3'	-3.37	102.53	115.18
5	B	1262	CH	C4'-O4'-C1'	-3.29	106.71	109.85
5	B	1262	CH	C5-C4-N4	-2.90	121.06	123.88
5	B	1262	CH	OP2-P-O5'	2.26	112.75	106.73
5	B	1262	CH	OP3-P-O5'	-2.21	100.85	106.73
5	A	1264	CH	C5-C4-N4	-2.14	121.80	123.88
5	B	1262	CH	O5'-P-OP1	2.10	112.36	106.47
5	A	1264	CH	O5'-P-OP1	2.05	112.22	106.47
5	A	1264	CH	P-O5'-C5'	2.02	123.85	118.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1263	MPD	C2-C3-C4-C5
5	B	1262	CH	C3'-C4'-C5'-O5'
6	A	1266	EDO	O1-C1-C2-O2
6	B	1263	EDO	O1-C1-C2-O2
5	B	1262	CH	C5'-O5'-P-OP1
5	B	1262	CH	O4'-C4'-C5'-O5'
5	B	1262	CH	C4'-C5'-O5'-P
5	A	1264	CH	C4'-C5'-O5'-P
5	A	1264	CH	C5'-O5'-P-OP3
4	A	1263	MPD	C2-C3-C4-O4

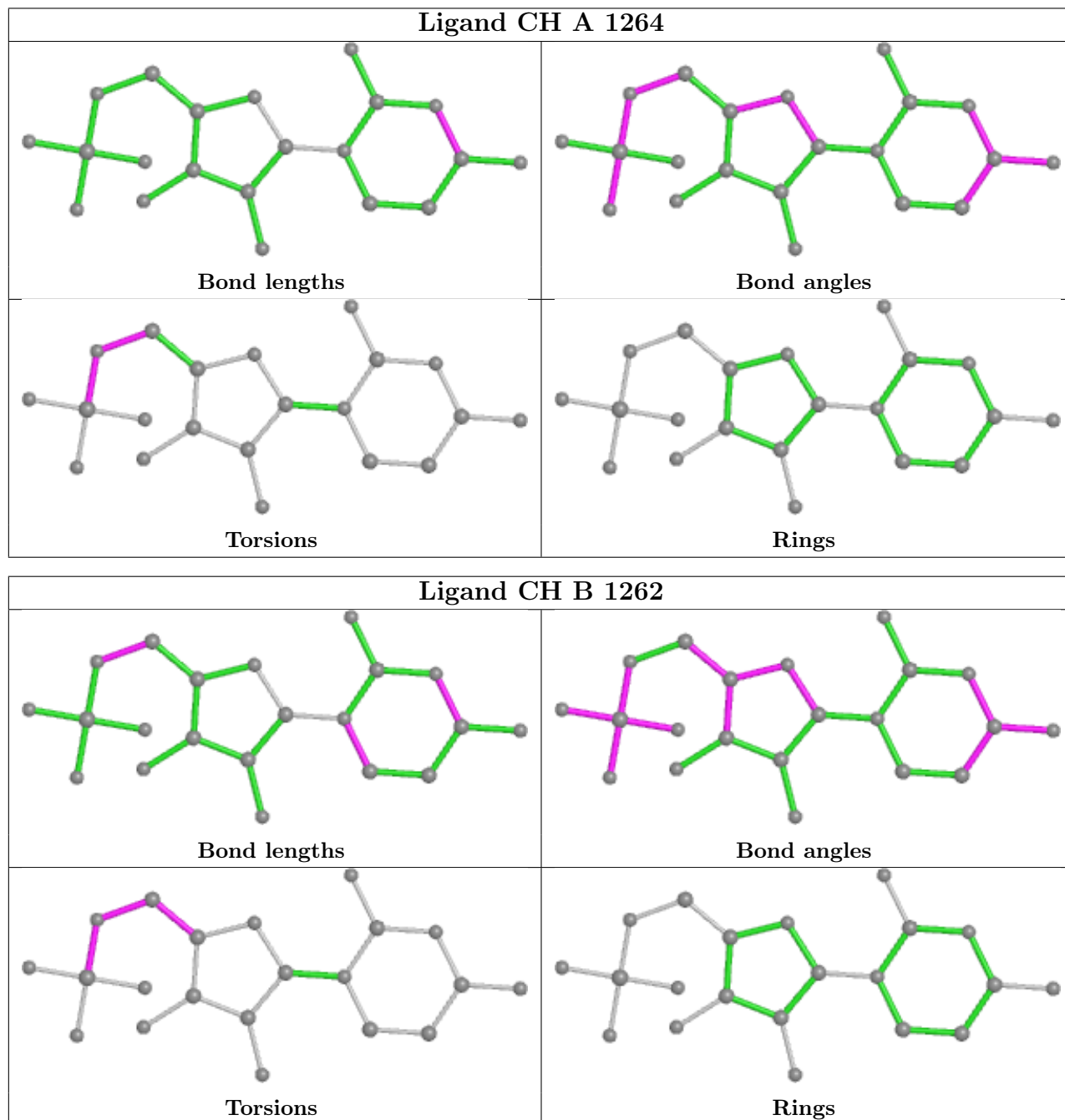
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1262	CH	5	0
4	A	1263	MPD	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	245/258 (94%)	0.20	7 (2%) 51 60	21, 32, 49, 55	3 (1%)
1	B	243/258 (94%)	0.28	11 (4%) 33 43	24, 38, 62, 73	7 (2%)
All	All	488/516 (94%)	0.24	18 (3%) 41 51	21, 34, 56, 73	10 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ASN	3.6
1	B	237	ASN	3.2
1	B	238	ASN	3.0
1	A	24	ASP	3.0
1	B	258	ILE	2.7
1	B	255	SER	2.6
1	A	49	PHE	2.5
1	B	23	ASN	2.5
1	B	166	THR	2.4
1	B	164	PHE	2.4
1	B	157	GLN	2.3
1	A	258	ILE	2.3
1	B	191	ASN	2.2
1	A	78	CYS	2.2
1	A	189	SER	2.1
1	A	30	CYS	2.1
1	B	190	LYS	2.1
1	B	177	ASN	2.0

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

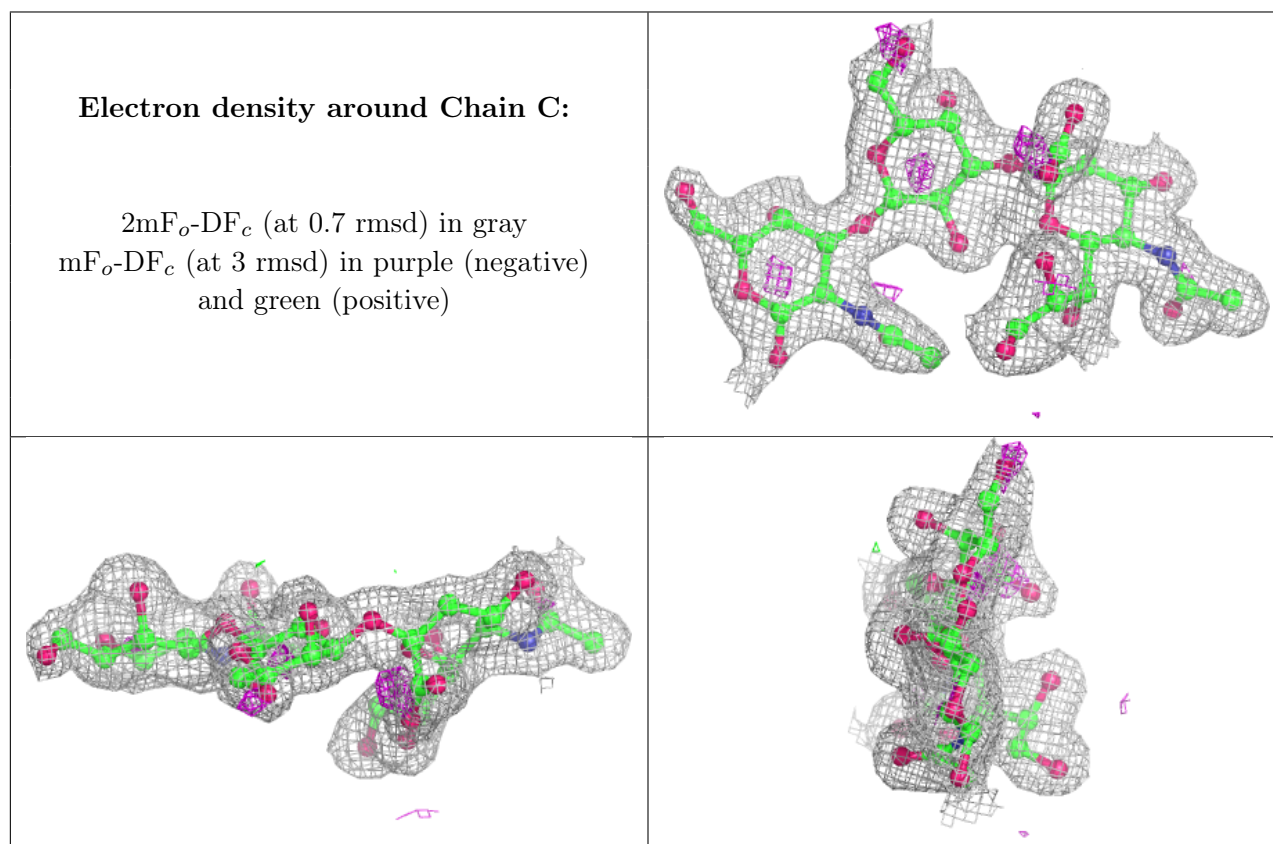
There are no non-standard protein/DNA/RNA residues in this entry.

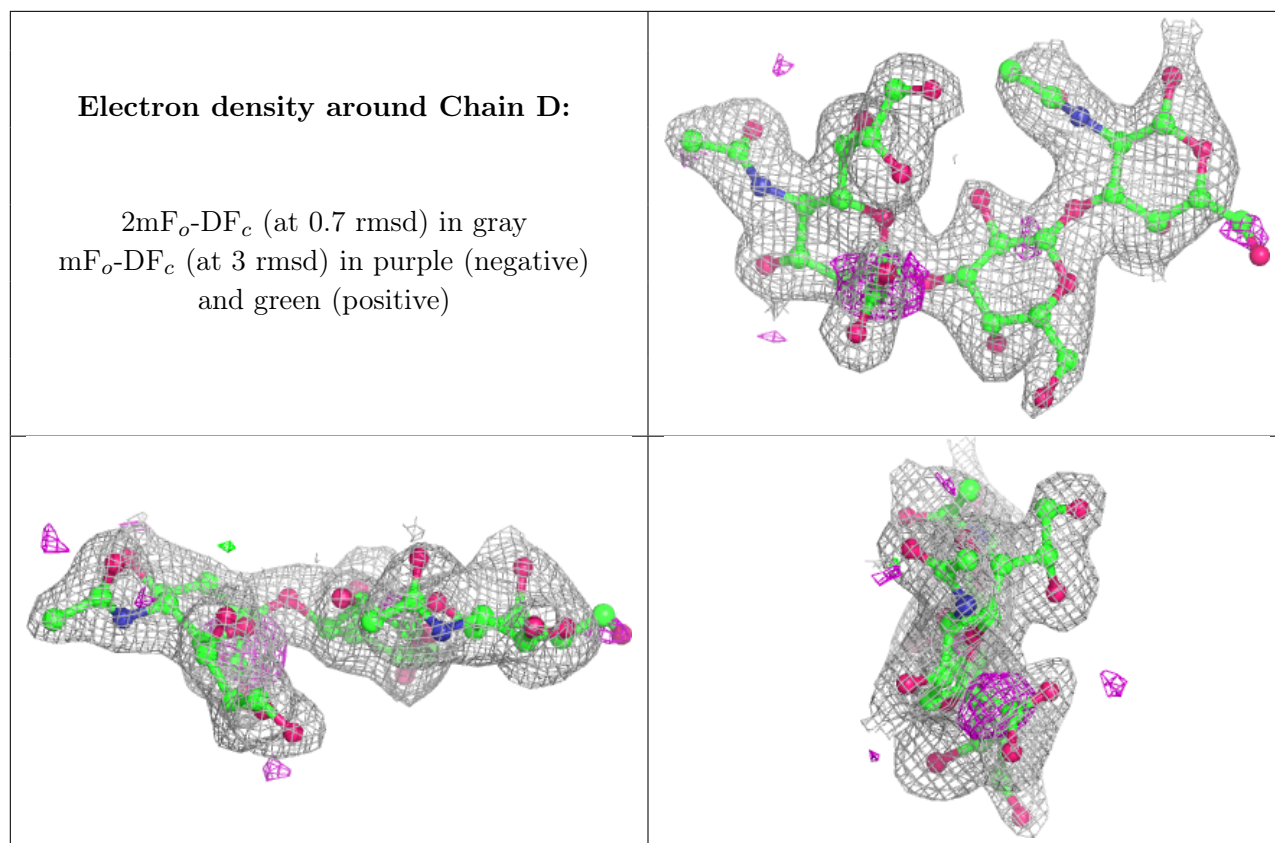
### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NGA	D	1	15/15	0.83	0.22	57,61,63,65	0
2	GAL	D	2	11/12	0.85	0.16	47,53,55,56	0
2	NGA	C	1	15/15	0.87	0.22	45,49,55,58	0
2	SIA	D	3	20/21	0.89	0.14	39,42,48,51	0
2	SIA	C	3	20/21	0.92	0.13	27,32,40,44	0
2	GAL	C	2	11/12	0.93	0.11	37,40,44,48	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.





## 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, 95<sup>th</sup> 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.

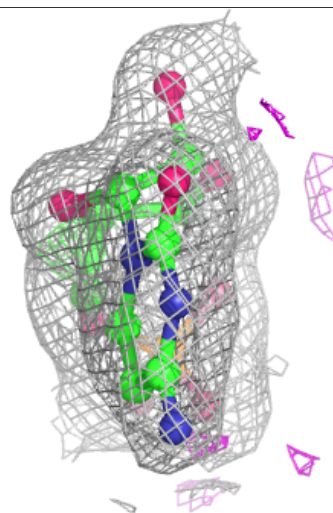
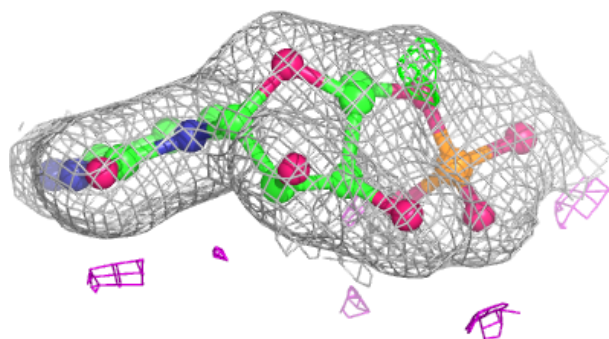
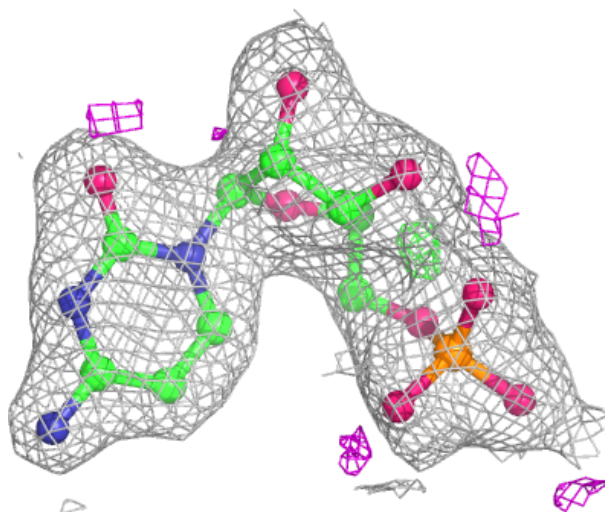
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	B	1263	4/4	0.80	0.26	71,71,72,72	0
6	EDO	A	1266	4/4	0.82	0.13	66,67,67,67	0
4	MPD	A	1263	8/8	0.85	0.24	45,48,51,51	0
3	ACT	A	1265	4/4	0.88	0.10	70,70,70,70	0
3	ACT	B	1264	4/4	0.90	0.10	66,66,66,66	0
3	ACT	A	1262	4/4	0.91	0.13	62,62,62,62	0
5	CH	B	1262	21/21	0.93	0.13	39,41,44,46	0
5	CH	A	1264	21/21	0.97	0.14	25,28,29,29	0

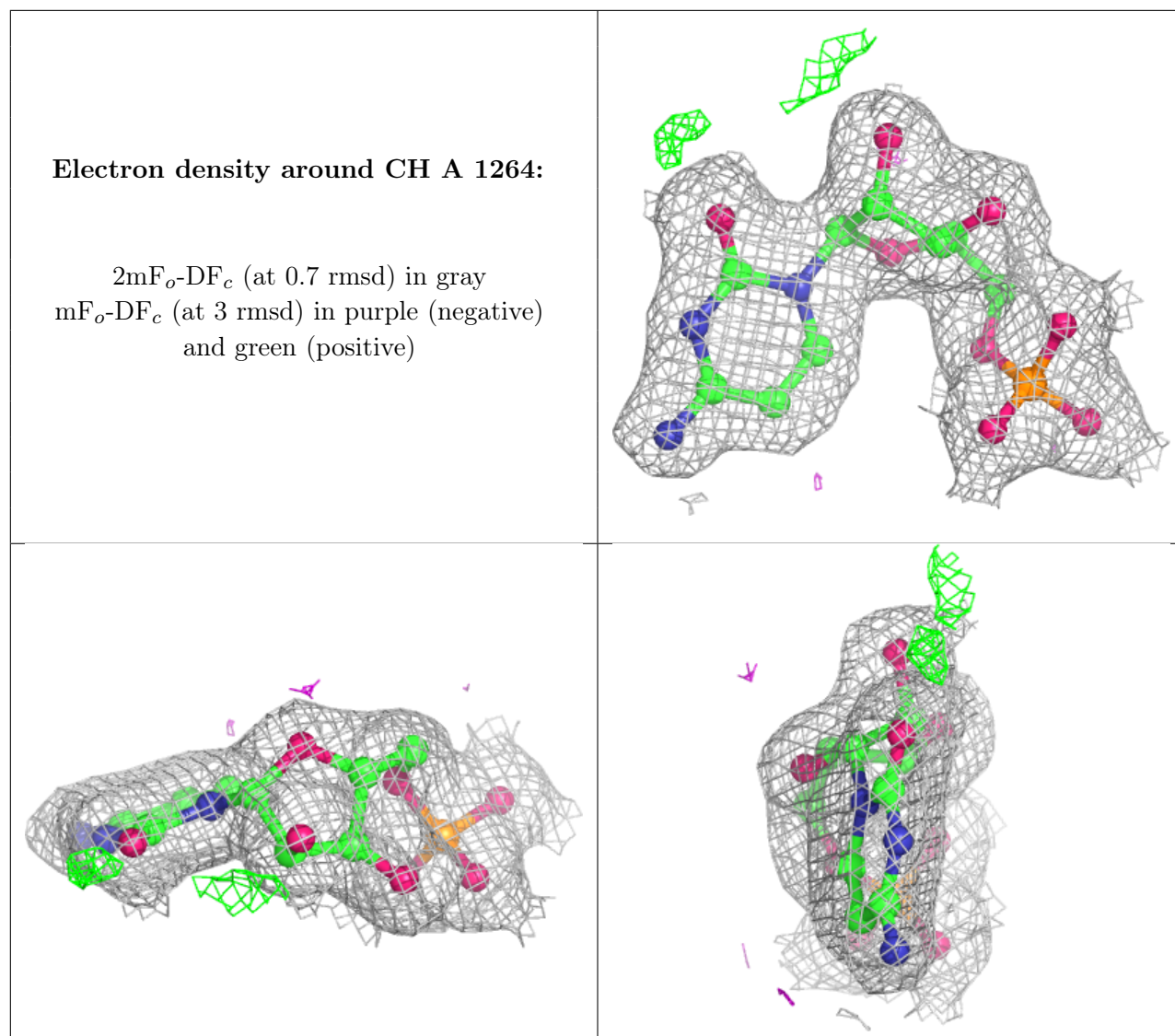
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around CH B 1262:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.