



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:05 pm GMT

PDB ID : 4CPY  
Title : Structure of the Neuraminidase from the B/Lyon/CHU/15.216/2011 virus in complex with Oseltamivir  
Authors : Vachieri, S.G.; Collins, P.J.; Escuret, V.; Casalegno, J.S.; Cattle, N.; Ferraris, O.; Sabatier, M.; Frobert, E.; Caro, V.; Skehel, J.J.; Gamblin, S.J.; Valla, F.; Valette, M.; Ottmann, M.; McCauley, J.W.; Daniels, R.S.; Lina, B.  
Deposited on : 2014-02-09  
Resolution : 1.80 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (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

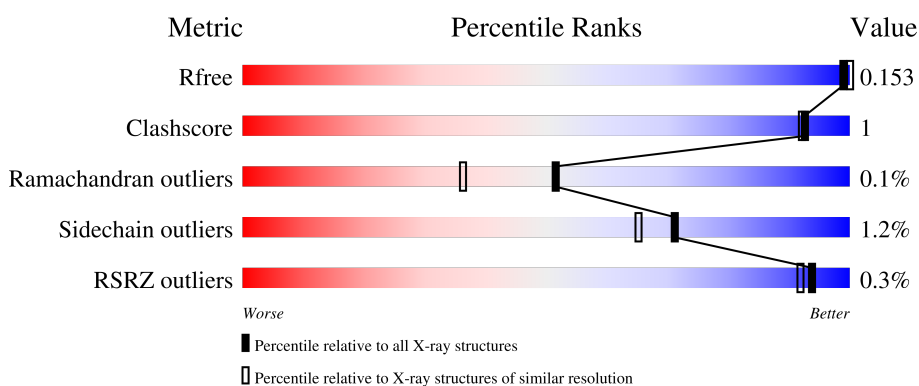
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	466	
1	B	466	
2	C	2	
2	D	2	

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	NAG	B	1469	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6958 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	Total 3037	C 1904	N 521	O 583	S 29	0	5	0
1	B	390	Total 3024	C 1896	N 520	O 579	S 29	0	2	0

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



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

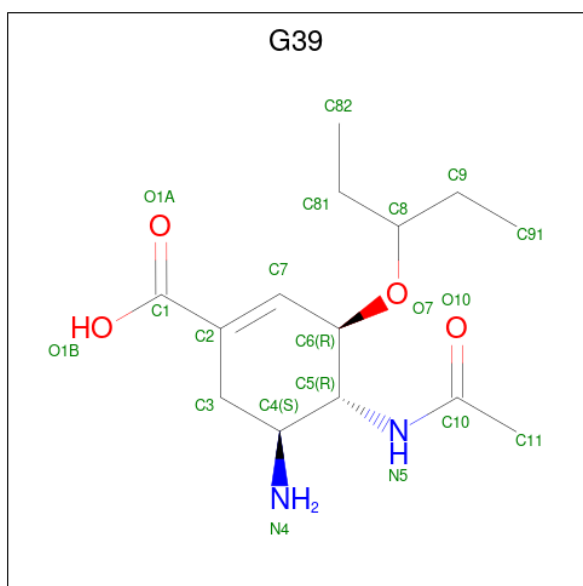
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

- Molecule 5 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (three-letter code: G39) (formula:  $C_{14}H_{24}N_2O_4$ ).



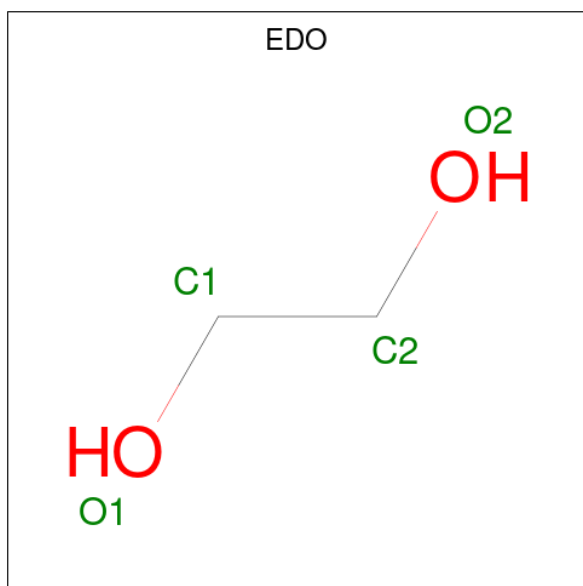
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	20	14	2	4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	B	1	20	14	2	4	0	0

- 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
			Total	C	O		
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0

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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
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	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	381	Total O 381 381	0	0
7	B	322	Total O 322 322	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: NEURAMINIDASE

Chain A:  80% 16%

MET LEU LEU PRO SER THR ILE GLN THR LEU LEU THR LEU LEU PHE LEU THR LEU LEU SER PRO GLY VAL GLY LEU LEU SER LEU LEU TYR TYR VAL VAL SER ALA LEU LEU LEU TYR TYR TYR SER ASP ILE LEU LEU LYS PHE SER PRO THR GLU ILE THR ALA ALA THR MET SER SER LEU ASP CYS ALA ASN ALA SER ASN VAL

GLN ALA VAL ASN ARG ARG ALA THR LYS LEU VAL VAL PHE LEU LEU SER PRO GLY VAL G66 T105 H133 Y134 M150 L200 T212 M238 G246 K271 H272 T273 E274 Y295 R314 W387 W455 L465

- Molecule 1: NEURAMINIDASE

Chain B:  81% 16%

MET LEU LEU PRO SER THR ILE GLN THR LEU LEU THR LEU LEU PHE LEU THR LEU LEU SER PRO GLY VAL GLY LEU LEU SER LEU LEU TYR TYR SER ASP ILE LEU LEU LYS PHE SER PRO THR GLU ILE THR ALA ALA THR MET SER SER LEU ASP CYS ALA ASN ALA SER ASN VAL

GLN ALA VAL ASN ARG ARG ALA THR LYS LEU VAL VAL PHE LEU LEU SER PRO GLY VAL G76 P77 Y134 L220 Q224 M238 V302 T313 R314 W387 S401 W455 L465

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

Chain C:  50% 50%

MAG1  
MAG2

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

Chain D:  100%

MAG1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.09Å 160.09Å 89.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.26 – 1.80 45.26 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.26-1.80) 99.5 (45.26-1.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, $R_{free}$	0.172 , 0.179 0.145 , 0.153	Depositor DCC
$R_{free}$ test set	6106 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 22.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.316 for -h,-k,l	Xtriage
Reported twinning fraction	0.673 for H, K, L 0.327 for -h,-k,l	Depositor
Outliers	2 of 121682 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, G39, 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	0.42	0/3120	0.66	0/4217
1	B	0.43	0/3104	0.67	0/4194
All	All	0.43	0/6224	0.67	0/8411

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	2911	10	0
1	B	3024	0	2903	4	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	20	0	23	1	0
5	B	20	0	23	2	0
6	A	44	0	66	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	24	0	36	0	0
7	A	381	0	0	2	11
7	B	322	0	0	0	12
All	All	6958	0	6038	18	12

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 1.

All (18) 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:224:GLN:HE21	1:B:238:MET:H	1.27	0.82
1:A:246:GLY:O	1:A:272:HIS:HD2	1.76	0.68
1:A:86:CYS:HB2	7:A:2016:HOH:O	1.98	0.62
1:A:272:HIS:HE1	1:A:274:GLU:OE2	1.82	0.61
1:A:133:HIS:HD2	1:A:150:ASN:HD21	1.55	0.55
1:A:271:LYS:HE3	1:A:295:TYR:CD2	2.43	0.54
1:B:314:ARG:HB2	1:B:387:TRP:CD1	2.43	0.53
1:B:224:GLN:NE2	1:B:238:MET:H	2.04	0.52
1:A:133:HIS:CD2	1:A:150:ASN:HD21	2.30	0.49
1:B:302:VAL:HG22	1:B:313:ILE:HG12	1.93	0.49
5:A:1470:G39:H823	5:A:1470:G39:H912	1.98	0.46
2:D:1:NAG:O4	2:D:2:NAG:H83	2.15	0.45
1:A:200[B]:LEU:HD11	1:A:212:THR:HB	1.97	0.45
5:B:1470:G39:H913	5:B:1470:G39:H7	1.98	0.44
1:A:314:ARG:HB2	1:A:387:TRP:CD1	2.52	0.44
5:B:1470:G39:H823	5:B:1470:G39:H912	1.99	0.44
1:A:105[B]:THR:HG22	7:A:2040:HOH:O	2.19	0.41
1:A:272:HIS:CE1	1:A:274:GLU:OE2	2.69	0.41

All (12) 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)
7:A:2123:HOH:O	7:B:2103:HOH:O[6_555]	0.95	1.25
7:A:2080:HOH:O	7:B:2037:HOH:O[6_555]	1.03	1.17
7:A:2105:HOH:O	7:B:2027:HOH:O[6_555]	1.03	1.17
7:A:2149:HOH:O	7:B:2028:HOH:O[6_555]	1.07	1.13
7:A:2126:HOH:O	7:B:2047:HOH:O[6_555]	1.12	1.08
7:A:2376:HOH:O	7:B:2033:HOH:O[6_555]	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2289:HOH:O	7:B:2267:HOH:O[4_565]	1.33	0.87
7:A:2201:HOH:O	7:B:2239:HOH:O[4_565]	1.34	0.86
7:A:2226:HOH:O	7:B:2144:HOH:O[5_665]	1.78	0.42
7:A:2147:HOH:O	7:B:2202:HOH:O[6_554]	1.90	0.30
7:B:2237:HOH:O	7:B:2306:HOH:O[2_564]	1.94	0.26
7:A:2124:HOH:O	7:B:2101:HOH:O[6_555]	1.95	0.25

## 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	393/466 (84%)	383 (98%)	10 (2%)	0	100	100
1	B	390/466 (84%)	378 (97%)	11 (3%)	1 (0%)	41	27
All	All	783/932 (84%)	761 (97%)	21 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	LEU

### 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	327/390 (84%)	324 (99%)	3 (1%)	78	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	325/390 (83%)	320 (98%)	5 (2%)	65	56
All	All	652/780 (84%)	644 (99%)	8 (1%)	71	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	TYR
1	A	238	MET
1	A	455	TRP
1	B	77	PRO
1	B	134	TYR
1	B	238	MET
1	B	401	SER
1	B	455	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	272	HIS
1	B	214	HIS
1	B	224	GLN

### 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](#)

4 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	2,1	14,14,15	0.60	0	17,19,21	0.98	2 (11%)
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	1.03	0
2	NAG	D	1	2,1	14,14,15	0.45	0	17,19,21	1.23	3 (17%)
2	NAG	D	2	2	14,14,15	0.48	0	17,19,21	1.45	4 (23%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C8-C7-N2	3.45	121.94	116.10
2	D	1	NAG	C8-C7-N2	2.58	120.46	116.10
2	D	1	NAG	C2-N2-C7	2.55	126.53	122.90
2	D	2	NAG	C1-C2-N2	2.50	114.77	110.49
2	D	2	NAG	O7-C7-C8	-2.27	117.84	122.06
2	C	1	NAG	C1-C2-N2	-2.20	106.74	110.49
2	C	1	NAG	C1-O5-C5	2.16	115.12	112.19
2	D	2	NAG	O5-C1-C2	-2.13	107.93	111.29
2	D	1	NAG	C1-C2-N2	-2.01	107.05	110.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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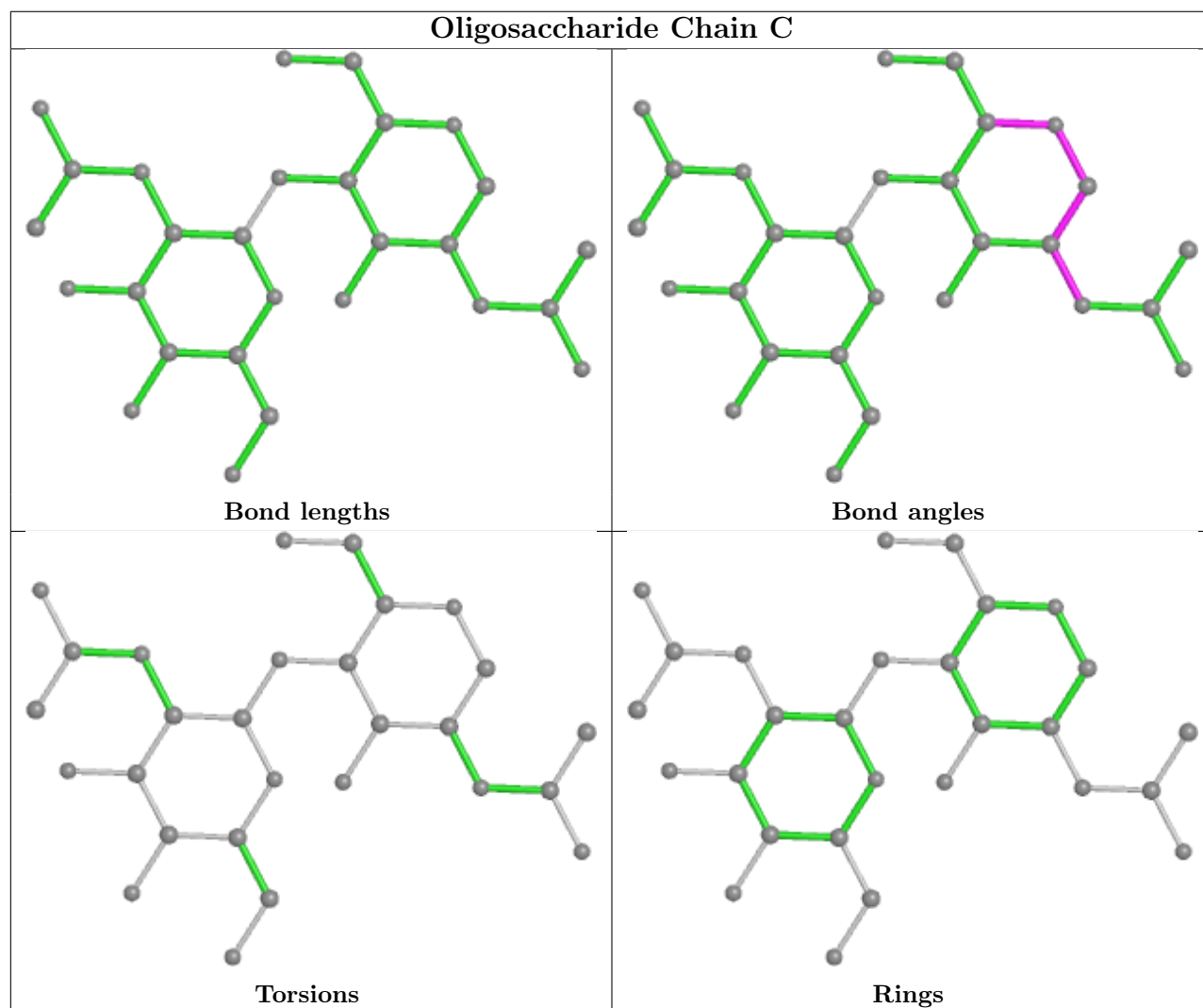
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2

There are no ring outliers.

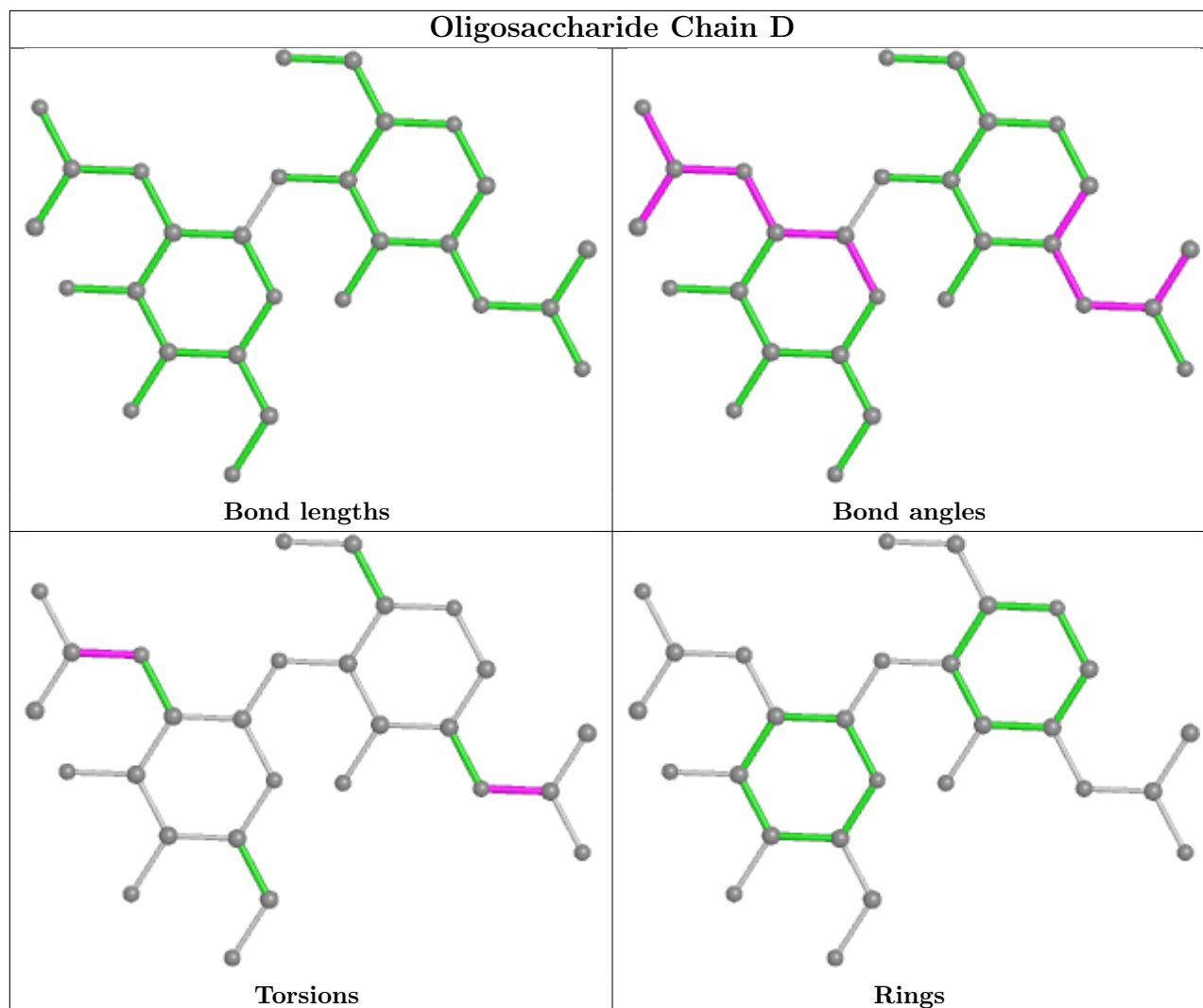
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	D	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.







## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\# Z  > 2$
6	EDO	A	1476	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	A	1479	-	3,3,3	0.39	0	2,2,2	0.43	0
6	EDO	A	1481	-	3,3,3	0.55	0	2,2,2	0.20	0
6	EDO	B	1476	-	3,3,3	0.50	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	G39	B	1470	-	20,20,20	0.73	0	19,27,27	0.85	0
6	EDO	A	1477	-	3,3,3	0.49	0	2,2,2	0.14	0
6	EDO	B	1472	-	3,3,3	0.47	0	2,2,2	0.09	0
6	EDO	A	1475	-	3,3,3	0.48	0	2,2,2	0.28	0
6	EDO	A	1478	-	3,3,3	0.36	0	2,2,2	0.45	0
6	EDO	A	1471	-	3,3,3	0.50	0	2,2,2	0.13	0
6	EDO	B	1473	-	3,3,3	0.45	0	2,2,2	0.56	0
6	EDO	A	1480	-	3,3,3	0.41	0	2,2,2	0.39	0
4	NAG	A	1469	1	14,14,15	0.48	0	17,19,21	0.79	0
6	EDO	A	1472	-	3,3,3	0.33	0	2,2,2	0.49	0
4	NAG	B	1469	1	14,14,15	0.74	0	17,19,21	1.57	2 (11%)
6	EDO	A	1474	-	3,3,3	0.46	0	2,2,2	0.29	0
5	G39	A	1470	-	20,20,20	0.69	0	19,27,27	1.03	0
6	EDO	B	1474	-	3,3,3	0.65	0	2,2,2	0.19	0
6	EDO	A	1473	-	3,3,3	0.39	0	2,2,2	0.41	0
6	EDO	B	1471	-	3,3,3	0.46	0	2,2,2	0.40	0
6	EDO	B	1475	-	3,3,3	0.56	0	2,2,2	0.22	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
6	EDO	A	1476	-	-	1/1/1/1	-
6	EDO	A	1479	-	-	1/1/1/1	-
6	EDO	A	1481	-	-	1/1/1/1	-
6	EDO	B	1476	-	-	0/1/1/1	-
5	G39	B	1470	-	-	2/16/32/32	0/1/1/1
6	EDO	A	1477	-	-	0/1/1/1	-
6	EDO	B	1472	-	-	0/1/1/1	-
6	EDO	A	1475	-	-	0/1/1/1	-
6	EDO	A	1478	-	-	0/1/1/1	-
6	EDO	A	1471	-	-	0/1/1/1	-
6	EDO	B	1473	-	-	1/1/1/1	-
6	EDO	A	1480	-	-	1/1/1/1	-
4	NAG	A	1469	1	-	0/6/23/26	0/1/1/1
6	EDO	A	1472	-	-	0/1/1/1	-
4	NAG	B	1469	1	1/1/5/7	0/6/23/26	0/1/1/1
6	EDO	A	1474	-	-	0/1/1/1	-
5	G39	A	1470	-	-	3/16/32/32	0/1/1/1
6	EDO	B	1474	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1473	-	-	0/1/1/1	-
6	EDO	B	1471	-	-	1/1/1/1	-
6	EDO	B	1475	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1469	NAG	O5-C1-C2	-4.96	103.45	111.29
4	B	1469	NAG	C1-C2-N2	2.30	114.41	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1469	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1470	G39	O7-C8-C81-C82
5	B	1470	G39	O7-C8-C81-C82
6	A	1481	EDO	O1-C1-C2-O2
6	B	1471	EDO	O1-C1-C2-O2
5	A	1470	G39	C9-C8-C81-C82
6	A	1479	EDO	O1-C1-C2-O2
6	B	1473	EDO	O1-C1-C2-O2
5	B	1470	G39	C9-C8-C81-C82
6	B	1475	EDO	O1-C1-C2-O2
5	A	1470	G39	O7-C8-C9-C91
6	A	1476	EDO	O1-C1-C2-O2
6	A	1480	EDO	O1-C1-C2-O2

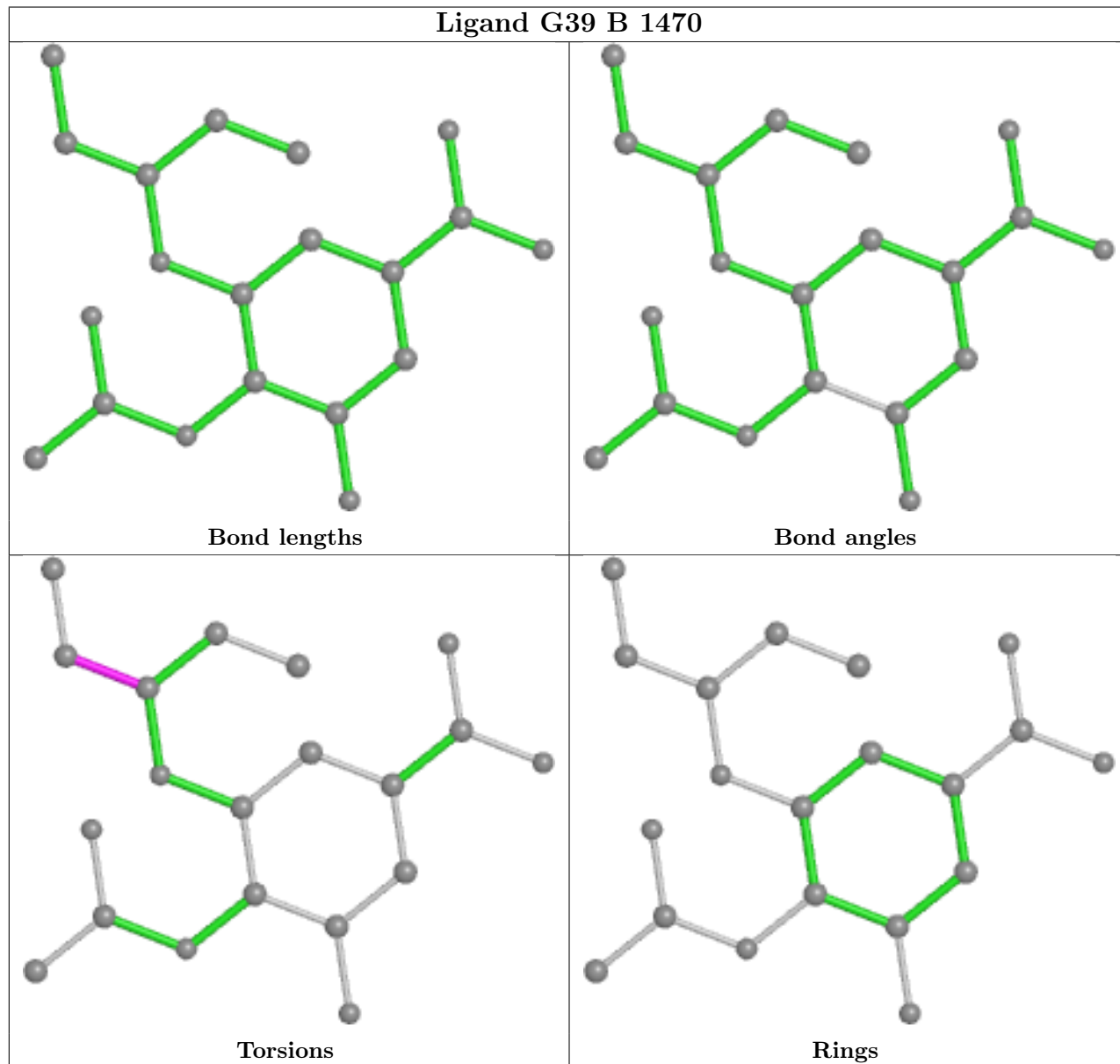
There are no ring outliers.

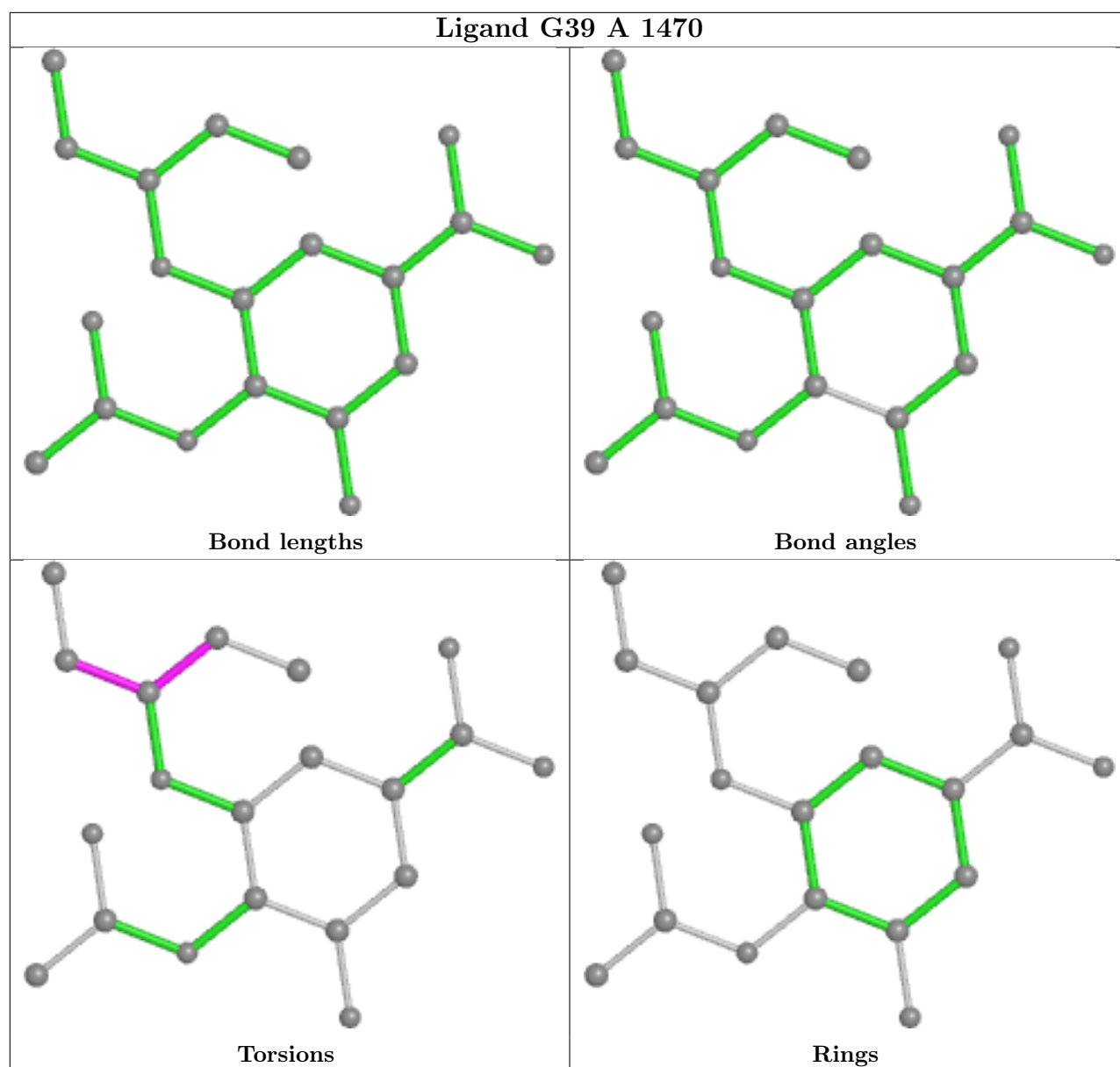
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1470	G39	2	0
5	A	1470	G39	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 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 [\(i\)](#)

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	390/466 (83%)	-0.82	1 (0%) 94 92	10, 15, 22, 54	0
1	B	390/466 (83%)	-0.82	1 (0%) 94 92	10, 15, 22, 52	0
All	All	780/932 (83%)	-0.82	2 (0%) 94 92	10, 15, 22, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	GLU	3.7
1	B	76	GLU	3.6

### 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](#)

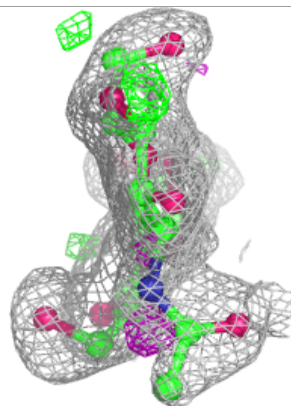
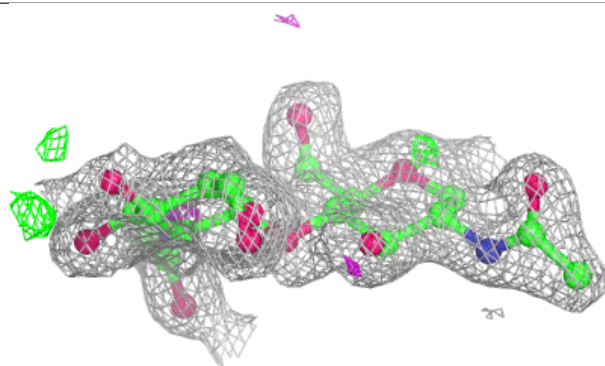
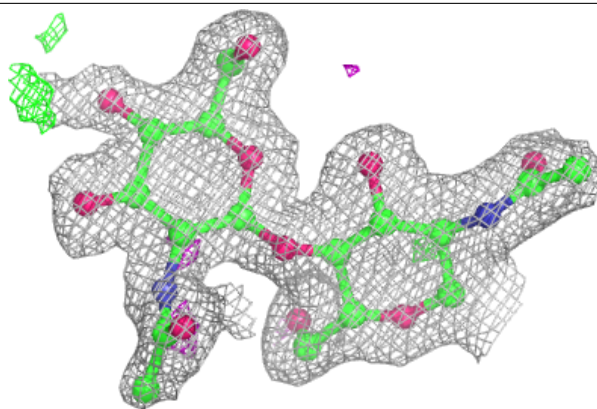
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	NAG	D	2	14/15	0.84	0.23	35,39,40,41	0
2	NAG	C	2	14/15	0.85	0.21	37,39,41,43	0
2	NAG	D	1	14/15	0.92	0.10	28,30,31,33	0
2	NAG	C	1	14/15	0.95	0.14	27,29,31,34	0

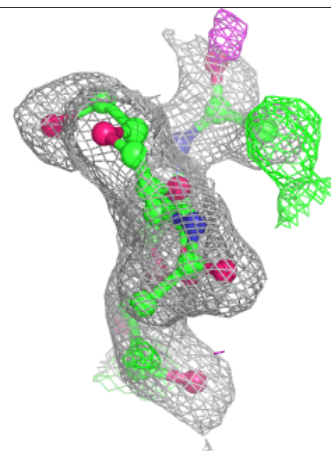
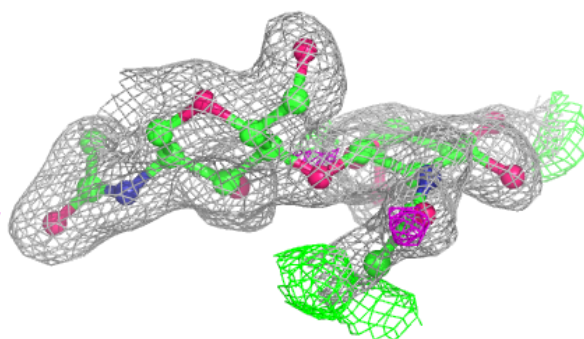
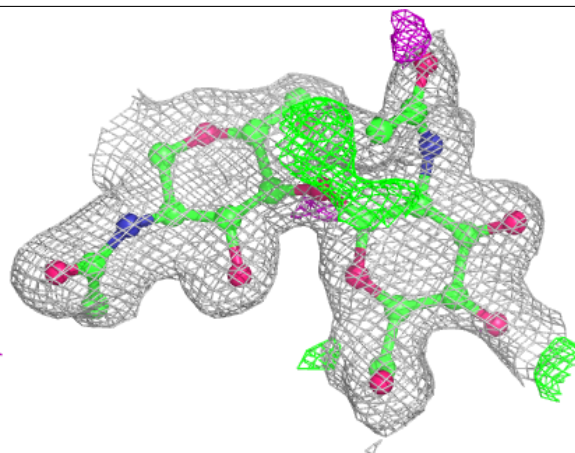
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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 D:**

$2mF_o-DF_c$  (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, 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.

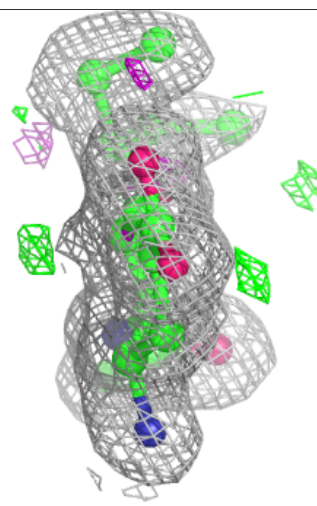
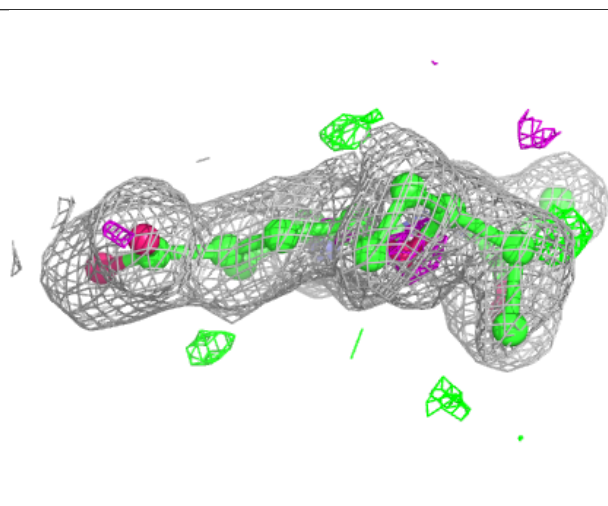
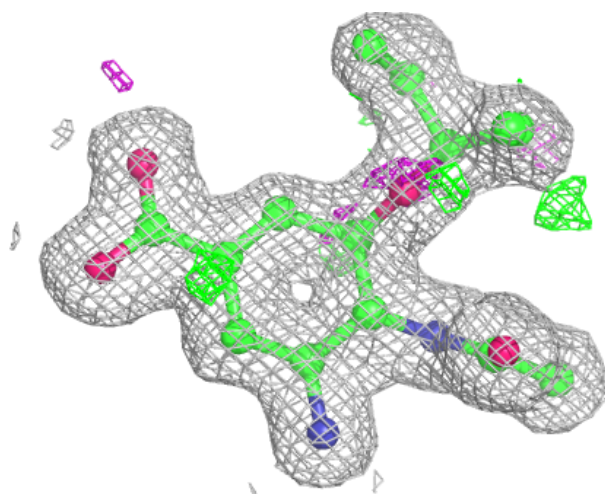
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	1469	14/15	0.77	0.29	40,48,51,51	0
6	EDO	B	1473	4/4	0.78	0.22	36,37,37,37	0
6	EDO	A	1475	4/4	0.79	0.23	35,36,36,37	0
4	NAG	A	1469	14/15	0.79	0.20	31,37,39,39	0
6	EDO	A	1479	4/4	0.86	0.21	32,32,33,33	0
6	EDO	A	1481	4/4	0.88	0.14	29,30,30,32	0
6	EDO	B	1474	4/4	0.90	0.15	21,25,26,27	0
6	EDO	B	1476	4/4	0.90	0.17	25,28,29,30	0
6	EDO	A	1476	4/4	0.91	0.17	40,40,40,41	0
6	EDO	A	1471	4/4	0.92	0.10	25,25,26,26	0
6	EDO	A	1478	4/4	0.92	0.12	36,36,36,37	0
6	EDO	B	1471	4/4	0.92	0.15	25,27,27,30	0
6	EDO	B	1475	4/4	0.93	0.15	27,27,27,28	0
6	EDO	A	1480	4/4	0.93	0.16	21,26,26,29	0
5	G39	A	1470	20/20	0.96	0.09	14,16,22,23	0
5	G39	B	1470	20/20	0.97	0.09	14,18,23,24	0
6	EDO	A	1473	4/4	0.97	0.06	15,16,16,17	0
6	EDO	A	1477	4/4	0.97	0.09	20,21,22,22	0
6	EDO	A	1474	4/4	0.98	0.07	14,15,16,16	0
6	EDO	A	1472	4/4	0.99	0.05	14,15,15,15	0
6	EDO	B	1472	4/4	0.99	0.05	16,16,16,16	0
3	CA	B	1466	1/1	1.00	0.05	16,16,16,16	0
3	CA	A	1466	1/1	1.00	0.06	13,13,13,13	0

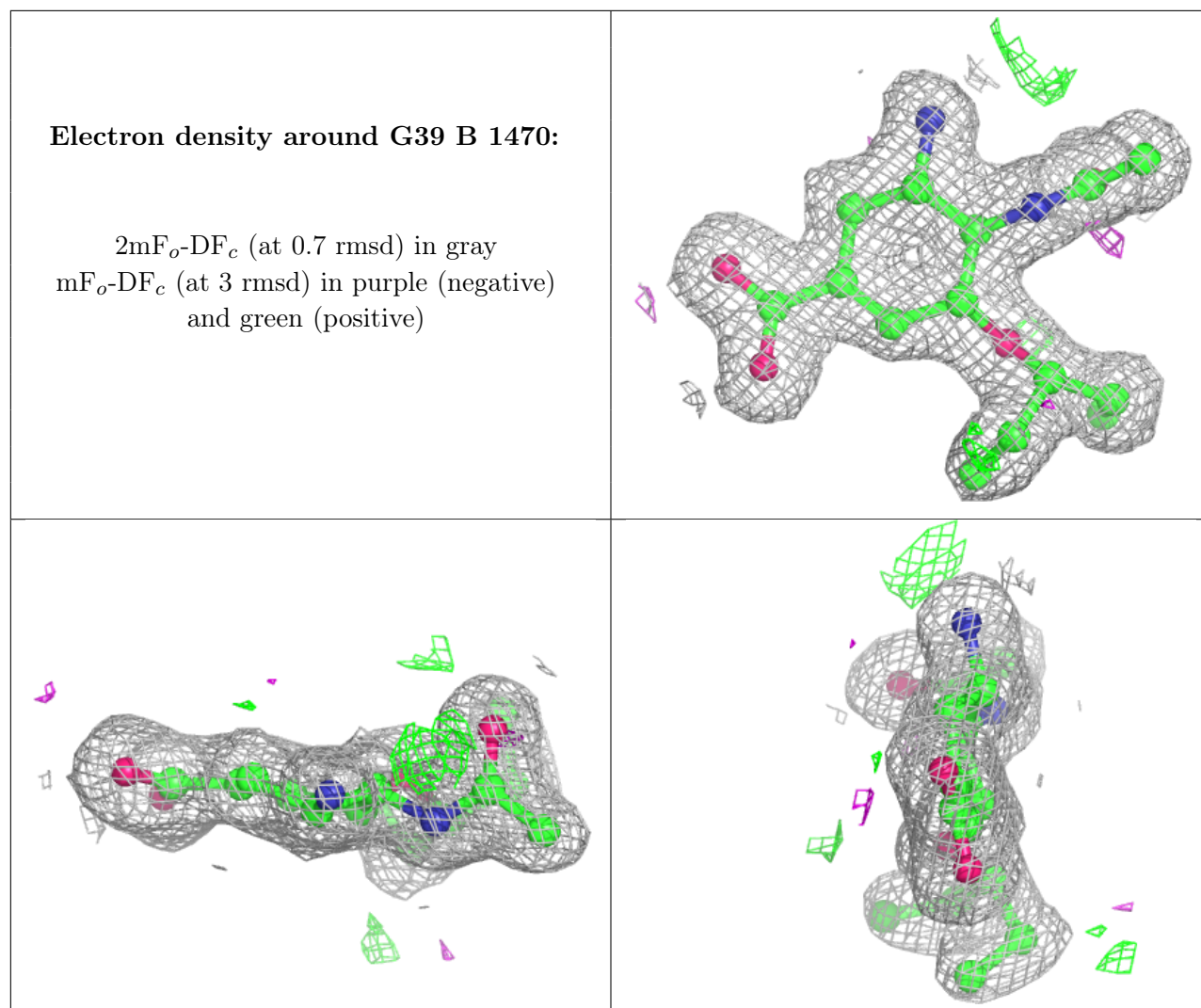
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around G39 A 1470:**

$2mF_o-DF_c$  (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.