



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 05:10 AM EDT

PDB ID : 3TI5  
Title : Crystal structure of 2009 pandemic H1N1 neuraminidase complexed with Zanamivir  
Authors : Vavricka, C.J.; Li, Q.; Wu, Y.; Qi, J.; Wang, M.; Liu, Y.; Gao, F.; Liu, J.; Feng, E.; He, J.; Wang, J.; Liu, H.; Jiang, H.; Gao, G.F.  
Deposited on : 2011-08-20  
Resolution : 1.90 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 : 1.8.5 (274361), 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

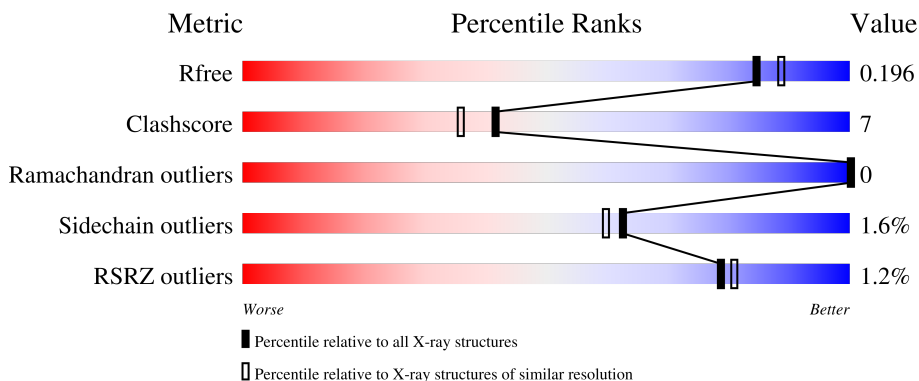
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	388	 2% 89% 10%
1	B	388	 1% 88% 12%
2	C	3	 67% 33%

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
6	GOL	A	1	-	-	X	-
7	ACT	A	471	-	-	X	-
7	ACT	B	1	-	-	X	-
7	ACT	B	471	-	-	X	-
7	ACT	B	472	-	-	X	-

## 2 Entry composition [i](#)

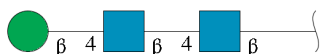
There are 8 unique types of molecules in this entry. The entry contains 6915 atoms, of which 1 is hydrogen and 0 are deuteriums.

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	387	2991	1877	516	577	21	0	0	0
1	B	387	2991	1877	516	577	21	0	0	0

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

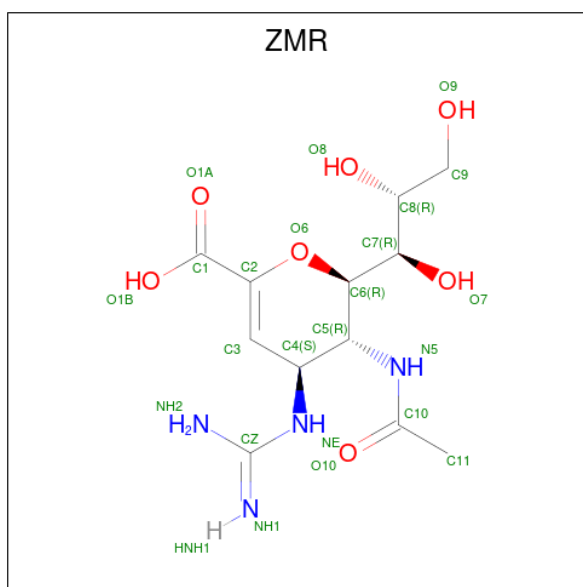


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

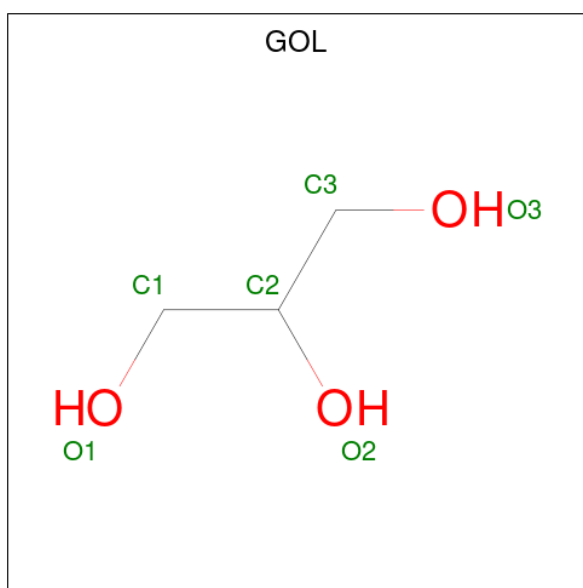
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	3	3	3	0	0
4	B	2	2	2	0	0

- Molecule 5 is ZANAMIVIR (three-letter code: ZMR) (formula: C<sub>12</sub>H<sub>20</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	A	1	23	12	4	7	0	0
5	B	1	23	12	4	7	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



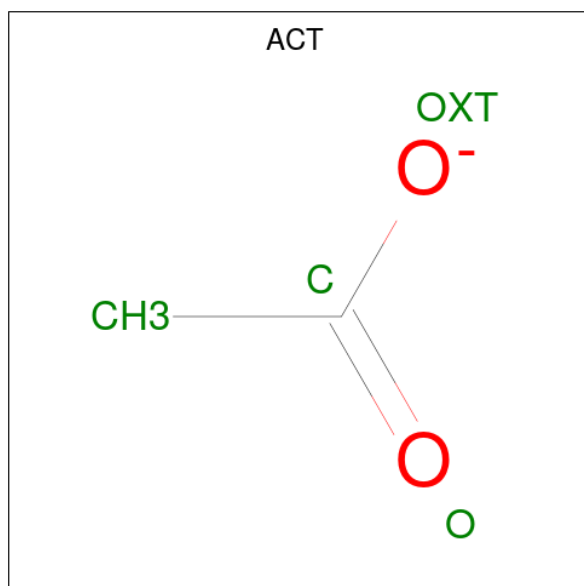
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
6	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	7	3	1	3	0	0

- Molecule 7 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
			Total	C	O		
7	A	1	4	2	2	0	0
7	B	1	4	2	2	0	0
7	B	1	4	2	2	0	0
7	B	1	4	2	2	0	0
7	B	1	4	2	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	384	384	384	0	0
8	B	378	378	378	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.45Å 136.96Å 118.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.13 – 1.90 36.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.6 (36.13-1.90) 98.9 (36.13-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.10 (at 1.89Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.167 , 0.193 0.172 , 0.196	Depositor DCC
$R_{free}$ test set	3770 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.4	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9010e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, ACT, BMA, NAG, CA, ZMR

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	0.23	0/3073	0.43	0/4177
1	B	0.23	0/3073	0.44	0/4177
All	All	0.23	0/6146	0.44	0/8354

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	2991	0	2820	32	0
1	B	2991	0	2820	52	0
2	C	39	0	34	0	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	A	23	0	15	0	0
5	B	23	0	15	0	0
6	A	12	0	16	9	0
6	B	6	1	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	3	2	0
7	B	16	0	12	27	0
8	A	384	0	0	3	0
8	B	378	0	0	3	0
All	All	6914	1	5782	84	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 (84) 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:432:LYS:H	7:B:1:ACT:H2	1.32	0.94
1:B:431:PRO:HD2	7:B:1:ACT:CH3	1.99	0.92
1:B:432:LYS:CG	7:B:1:ACT:H3	1.99	0.92
1:B:431:PRO:HD2	7:B:1:ACT:H1	1.51	0.91
1:A:432:LYS:HB2	6:A:1:GOL:H12	1.54	0.89
1:B:396:ASP:H	7:B:471:ACT:CH3	1.93	0.82
1:B:395:GLN:HA	7:B:471:ACT:H1	1.61	0.81
1:B:432:LYS:HG2	7:B:1:ACT:H3	1.62	0.78
1:A:468:ILE:O	1:A:469:ASP:HB2	1.84	0.78
1:B:455:GLY:HA3	7:B:471:ACT:CH3	2.15	0.76
1:B:259:LYS:HD2	8:B:687:HOH:O	1.87	0.75
1:B:468:ILE:O	1:B:469:ASP:HB2	1.86	0.75
1:A:129:CYS:H	7:A:471:ACT:H1	1.53	0.74
1:B:396:ASP:H	7:B:471:ACT:H1	1.52	0.73
1:B:432:LYS:H	7:B:1:ACT:CH3	2.01	0.73
1:A:431:PRO:HD2	6:A:1:GOL:O3	1.89	0.72
1:A:429:GLY:O	6:A:1:GOL:H11	1.90	0.71
1:B:432:LYS:CB	7:B:1:ACT:H3	2.21	0.71
1:B:129:CYS:H	7:B:472:ACT:CH3	2.05	0.69
1:B:129:CYS:H	7:B:472:ACT:H1	1.56	0.69
1:A:432:LYS:H	6:A:1:GOL:HO3	1.42	0.68
1:A:129:CYS:H	7:A:471:ACT:CH3	2.07	0.67
1:B:455:GLY:HA3	7:B:471:ACT:H3	1.77	0.64
1:B:215:ILE:C	1:B:215:ILE:HD13	2.18	0.63
1:B:396:ASP:H	7:B:471:ACT:H3	1.65	0.62
1:B:325:ASN:O	1:B:348:GLY:HA2	2.01	0.60
1:B:431:PRO:CD	7:B:1:ACT:CH3	2.79	0.58
1:B:455:GLY:HA3	7:B:471:ACT:H2	1.85	0.57
1:A:468:ILE:O	1:A:469:ASP:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LYS:HB2	7:B:1:ACT:H3	1.85	0.56
1:B:270:ALA:HB1	1:B:273:TYR:HB2	1.88	0.56
1:B:468:ILE:O	1:B:469:ASP:CB	2.54	0.55
1:A:378:TRP:HB3	1:A:392:ILE:HB	1.87	0.55
1:A:215:ILE:C	1:A:215:ILE:HD13	2.26	0.54
1:A:155:TYR:CE1	1:B:461:GLY:HA3	2.43	0.53
1:B:378:TRP:HB3	1:B:392:ILE:HB	1.89	0.53
1:B:431:PRO:CD	7:B:1:ACT:H1	2.32	0.52
1:B:125:SER:HB2	1:B:126:PRO:CD	2.39	0.52
1:B:412(B):PRO:HB3	1:B:415:LEU:O	2.10	0.52
1:A:432:LYS:N	6:A:1:GOL:O3	2.39	0.51
6:A:472:GOL:H12	8:A:767:HOH:O	2.10	0.51
1:A:125:SER:HB2	1:A:126:PRO:CD	2.40	0.51
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.10	0.51
1:A:125:SER:HB2	1:A:126:PRO:HD2	1.93	0.50
1:B:102:LYS:HG3	1:B:444:ILE:HG22	1.93	0.50
1:B:431:PRO:HD2	7:B:1:ACT:H2	1.88	0.50
1:B:125:SER:HB2	1:B:126:PRO:HD2	1.93	0.50
1:A:431:PRO:HD2	6:A:1:GOL:C3	2.41	0.49
1:B:128:GLU:HA	7:B:472:ACT:H2	1.93	0.49
1:B:396:ASP:N	7:B:471:ACT:H1	2.24	0.49
1:A:284:SER:HB3	8:A:478:HOH:O	2.12	0.49
1:B:203:ALA:HB3	1:B:215:ILE:CG2	2.44	0.48
1:A:367:SER:HB2	1:A:372:ASN:ND2	2.29	0.47
1:B:457:SER:O	1:B:459:PRO:HD3	2.14	0.46
1:A:325:ASN:O	1:A:348:GLY:HA2	2.15	0.46
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.97	0.46
1:B:320:GLY:HA3	1:B:331:LYS:O	2.15	0.46
1:A:121:PHE:CG	1:A:228:SER:HA	2.51	0.45
1:A:203:ALA:HB3	1:A:215:ILE:CG2	2.46	0.45
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.99	0.45
1:B:128:GLU:CA	7:B:472:ACT:H2	2.47	0.45
1:B:129:CYS:H	7:B:472:ACT:H2	1.82	0.45
1:B:283:ASP:HB3	8:B:808:HOH:O	2.17	0.45
1:A:431:PRO:CD	6:A:1:GOL:O3	2.63	0.44
1:B:121:PHE:CG	1:B:228:SER:HA	2.52	0.44
1:B:431:PRO:CD	7:B:1:ACT:H2	2.46	0.43
1:A:283:ASP:HB3	8:A:576:HOH:O	2.18	0.43
1:B:322:PHE:HB2	1:B:327:ARG:HD2	2.01	0.43
1:B:203:ALA:HB3	1:B:215:ILE:HG23	2.01	0.43
1:A:432:LYS:HG2	6:A:1:GOL:O3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:HB2	7:B:472:ACT:H2	2.00	0.42
1:A:346:ALA:O	1:A:347:ASN:HB2	2.18	0.42
1:A:379:ASP:HA	1:A:380:PRO:HD2	1.90	0.42
1:B:188:ASN:HB2	1:B:207:TYR:CZ	2.55	0.42
1:B:379:ASP:HA	1:B:380:PRO:HD2	1.86	0.41
1:B:228:SER:HB3	1:B:350:LYS:HE2	2.02	0.41
1:B:355:LYS:HE2	1:B:383:TRP:CD1	2.54	0.41
1:B:347:ASN:HB3	8:B:507:HOH:O	2.20	0.41
1:A:122:ILE:HD13	1:A:163:ILE:CD1	2.51	0.41
1:B:432:LYS:HB2	7:B:1:ACT:CH3	2.50	0.41
1:A:108:ILE:HD12	1:A:166:VAL:CG1	2.51	0.41
1:A:320:GLY:HA3	1:A:331:LYS:O	2.20	0.41
1:B:457:SER:C	1:B:459:PRO:HD3	2.41	0.41
1:A:188:ASN:HB2	1:A:207:TYR:CZ	2.56	0.40

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	385/388 (99%)	368 (96%)	17 (4%)	0	100	100
1	B	385/388 (99%)	369 (96%)	16 (4%)	0	100	100
All	All	770/776 (99%)	737 (96%)	33 (4%)	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	334/335 (100%)	328 (98%)	6 (2%)	59	55
1	B	334/335 (100%)	329 (98%)	5 (2%)	65	62
All	All	668/670 (100%)	657 (98%)	11 (2%)	62	60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ILE
1	A	230	CYS
1	A	296	HIS
1	A	372	ASN
1	A	435	ASN
1	A	463	GLU
1	B	215	ILE
1	B	230	CYS
1	B	296	HIS
1	B	372	ASN
1	B	463	GLU

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	401	ASN
1	A	435	ASN
1	B	401	ASN
1	B	435	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

3 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	0.57	0	17,19,21	0.65	0
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	1.03	1 (5%)
2	BMA	C	3	2	11,11,12	0.62	0	15,15,17	0.86	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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C3-C4-C5	2.27	114.28	110.24

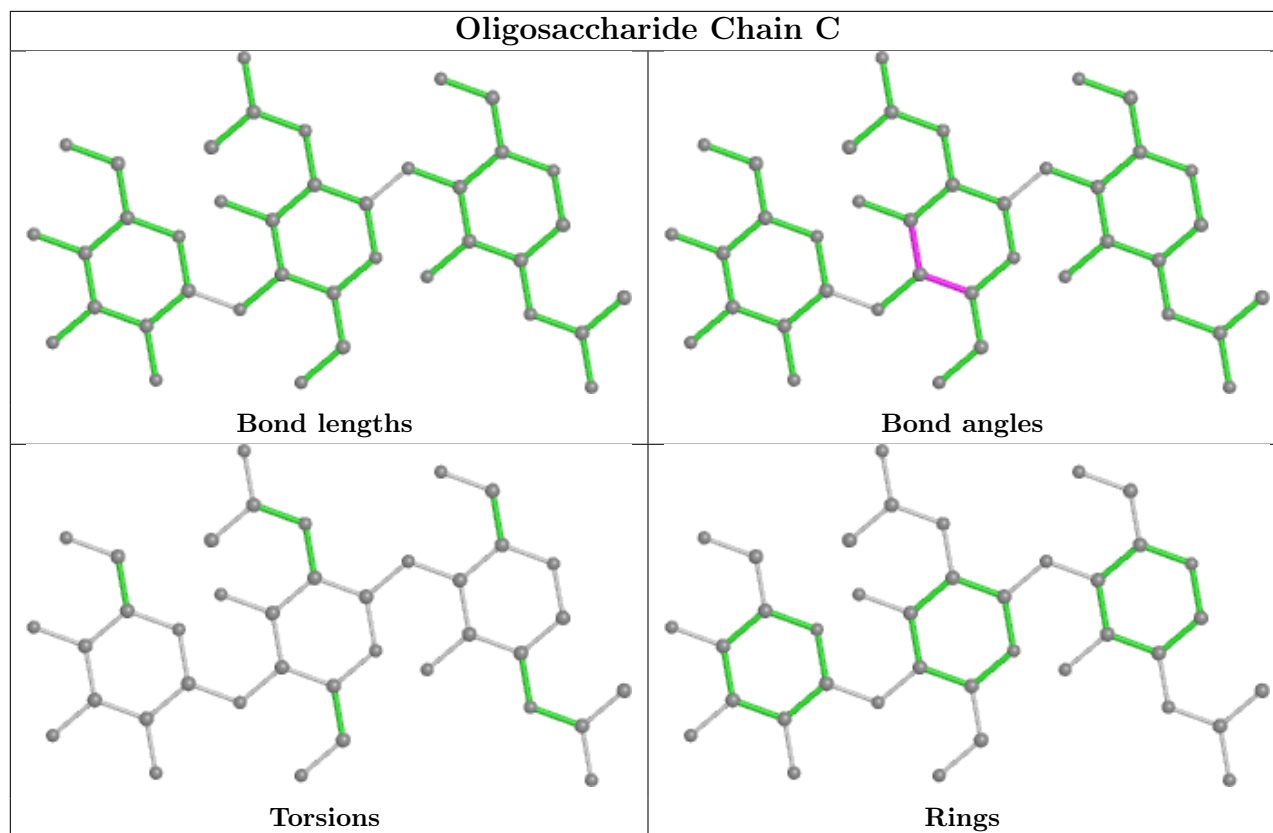
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	ACT	A	471	-	3,3,3	0.76	0	3,3,3	1.36	0
6	GOL	B	473	-	5,5,5	0.36	0	5,5,5	0.35	0
3	NAG	B	501	1	14,14,15	0.57	0	17,19,21	0.97	1 (5%)
6	GOL	A	1	-	5,5,5	0.37	0	5,5,5	0.48	0
7	ACT	B	1	-	3,3,3	0.79	0	3,3,3	1.31	0
3	NAG	B	502	1	14,14,15	0.57	0	17,19,21	0.73	0
5	ZMR	B	1002	-	22,23,23	4.00	11 (50%)	24,32,32	1.95	5 (20%)
5	ZMR	A	1002	-	22,23,23	3.94	10 (45%)	24,32,32	1.73	6 (25%)
7	ACT	B	474	-	3,3,3	0.76	0	3,3,3	1.35	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ACT	B	471	-	3,3,3	0.76	0	3,3,3	1.32	0
7	ACT	B	472	-	3,3,3	0.78	0	3,3,3	1.32	0
6	GOL	A	472	-	5,5,5	0.36	0	5,5,5	0.25	0
3	NAG	A	505	1	14,14,15	0.58	0	17,19,21	0.73	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	GOL	B	473	-	-	4/4/4/4	-
3	NAG	B	501	1	-	2/6/23/26	0/1/1/1
6	GOL	A	1	-	-	2/4/4/4	-
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
5	ZMR	B	1002	-	-	0/22/38/38	0/1/1/1
5	ZMR	A	1002	-	-	0/22/38/38	0/1/1/1
6	GOL	A	472	-	-	4/4/4/4	-
3	NAG	A	505	1	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	ZMR	C3-C2	14.84	1.56	1.33
5	A	1002	ZMR	C3-C2	14.56	1.55	1.33
5	B	1002	ZMR	CZ-NE	5.97	1.43	1.33
5	A	1002	ZMR	CZ-NE	5.35	1.42	1.33
5	B	1002	ZMR	O8-C8	-4.52	1.33	1.43
5	A	1002	ZMR	C4-NE	-4.36	1.40	1.46
5	A	1002	ZMR	O8-C8	-4.11	1.34	1.43
5	A	1002	ZMR	O7-C7	-4.11	1.33	1.43
5	B	1002	ZMR	C4-NE	-3.92	1.41	1.46
5	B	1002	ZMR	O7-C7	-3.35	1.35	1.43
5	A	1002	ZMR	O10-C10	-3.16	1.16	1.23
5	B	1002	ZMR	O10-C10	-3.01	1.16	1.23
5	A	1002	ZMR	C5-N5	-2.67	1.41	1.45
5	B	1002	ZMR	C5-N5	-2.53	1.41	1.45
5	B	1002	ZMR	O9-C9	-2.50	1.31	1.42
5	B	1002	ZMR	O6-C6	-2.49	1.41	1.46
5	A	1002	ZMR	O9-C9	-2.44	1.32	1.42
5	A	1002	ZMR	C4-C3	2.42	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1002	ZMR	C7-C6	-2.39	1.49	1.53
5	A	1002	ZMR	O6-C6	-2.16	1.42	1.46
5	B	1002	ZMR	C4-C3	2.12	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1002	ZMR	O6-C2-C3	-4.49	119.37	124.61
5	B	1002	ZMR	C6-C5-N5	3.76	117.16	110.91
5	B	1002	ZMR	C3-C4-NE	3.64	116.19	111.00
5	A	1002	ZMR	O6-C2-C3	-3.64	120.37	124.61
5	B	1002	ZMR	O8-C8-C7	3.54	117.70	109.10
5	A	1002	ZMR	C6-C5-N5	3.52	116.75	110.91
3	B	501	NAG	C1-O5-C5	2.99	116.25	112.19
5	A	1002	ZMR	O6-C2-C1	2.99	118.04	112.06
5	A	1002	ZMR	O8-C8-C7	2.79	115.87	109.10
5	A	1002	ZMR	O7-C7-C8	2.10	113.88	108.81
5	A	1002	ZMR	NE-CZ-NH1	-2.04	117.03	120.59
5	B	1002	ZMR	O7-C7-C8	2.02	113.70	108.81

There are no chirality outliers.

All (12) torsion outliers are listed below:

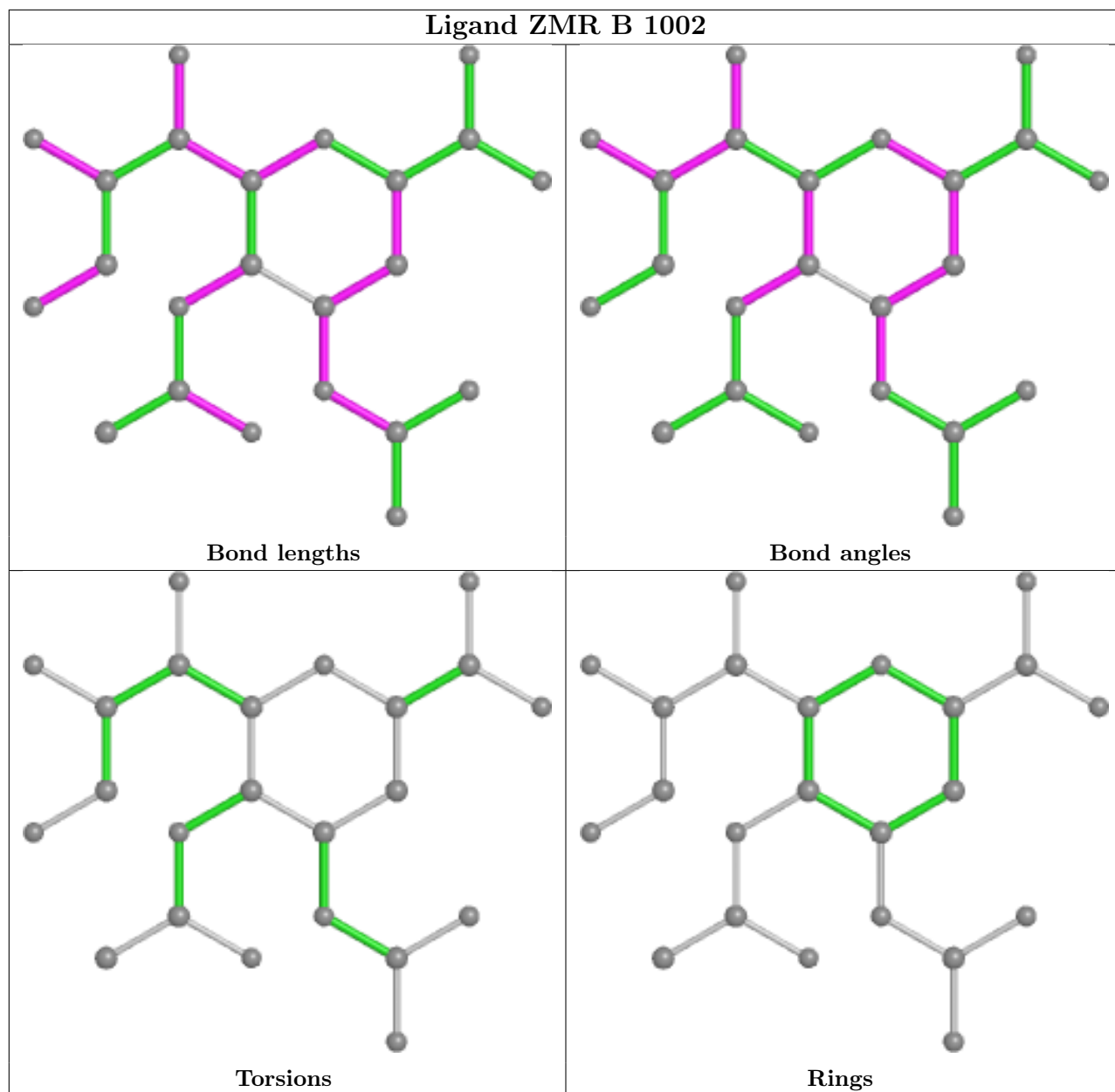
Mol	Chain	Res	Type	Atoms
6	A	1	GOL	O1-C1-C2-C3
6	A	472	GOL	O1-C1-C2-C3
3	B	501	NAG	C4-C5-C6-O6
6	A	472	GOL	O1-C1-C2-O2
3	B	501	NAG	O5-C5-C6-O6
6	A	472	GOL	C1-C2-C3-O3
6	B	473	GOL	O1-C1-C2-C3
6	B	473	GOL	C1-C2-C3-O3
6	A	472	GOL	O2-C2-C3-O3
6	A	1	GOL	O1-C1-C2-O2
6	B	473	GOL	O1-C1-C2-O2
6	B	473	GOL	O2-C2-C3-O3

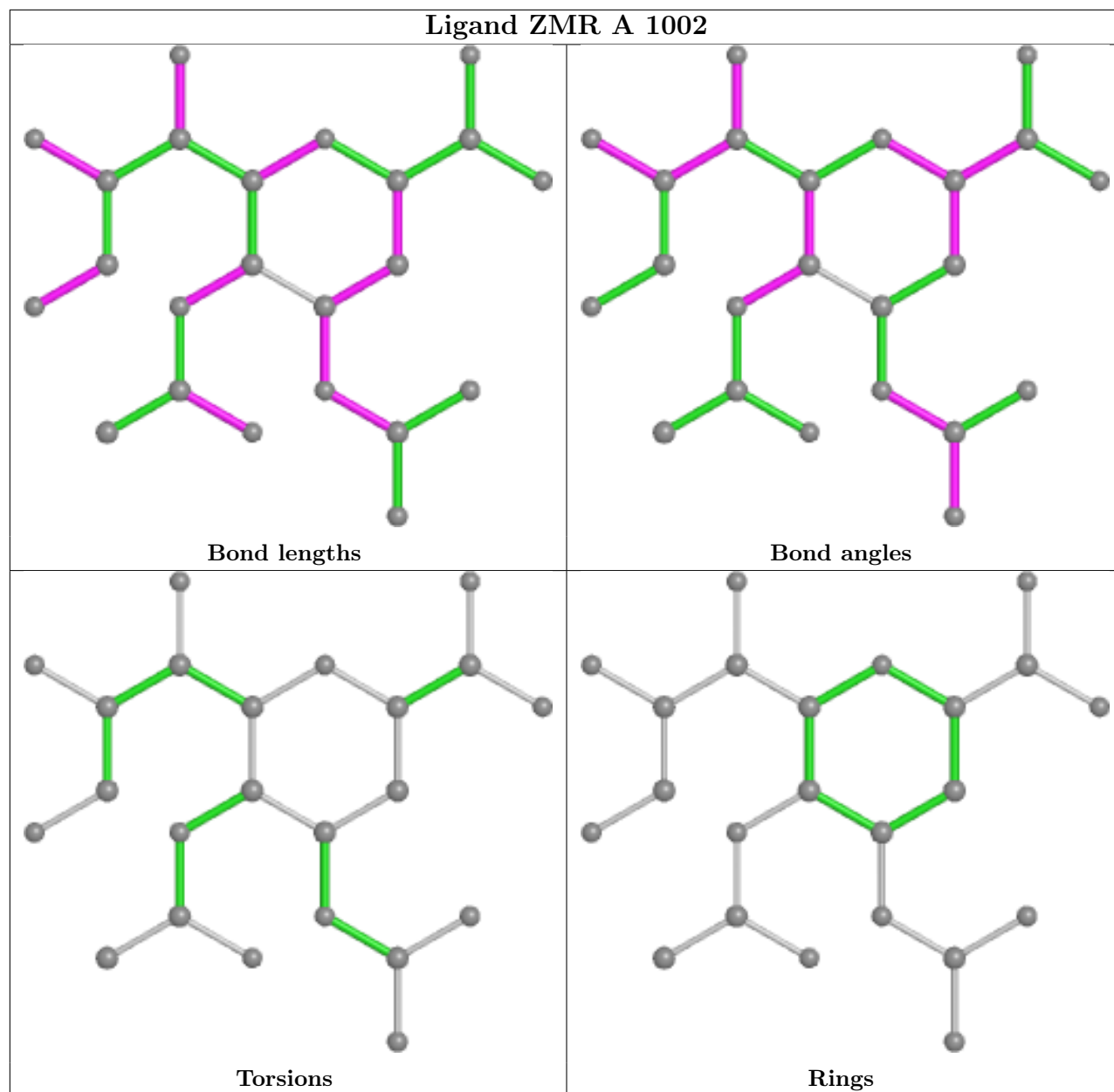
There are no ring outliers.

6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	471	ACT	2	0
6	A	1	GOL	8	0
7	B	1	ACT	13	0
7	B	471	ACT	8	0
7	B	472	ACT	6	0
6	A	472	GOL	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	387/388 (99%)	-0.11	6 (1%) 72 74	5, 10, 21, 34	0
1	B	387/388 (99%)	-0.20	3 (0%) 86 87	5, 10, 20, 32	0
All	All	774/776 (99%)	-0.15	9 (1%) 79 81	5, 10, 21, 34	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	ASP	3.0
1	B	469	ASP	3.0
1	B	83	VAL	2.9
1	A	83	VAL	2.8
1	A	82	SER	2.7
1	A	93	PRO	2.7
1	A	435	ASN	2.6
1	B	82	SER	2.5
1	A	416	ASP	2.3

### 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, 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.

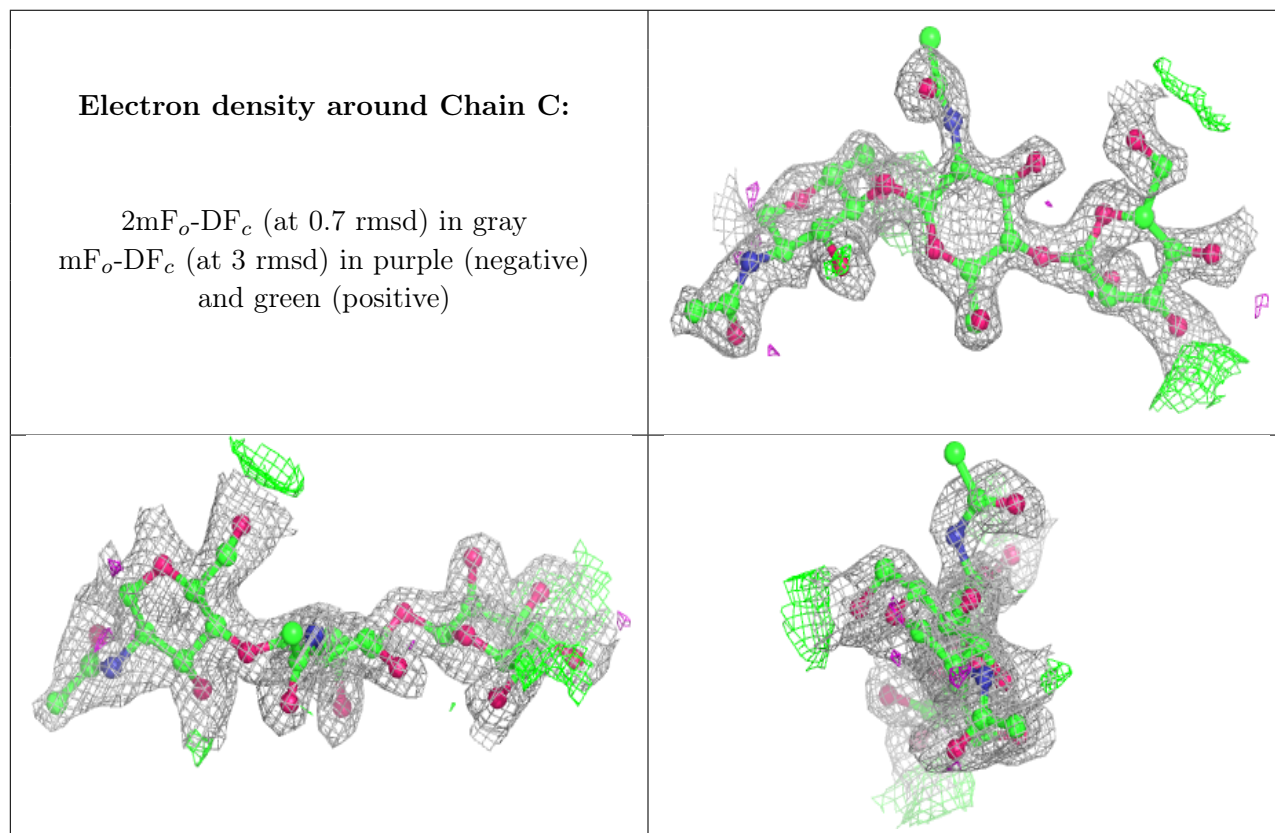
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	C	3	11/12	0.65	0.32	28,35,41,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	2	14/15	0.82	0.36	37,41,47,52	0
2	NAG	C	1	14/15	0.87	0.28	19,28,33,34	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.



## 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
3	NAG	B	501	14/15	0.64	0.26	55,67,80,83	0
6	GOL	B	473	6/6	0.79	0.21	35,38,42,50	0
3	NAG	A	505	14/15	0.80	0.27	32,43,50,50	0
6	GOL	A	472	6/6	0.81	0.23	32,34,43,52	0
3	NAG	B	502	14/15	0.84	0.26	30,38,47,49	0
6	GOL	A	1	6/6	0.84	0.33	6,23,27,30	0

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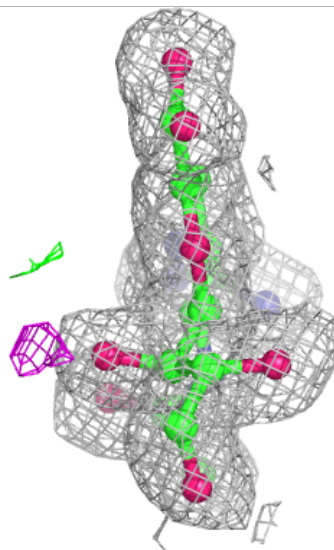
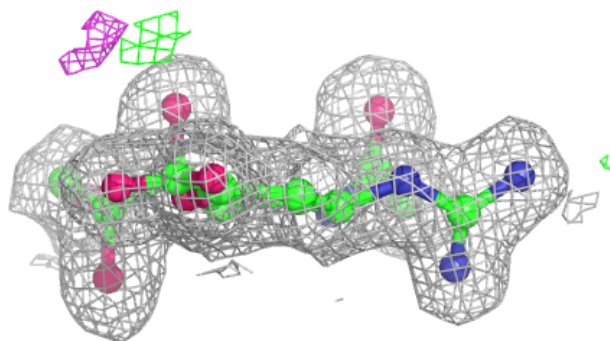
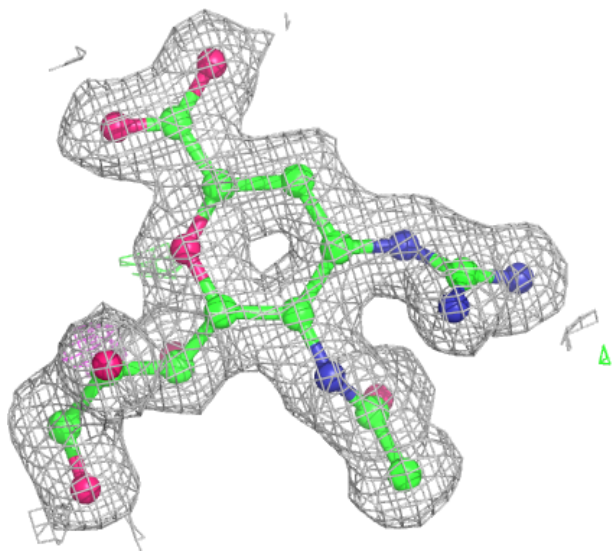
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ACT	B	471	4/4	0.85	0.22	17,24,37,42	0
7	ACT	A	471	4/4	0.91	0.15	14,16,27,32	0
7	ACT	B	1	4/4	0.92	0.21	5,12,23,24	0
7	ACT	B	474	4/4	0.92	0.12	23,28,28,36	0
7	ACT	B	472	4/4	0.94	0.14	18,21,30,34	0
5	ZMR	A	1002	23/23	0.96	0.10	6,10,12,16	0
5	ZMR	B	1002	23/23	0.96	0.09	8,9,15,16	0
4	CA	B	601	1/1	0.97	0.08	10,10,10,10	0
4	CA	A	601	1/1	0.98	0.09	11,11,11,11	0
4	CA	A	602	1/1	0.99	0.07	16,16,16,16	0
4	CA	B	602	1/1	0.99	0.05	14,14,14,14	0
4	CA	A	603	1/1	0.99	0.06	17,17,17,17	1

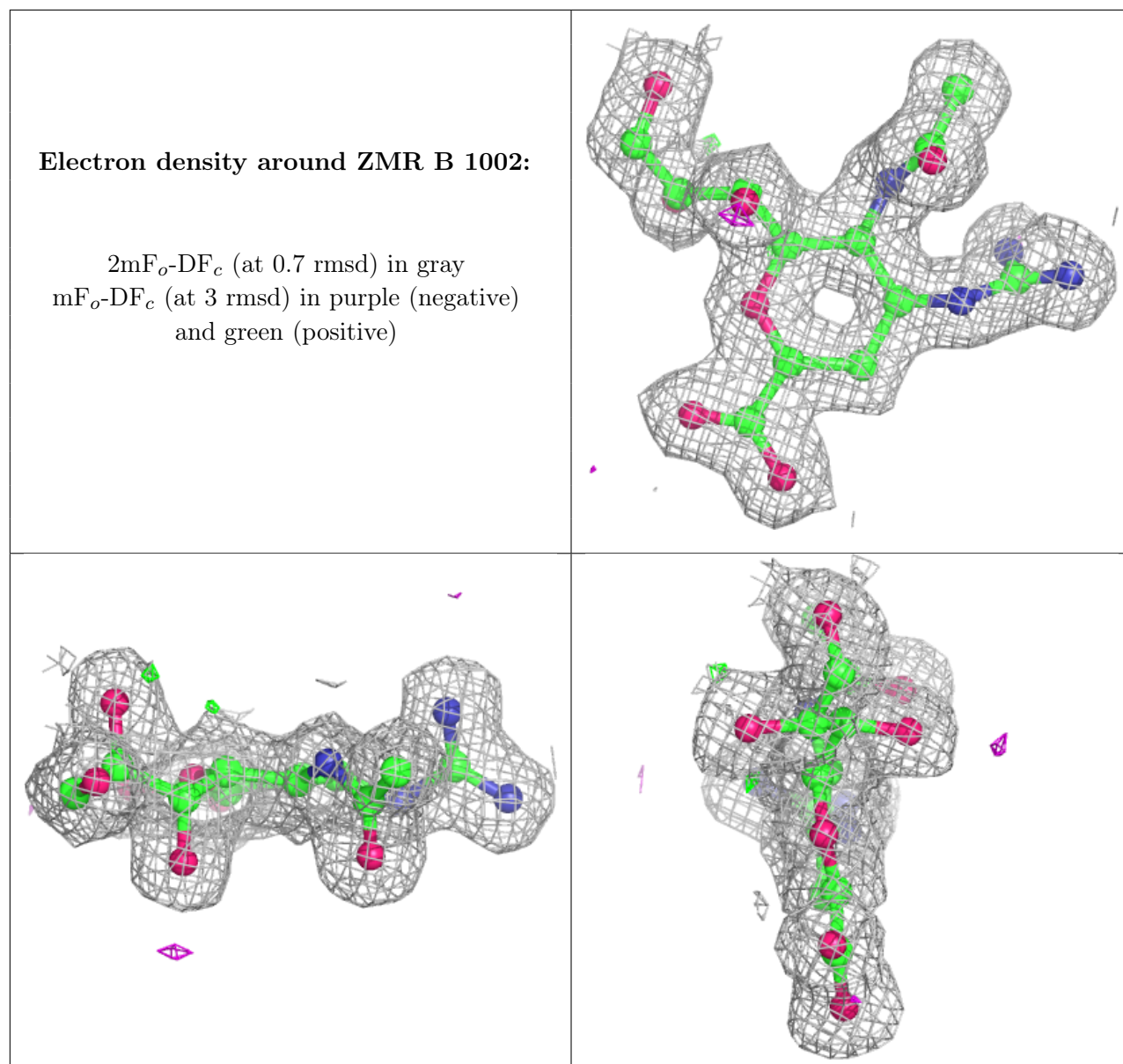
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around ZMR A 1002:**

$2mF_o-DF_c$  (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.