



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:47 AM BST

PDB ID : 2WNJ  
Title : CRYSTAL STRUCTURE OF APLYSIA ACHBP IN COMPLEX WITH DMXBA  
Authors : Sulzenbacher, G.; Hibbs, R.; Shi, J.; Talley, T.; Conrod, S.; Kem, W.; Taylor, P.; Marchot, P.; Bourne, Y.  
Deposited on : 2009-07-09  
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.

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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 : 2.13.1  
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) : 2.13.1

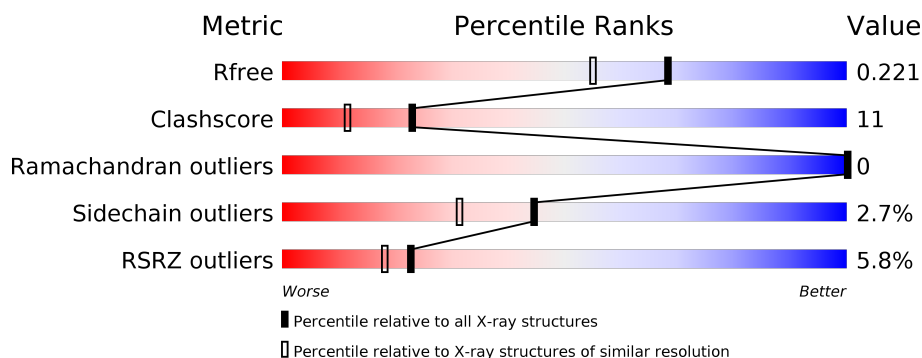
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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 on 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	228	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	B	228	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>
1	C	228	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	D	228	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>7%</div> </div> </div>
1	E	228	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
2	F	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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
3	ZY7	A	301[B]	-	-	X	-
3	ZY7	D	301[B]	-	-	X	-
3	ZY7	E	301[A]	-	-	X	-

## 2 Entry composition [i](#)

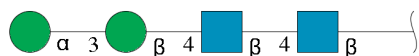
There are 5 unique types of molecules in this entry. The entry contains 10037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SOLUBLE ACETYLCHOLINE RECEPTOR.

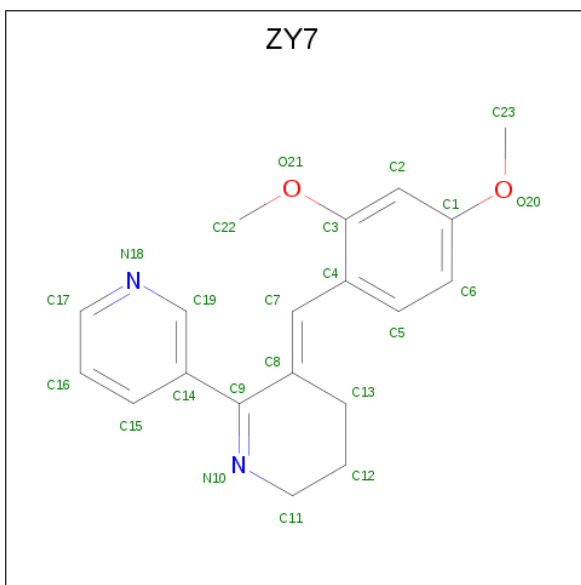
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	10	0
			1727	1098	283	336	10			
1	B	212	Total	C	N	O	S	0	8	0
			1746	1107	290	339	10			
1	C	214	Total	C	N	O	S	0	10	0
			1769	1120	291	347	11			
1	D	211	Total	C	N	O	S	0	8	0
			1733	1100	284	339	10			
1	E	217	Total	C	N	O	S	0	13	0
			1822	1162	297	353	10			

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



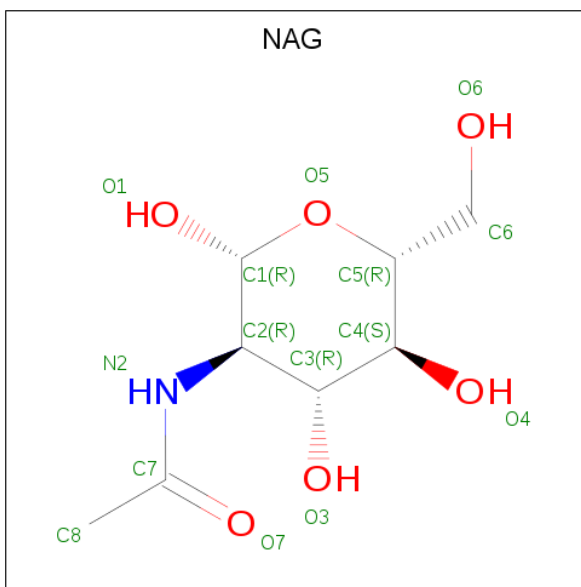
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is (3E)-3-[(2,4-DIMETHOXYPHENYL)METHYLIDENE]-3,4,5,6-TETRAHYDRO-2,3'-BIPYRIDINE (three-letter code: ZY7) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			46	38	4	4		
3	B	1	Total	C	N	O	0	0
			23	19	2	2		
3	C	1	Total	C	N	O	0	0
			23	19	2	2		
3	D	1	Total	C	N	O	0	1
			46	38	4	4		
3	E	1	Total	C	N	O	0	1
			46	38	4	4		

- 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
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

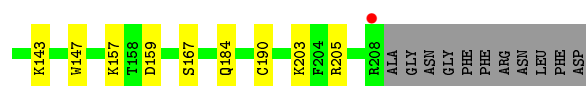
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total	O	0	0
			214	214		
5	B	177	Total	O	0	0
			177	177		
5	C	200	Total	O	0	0
			200	200		
5	D	193	Total	O	0	0
			193	193		
5	E	208	Total	O	0	0
			208	208		

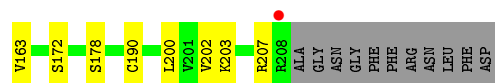
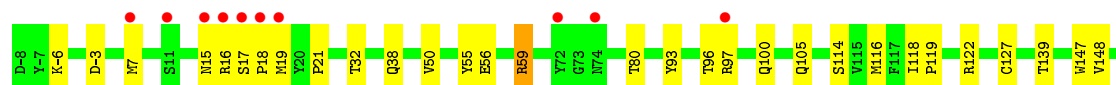
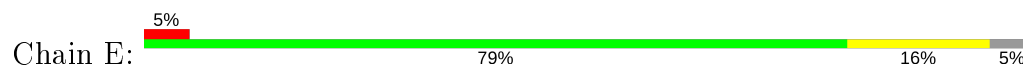


- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR





• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.22Å 114.80Å 131.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 47.71 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.80) 99.8 (47.71-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.169 , 0.206 0.191 , 0.221	Depositor DCC
$R_{free}$ test set	6069 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: ZY7, BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.71	1/1799 (0.1%)	0.76	0/2451
1	B	0.69	1/1812 (0.1%)	0.76	2/2466 (0.1%)
1	C	0.67	0/1836	0.74	0/2496
1	D	0.76	0/1799	0.81	1/2450 (0.0%)
1	E	0.77	0/1902	0.79	0/2590
All	All	0.72	2/9148 (0.0%)	0.77	3/12453 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CB-CG	-5.42	1.41	1.52
1	B	56	GLU	CB-CG	-5.05	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59[A]	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	59[B]	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	D	68	ASP	CB-CG-OD1	5.61	123.35	118.30

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	1727	0	1690	34	0
1	B	1746	0	1707	22	0
1	C	1769	0	1728	46	0
1	D	1733	0	1688	48	0
1	E	1822	0	1791	61	0
2	F	50	0	43	0	0
3	A	46	0	39	15	0
3	B	23	0	20	8	0
3	C	23	0	20	4	0
3	D	46	0	37	24	0
3	E	46	0	37	26	0
4	B	14	0	13	0	0
5	A	214	0	0	4	0
5	B	177	0	0	2	0
5	C	200	0	0	6	0
5	D	193	0	0	6	0
5	E	208	0	0	6	0
All	All	10037	0	8813	204	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 11.

All (204) 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:E:93[A]:TYR:CE2	3:E:301[A]:ZY7:H121	1.12	1.61
1:E:93[A]:TYR:CE2	3:E:301[A]:ZY7:C12	2.03	1.40
1:D:57[B]:GLN:OE1	3:E:301[B]:ZY7:C2	1.76	1.33
1:E:93[A]:TYR:OH	3:E:301[A]:ZY7:H111	1.17	1.33
1:E:93[A]:TYR:OH	3:E:301[A]:ZY7:C11	1.81	1.29
1:D:57[B]:GLN:OE1	3:E:301[B]:ZY7:H2	1.35	1.18
1:E:93[A]:TYR:CZ	3:E:301[A]:ZY7:C11	2.29	1.14
1:C:118:ILE:HD12	3:D:301[B]:ZY7:C7	1.90	1.00
1:C:118:ILE:HD11	3:D:301[B]:ZY7:C3	1.92	0.99
1:C:118:ILE:CD1	3:D:301[B]:ZY7:C4	2.43	0.97
1:E:93[A]:TYR:CZ	3:E:301[A]:ZY7:H121	2.01	0.92
1:D:57[B]:GLN:CD	3:E:301[B]:ZY7:C1	2.33	0.91
1:C:118:ILE:CD1	3:D:301[B]:ZY7:C7	2.48	0.91
1:D:57[B]:GLN:HG3	1:D:118:ILE:CD1	2.00	0.91
1:E:93[A]:TYR:CZ	3:E:301[A]:ZY7:H112	2.03	0.90
1:E:200[B]:LEU:CD1	1:E:202[B]:VAL:HG23	2.02	0.90
1:D:57[B]:GLN:OE1	3:E:301[B]:ZY7:C1	2.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301[A]:ZY7:H132	3:A:301[A]:ZY7:H5	1.59	0.85
1:D:57[B]:GLN:CD	3:E:301[B]:ZY7:C2	2.46	0.84
1:E:93[A]:TYR:CD2	3:E:301[A]:ZY7:H121	2.07	0.83
1:C:59[B]:ARG:CG	1:C:59[B]:ARG:HH21	1.91	0.83
1:B:59[A]:ARG:HE	1:B:114:SER:HB2	1.43	0.82
3:A:301[B]:ZY7:C22	1:E:116[B]:MET:SD	2.69	0.80
1:A:157:LYS:NZ	5:A:2163:HOH:O	2.12	0.80
1:D:57[B]:GLN:HG3	1:D:118:ILE:HD12	1.62	0.79
1:B:7[B]:MET:HE2	1:C:21:PRO:HD3	1.66	0.78
1:E:59[B]:ARG:CG	1:E:59[B]:ARG:HH21	1.97	0.78
1:C:118:ILE:CD1	3:D:301[B]:ZY7:C3	2.61	0.77
1:E:93[A]:TYR:OH	3:E:301[A]:ZY7:H112	1.83	0.77
1:C:-6:LYS:N	1:C:-6:LYS:HD3	2.00	0.77
1:C:118:ILE:HD12	3:D:301[B]:ZY7:H7	1.67	0.77
1:B:59[B]:ARG:NH2	1:B:159:ASP:OD2	2.18	0.76
1:C:118:ILE:HD13	3:D:301[B]:ZY7:C4	2.14	0.75
1:E:93[A]:TYR:CZ	3:E:301[A]:ZY7:C12	2.53	0.75
1:E:59[B]:ARG:HE	1:E:114:SER:HB2	1.50	0.75
1:E:105:GLN:NE2	5:E:2127:HOH:O	2.22	0.72
1:D:159:ASP:OD2	5:D:2146:HOH:O	2.08	0.72
1:D:190:CYS:HB2	3:D:301[B]:ZY7:C4	2.20	0.72
1:C:59[B]:ARG:HH21	1:C:59[B]:ARG:HG3	1.53	0.71
1:A:57[B]:GLN:OE1	3:B:301:ZY7:C2	2.38	0.71
1:E:93[A]:TYR:HE2	3:E:301[A]:ZY7:C12	1.66	0.69
1:C:143[A]:LYS:NZ	5:C:2145:HOH:O	2.24	0.69
1:A:100:GLN:HE22	1:B:97[A]:ARG:HH21	1.39	0.68
3:A:301[B]:ZY7:O21	1:E:116[B]:MET:SD	2.51	0.68
1:D:57[A]:GLN:OE1	5:D:2063:HOH:O	0.68	0.68
1:E:93[A]:TYR:HE2	3:E:301[A]:ZY7:H121	0.86	0.68
3:C:301:ZY7:H5	3:C:301:ZY7:H131	1.77	0.67
1:A:160:THR:OG1	5:A:2168:HOH:O	2.11	0.67
1:E:105:GLN:OE1	5:E:2127:HOH:O	2.12	0.67
1:E:200[B]:LEU:HD13	1:E:202[B]:VAL:HG23	1.76	0.67
1:E:200[B]:LEU:HD11	1:E:202[B]:VAL:CG2	2.25	0.67
1:D:190:CYS:HB2	3:D:301[B]:ZY7:C3	2.25	0.67
1:A:116[B]:MET:SD	3:B:301:ZY7:O21	2.52	0.66
1:B:7[B]:MET:CE	1:C:21:PRO:HD3	2.25	0.66
1:E:200[B]:LEU:HD11	1:E:202[B]:VAL:HG23	1.78	0.66
3:B:301:ZY7:H5	3:B:301:ZY7:H132	1.76	0.66
1:A:21:PRO:HB3	1:E:7:MET:CE	2.26	0.66
1:B:59[A]:ARG:HH11	1:B:59[A]:ARG:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97[A]:ARG:HH21	1:E:100:GLN:HE22	1.41	0.65
1:A:57[B]:GLN:OE1	3:B:301:ZY7:H2	1.97	0.65
1:B:105:GLN:NE2	5:B:2113:HOH:O	2.29	0.65
1:C:7[A]:MET:CE	1:D:21:PRO:HD3	2.26	0.65
3:A:301[B]:ZY7:H221	1:E:116[B]:MET:CE	2.26	0.65
1:B:59[A]:ARG:HH11	1:B:59[A]:ARG:CG	2.11	0.64
1:C:57[B]:GLN:HG2	3:D:301[B]:ZY7:C23	2.27	0.64
1:D:97[B]:ARG:NH2	5:D:2098:HOH:O	2.29	0.64
1:A:116[B]:MET:SD	3:B:301:ZY7:C22	2.86	0.64
1:C:118:ILE:HD11	3:D:301[B]:ZY7:O21	1.96	0.64
1:E:59[B]:ARG:HH21	1:E:59[B]:ARG:HG2	1.63	0.64
1:E:163:VAL:HG21	1:E:200[B]:LEU:HD21	1.80	0.64
1:C:59[B]:ARG:NH2	5:C:2071:HOH:O	2.31	0.63
1:C:7[B]:MET:HE3	5:C:2008:HOH:O	1.98	0.63
3:A:301[B]:ZY7:H221	1:E:116[B]:MET:SD	2.38	0.63
1:C:7[A]:MET:HE2	1:D:21:PRO:HD3	1.80	0.62
1:D:25:LYS:NZ	5:D:2015:HOH:O	2.32	0.62
1:E:105:GLN:CD	5:E:2127:HOH:O	2.38	0.62
1:E:163:VAL:HG21	1:E:200[B]:LEU:CD2	2.30	0.62
1:C:57[B]:GLN:OE1	5:C:2060:HOH:O	0.63	0.62
1:A:56:GLU:O	1:A:119:PRO:HD2	2.00	0.61
3:A:301[A]:ZY7:H132	3:A:301[A]:ZY7:C5	2.30	0.60
3:A:301[B]:ZY7:H131	3:A:301[B]:ZY7:H5	1.83	0.60
1:A:116[B]:MET:SD	3:B:301:ZY7:H221	2.43	0.59
1:C:59[B]:ARG:HH21	1:C:59[B]:ARG:HG2	1.64	0.59
1:C:-6:LYS:H3	1:C:-6:LYS:HD3	1.67	0.59
1:D:57[A]:GLN:HG3	3:E:301[A]:ZY7:H221	1.83	0.59
1:C:59[B]:ARG:HE	1:C:114:SER:HB2	1.68	0.59
1:E:7:MET:HA	1:E:7:MET:CE	2.33	0.58
1:C:167:SER:OG	3:D:301[A]:ZY7:H232	2.03	0.58
1:A:191:CYS:SG	3:A:301[B]:ZY7:H223	2.44	0.58
1:C:-6:LYS:H1	1:C:-6:LYS:HD3	1.69	0.57
1:C:59[B]:ARG:NH2	1:C:59[B]:ARG:HG3	2.18	0.57
1:E:59[B]:ARG:NH2	5:E:2077:HOH:O	2.36	0.57
3:C:301:ZY7:H5	3:C:301:ZY7:C13	2.34	0.57
1:E:38:GLN:OE1	1:E:55[A]:TYR:CE1	2.57	0.57
1:E:32:THR:HG21	1:E:59[A]:ARG:HH22	1.69	0.57
1:E:59[B]:ARG:HG3	1:E:59[B]:ARG:HH21	1.69	0.57
1:D:143:LYS:HE3	1:D:184:GLN:HE22	1.69	0.57
1:B:57[B]:GLN:HG2	3:C:301:ZY7:C1	2.35	0.57
3:B:301:ZY7:H5	3:B:301:ZY7:C13	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57[B]:GLN:HG3	1:D:118:ILE:HD11	1.84	0.56
1:A:143:LYS:NZ	1:A:184:GLN:HE22	2.04	0.56
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.45	0.56
1:A:12:ASP:HA	1:A:16:ARG:HE	1.71	0.56
1:C:7[A]:MET:SD	1:D:18:PRO:HG2	2.46	0.56
1:C:57[B]:GLN:HG2	3:D:301[B]:ZY7:C1	2.36	0.55
1:D:11:SER:OG	1:D:16:ARG:CZ	2.53	0.55
1:A:190:CYS:HB2	3:A:301[B]:ZY7:C1	2.37	0.55
3:D:301[A]:ZY7:H5	3:D:301[A]:ZY7:H132	1.88	0.55
1:C:59[B]:ARG:CG	1:C:59[B]:ARG:NH2	2.58	0.55
1:D:30:THR:HG21	1:D:157[A]:LYS:HE3	1.88	0.55
1:A:100:GLN:HE22	1:B:97[A]:ARG:NH2	2.05	0.54
3:D:301[A]:ZY7:C5	3:D:301[A]:ZY7:H132	2.37	0.54
1:D:147:TRP:CE2	3:D:301[A]:ZY7:H19	2.43	0.54
1:D:55[A]:TYR:CE2	1:E:147:TRP:HH2	2.27	0.54
3:E:301[A]:ZY7:H132	3:E:301[A]:ZY7:H5	1.91	0.53
1:A:11:SER:O	1:A:16:ARG:HG3	2.09	0.53
1:E:56:GLU:O	1:E:119:PRO:HD2	2.09	0.53
1:D:147:TRP:NE1	3:D:301[A]:ZY7:H19	2.23	0.53
1:B:136:GLU:O	1:B:203[B]:LYS:HE3	2.10	0.52
1:B:191:CYS:SG	3:B:301:ZY7:H223	2.50	0.52
1:A:96:THR:O	1:E:122:ARG:HD2	2.08	0.52
1:A:161:ASP:HB3	5:A:2192:HOH:O	2.09	0.52
3:D:301[A]:ZY7:C13	3:D:301[A]:ZY7:H5	2.40	0.52
1:D:15:ASN:N	1:D:15:ASN:HD22	2.07	0.52
1:D:190:CYS:CB	3:D:301[B]:ZY7:C4	2.87	0.52
1:A:21:PRO:HB3	1:E:7:MET:HE3	1.93	0.51
1:B:59[A]:ARG:CG	1:B:59[A]:ARG:NH1	2.73	0.51
1:E:172:SER:O	1:E:207[B]:ARG:HD3	2.11	0.51
1:C:56:GLU:O	1:C:119:PRO:HD2	2.10	0.51
1:D:136:GLU:O	1:D:203:LYS:HE2	2.11	0.51
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.51	0.50
1:D:167:SER:OG	3:E:301[A]:ZY7:H232	2.11	0.50
3:E:301[A]:ZY7:H132	3:E:301[A]:ZY7:C5	2.41	0.50
1:D:57[A]:GLN:HG3	3:E:301[A]:ZY7:C22	2.41	0.50
1:C:7[B]:MET:SD	1:D:21:PRO:HB3	2.52	0.50
1:A:190:CYS:HB2	3:A:301[B]:ZY7:C6	2.41	0.50
1:A:122:ARG:HD2	1:B:96:THR:O	2.10	0.50
1:C:97[B]:ARG:NH1	5:C:2107:HOH:O	2.43	0.49
1:D:190:CYS:CB	3:D:301[B]:ZY7:C5	2.90	0.49
3:C:301:ZY7:C5	3:C:301:ZY7:H131	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-6:LYS:O	1:C:-2:ASP:N	2.43	0.48
3:A:301[A]:ZY7:C13	3:A:301[A]:ZY7:H5	2.39	0.48
1:B:139:THR:OG1	1:B:203[B]:LYS:NZ	2.41	0.48
1:C:-6:LYS:N	1:C:-6:LYS:CD	2.74	0.48
3:D:301[B]:ZY7:H131	3:D:301[B]:ZY7:H5	1.95	0.47
1:C:122:ARG:HD2	1:D:96:THR:O	2.13	0.47
1:D:7:MET:CE	1:E:21:PRO:HD3	2.44	0.47
1:E:97[B]:ARG:NH2	5:E:2109:HOH:O	2.26	0.47
1:A:61:LYS:HE3	1:A:112:ASP:O	2.14	0.47
1:B:193:GLU:CD	1:B:193:GLU:H	2.18	0.47
1:B:7[B]:MET:SD	1:C:18:PRO:HB2	2.54	0.47
1:C:7[A]:MET:HE3	1:D:21:PRO:HD3	1.97	0.46
3:E:301[B]:ZY7:H131	3:E:301[B]:ZY7:H5	1.98	0.46
1:E:190:CYS:HB2	3:E:301[B]:ZY7:C3	2.46	0.46
1:E:55[B]:TYR:CD1	1:E:118[B]:ILE:CG2	2.99	0.46
1:D:190:CYS:HB3	3:D:301[B]:ZY7:C5	2.47	0.45
1:D:106:ILE:HB	1:E:148:VAL:HG11	1.97	0.45
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.56	0.45
1:D:122:ARG:HD2	1:E:96:THR:O	2.15	0.45
1:D:56:GLU:O	1:D:119:PRO:HD2	2.17	0.45
1:D:99[A]:VAL:HG22	1:D:123:LEU:HD13	1.99	0.45
1:E:59[A]:ARG:HD3	5:E:2076:HOH:O	2.17	0.45
1:E:139:THR:OG1	1:E:203[B]:LYS:HG2	2.16	0.45
1:B:106:ILE:HB	1:C:148:VAL:HG11	1.99	0.44
1:C:43:ALA:HA	1:C:50:VAL:HG22	1.99	0.44
1:D:59:ARG:NH2	1:D:61:LYS:HE3	2.32	0.44
1:E:59[B]:ARG:HG3	1:E:59[B]:ARG:NH2	2.31	0.44
1:A:57[B]:GLN:HG3	1:A:118:ILE:CD1	2.46	0.44
1:A:57[B]:GLN:HG2	5:A:2039:HOH:O	2.16	0.44
1:B:122:ARG:HD2	1:C:96:THR:O	2.17	0.44
1:A:147:TRP:HH2	1:E:55[A]:TYR:CZ	2.36	0.44
1:C:143[A]:LYS:NZ	1:C:184:GLN:HE22	2.15	0.44
1:D:11:SER:O	1:D:16:ARG:HD2	2.18	0.43
1:D:57[B]:GLN:CG	1:D:118:ILE:HD12	2.42	0.43
1:E:147:TRP:O	3:E:301[A]:ZY7:N10	2.52	0.43
1:A:147:TRP:CE2	3:A:301[A]:ZY7:H19	2.54	0.43
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.58	0.43
1:C:163:VAL:HG21	1:C:200:LEU:CD1	2.48	0.43
3:A:301[B]:ZY7:H5	1:E:55[B]:TYR:CE1	2.54	0.43
1:B:163:VAL:HG21	1:B:200:LEU:CD1	2.49	0.43
1:A:14:PHE:C	1:A:16:ARG:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:CYS:HB2	3:D:301[B]:ZY7:C5	2.49	0.43
3:D:301[A]:ZY7:C13	3:D:301[A]:ZY7:C5	2.97	0.42
1:E:32:THR:CG2	1:E:59[A]:ARG:HH22	2.31	0.42
1:E:147:TRP:NE1	3:E:301[A]:ZY7:H19	2.35	0.42
1:D:55[A]:TYR:CZ	1:E:147:TRP:HH2	2.37	0.42
1:C:136:GLU:HG2	5:C:2140:HOH:O	2.20	0.41
1:E:178:SER:OG	1:E:203[B]:LYS:HD2	2.20	0.41
1:A:147:TRP:NE1	3:A:301[A]:ZY7:H19	2.35	0.41
3:A:301[B]:ZY7:C13	3:A:301[B]:ZY7:H5	2.48	0.41
1:C:59[B]:ARG:HD2	1:C:115:VAL:O	2.21	0.41
1:E:50:VAL:CG2	1:E:127:CYS:SG	3.09	0.41
1:A:143:LYS:HZ3	1:A:184:GLN:HE22	1.68	0.41
1:C:61:LYS:NZ	1:C:112:ASP:O	2.52	0.41
1:A:99[A]:VAL:HG21	1:A:121:GLN:NE2	2.36	0.41
1:E:17:SER:HA	1:E:18:PRO:HD3	1.89	0.41
1:D:57[B]:GLN:NE2	5:D:2063:HOH:O	2.46	0.41
1:A:116[B]:MET:CG	1:A:118:ILE:HD11	2.50	0.41
1:E:59[B]:ARG:CG	1:E:59[B]:ARG:NH2	2.65	0.40
1:C:55:TYR:CE2	1:D:147:TRP:HH2	2.39	0.40
1:D:79:ARG:NH2	5:D:2078:HOH:O	2.29	0.40
1:A:3:GLN:HG2	5:B:2009:HOH:O	2.22	0.40
1:B:178:SER:OG	1:B:203[A]:LYS:HD3	2.22	0.40
1:E:163:VAL:CG2	1:E:200[B]:LEU:CD2	2.98	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	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
1	B	218/228 (96%)	216 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	221/228 (97%)	218 (99%)	3 (1%)	0	100	100
1	D	217/228 (95%)	214 (99%)	3 (1%)	0	100	100
1	E	228/228 (100%)	225 (99%)	3 (1%)	0	100	100
All	All	1101/1140 (97%)	1084 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	200/206 (97%)	195 (98%)	5 (2%)	47	34
1	B	201/206 (98%)	193 (96%)	8 (4%)	31	16
1	C	205/206 (100%)	201 (98%)	4 (2%)	55	44
1	D	200/206 (97%)	196 (98%)	4 (2%)	55	44
1	E	211/206 (102%)	203 (96%)	8 (4%)	33	18
All	All	1017/1030 (99%)	988 (97%)	29 (3%)	44	29

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MET
1	A	57[A]	GLN
1	A	57[B]	GLN
1	A	80	THR
1	A	193	GLU
1	B	17	SER
1	B	59[A]	ARG
1	B	59[B]	ARG
1	B	80	THR
1	B	157	LYS
1	B	162	GLN
1	B	193	GLU

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Mol	Chain	Res	Type
1	B	208	ARG
1	C	-6	LYS
1	C	17	SER
1	C	19	MET
1	C	136	GLU
1	D	0	LEU
1	D	15	ASN
1	D	17	SER
1	D	205	ARG
1	E	-6	LYS
1	E	-3	ASP
1	E	15	ASN
1	E	16	ARG
1	E	19	MET
1	E	59[A]	ARG
1	E	59[B]	ARG
1	E	80	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	100	GLN
1	A	121	GLN
1	A	184	GLN
1	A	187	HIS
1	B	15	ASN
1	B	187	HIS
1	C	15	ASN
1	C	70	ASN
1	C	184	GLN
1	D	15	ASN
1	D	184	GLN
1	D	199	ASN
1	E	100	GLN
1	E	162	GLN
1	E	199	ASN

### 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 ⓘ

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	F	1	1,2	14,14,15	0.46	0	17,19,21	1.90	3 (17%)
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	1.32	3 (17%)
2	BMA	F	3	2	11,11,12	0.33	0	15,15,17	0.71	0
2	MAN	F	4	2	11,11,12	0.43	0	15,15,17	0.89	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	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	5.92	120.21	112.19
2	F	1	NAG	C3-C4-C5	2.99	115.56	110.24
2	F	2	NAG	C2-N2-C7	-2.66	119.11	122.90
2	F	2	NAG	C1-C2-N2	-2.48	106.25	110.49
2	F	1	NAG	C2-N2-C7	-2.11	119.91	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O5-C1-C2	-2.05	108.05	111.29

There are no chirality outliers.

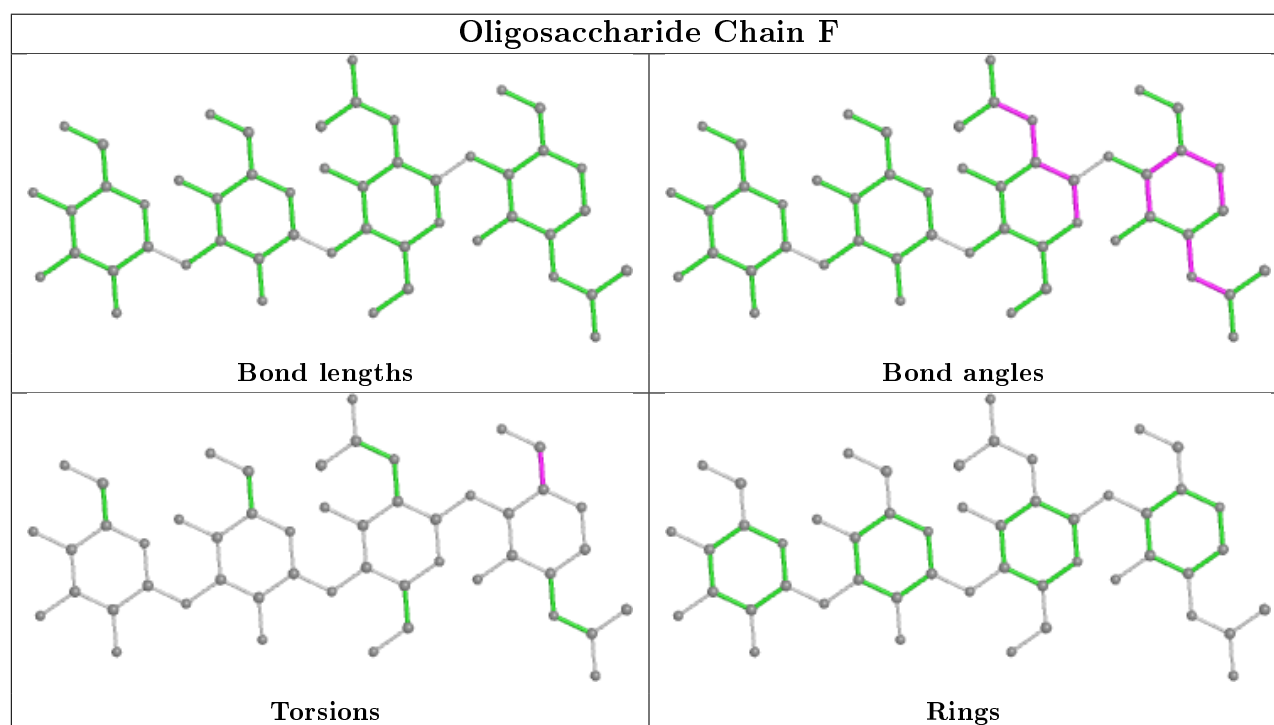
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

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 ⓘ

9 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	ZY7	A	301[B]	-	25,25,25	1.31	3 (12%)	30,33,33	2.15	9 (30%)
3	ZY7	D	301[B]	-	25,25,25	1.33	2 (8%)	30,33,33	2.19	10 (33%)
3	ZY7	A	301[A]	-	25,25,25	1.21	3 (12%)	30,33,33	2.40	5 (16%)
3	ZY7	E	301[B]	-	25,25,25	1.18	2 (8%)	30,33,33	2.15	6 (20%)
4	NAG	B	401	1	14,14,15	0.35	0	17,19,21	0.97	1 (5%)
3	ZY7	E	301[A]	-	25,25,25	1.21	3 (12%)	30,33,33	2.38	7 (23%)
3	ZY7	D	301[A]	-	25,25,25	1.10	2 (8%)	30,33,33	2.24	7 (23%)
3	ZY7	B	301	-	25,25,25	1.19	2 (8%)	30,33,33	2.03	11 (36%)
3	ZY7	C	301	-	25,25,25	2.02	2 (8%)	30,33,33	2.64	10 (33%)

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	ZY7	A	301[B]	-	-	8/12/23/23	0/3/3/3
3	ZY7	D	301[B]	-	-	6/12/23/23	0/3/3/3
3	ZY7	A	301[A]	-	-	2/12/23/23	0/3/3/3
3	ZY7	E	301[B]	-	-	6/12/23/23	0/3/3/3
4	NAG	B	401	1	-	4/6/23/26	0/1/1/1
3	ZY7	E	301[A]	-	-	1/12/23/23	0/3/3/3
3	ZY7	D	301[A]	-	-	1/12/23/23	0/3/3/3
3	ZY7	B	301	-	-	6/12/23/23	0/3/3/3
3	ZY7	C	301	-	-	8/12/23/23	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	ZY7	C9-N10	-9.01	1.22	1.28
3	D	301[B]	ZY7	C4-C3	4.66	1.50	1.41
3	A	301[B]	ZY7	C4-C3	4.17	1.49	1.41
3	B	301	ZY7	C4-C3	3.82	1.49	1.41
3	E	301[A]	ZY7	C4-C3	3.81	1.49	1.41
3	E	301[B]	ZY7	C4-C3	3.74	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301[A]	ZY7	C4-C3	3.71	1.48	1.41
3	D	301[A]	ZY7	C4-C3	3.68	1.48	1.41
3	C	301	ZY7	C4-C3	3.47	1.48	1.41
3	A	301[B]	ZY7	C9-N10	-3.39	1.26	1.28
3	D	301[B]	ZY7	C9-N10	-3.30	1.26	1.28
3	A	301[A]	ZY7	C9-N10	-2.82	1.26	1.28
3	E	301[B]	ZY7	C9-N10	-2.71	1.26	1.28
3	E	301[A]	ZY7	C4-C7	2.50	1.50	1.46
3	B	301	ZY7	C9-N10	-2.46	1.27	1.28
3	D	301[A]	ZY7	C9-N10	-2.32	1.27	1.28
3	A	301[A]	ZY7	C4-C7	2.29	1.50	1.46
3	E	301[A]	ZY7	C14-C9	2.10	1.51	1.48
3	A	301[B]	ZY7	C4-C7	2.10	1.50	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	ZY7	C11-N10-C9	11.27	130.68	116.09
3	A	301[A]	ZY7	C11-N10-C9	10.80	130.08	116.09
3	E	301[A]	ZY7	C11-N10-C9	10.31	129.45	116.09
3	D	301[A]	ZY7	C11-N10-C9	8.96	127.69	116.09
3	E	301[B]	ZY7	C11-N10-C9	8.47	127.06	116.09
3	A	301[B]	ZY7	C11-N10-C9	7.34	125.59	116.09
3	D	301[B]	ZY7	C11-N10-C9	6.80	124.90	116.09
3	B	301	ZY7	C11-N10-C9	5.17	122.79	116.09
3	D	301[B]	ZY7	C22-O21-C3	4.82	124.80	117.53
3	E	301[B]	ZY7	C14-C9-N10	4.20	122.15	118.04
3	B	301	ZY7	O21-C3-C4	4.13	121.51	115.92
3	B	301	ZY7	C22-O21-C3	3.87	123.38	117.53
3	D	301[B]	ZY7	C14-C9-N10	3.82	121.78	118.04
3	A	301[B]	ZY7	O21-C3-C4	3.61	120.81	115.92
3	A	301[B]	ZY7	C14-C9-N10	3.51	121.48	118.04
3	C	301	ZY7	O21-C3-C4	3.43	120.56	115.92
3	B	301	ZY7	C14-C9-N10	3.42	121.39	118.04
3	A	301[A]	ZY7	C12-C13-C8	-3.40	105.33	112.15
3	A	301[A]	ZY7	C22-O21-C3	3.30	122.51	117.53
3	D	301[A]	ZY7	C12-C11-N10	-3.28	103.67	113.34
3	D	301[A]	ZY7	O21-C3-C4	3.27	120.35	115.92
3	B	301	ZY7	C15-C14-C19	2.92	120.94	117.63
3	D	301[B]	ZY7	C17-N18-C19	2.91	121.88	116.85
3	A	301[B]	ZY7	C22-O21-C3	2.87	121.86	117.53
3	E	301[A]	ZY7	C22-O21-C3	2.86	121.85	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301[B]	ZY7	C12-C11-N10	-2.85	104.92	113.34
3	C	301	ZY7	C13-C8-C7	2.82	128.08	125.27
3	B	301	ZY7	C12-C11-N10	-2.81	105.04	113.34
3	A	301[B]	ZY7	C12-C11-N10	-2.77	105.17	113.34
3	A	301[B]	ZY7	C17-N18-C19	2.73	121.57	116.85
3	E	301[A]	ZY7	C12-C11-N10	-2.72	105.30	113.34
3	C	301	ZY7	C17-N18-C19	2.71	121.54	116.85
3	C	301	ZY7	C14-C19-N18	-2.71	119.48	123.49
3	C	301	ZY7	C12-C11-N10	-2.67	105.46	113.34
3	E	301[B]	ZY7	C17-N18-C19	2.65	121.44	116.85
3	B	301	ZY7	O21-C3-C2	-2.65	119.56	124.12
3	E	301[A]	ZY7	C23-O20-C1	2.59	123.14	117.51
3	D	301[B]	ZY7	C14-C19-N18	-2.57	119.69	123.49
3	A	301[A]	ZY7	C12-C11-N10	-2.56	105.79	113.34
3	A	301[B]	ZY7	O21-C3-C2	-2.52	119.78	124.12
3	C	301	ZY7	C7-C8-C9	-2.49	114.78	120.24
3	E	301[A]	ZY7	C17-N18-C19	2.45	121.09	116.85
3	C	301	ZY7	O21-C3-C2	-2.44	119.92	124.12
3	D	301[A]	ZY7	C23-O20-C1	2.43	122.79	117.51
3	B	301	ZY7	C14-C19-N18	-2.40	119.94	123.49
3	B	301	ZY7	C17-N18-C19	2.40	121.00	116.85
3	E	301[B]	ZY7	O21-C3-C4	2.39	119.16	115.92
3	C	301	ZY7	C15-C14-C19	2.32	120.26	117.63
3	D	301[A]	ZY7	C17-N18-C19	2.29	120.81	116.85
3	C	301	ZY7	C12-C13-C8	-2.29	107.56	112.15
3	E	301[B]	ZY7	C14-C19-N18	-2.27	120.14	123.49
3	E	301[A]	ZY7	C12-C13-C8	-2.24	107.66	112.15
3	D	301[B]	ZY7	O21-C3-C4	2.23	118.94	115.92
3	E	301[A]	ZY7	C8-C9-N10	-2.16	117.12	124.57
3	B	301	ZY7	C16-C15-C14	-2.13	117.82	120.34
3	A	301[B]	ZY7	C14-C19-N18	-2.13	120.34	123.49
3	D	301[A]	ZY7	C4-C7-C8	-2.13	124.81	128.45
3	D	301[B]	ZY7	C15-C14-C19	2.11	120.03	117.63
4	B	401	NAG	C1-C2-N2	-2.10	106.90	110.49
3	D	301[B]	ZY7	C12-C13-C8	-2.10	107.94	112.15
3	D	301[B]	ZY7	C7-C8-C9	-2.08	115.69	120.24
3	A	301[A]	ZY7	C8-C9-N10	-2.06	117.46	124.57
3	D	301[A]	ZY7	C12-C13-C8	-2.04	108.05	112.15
3	B	301	ZY7	C7-C8-C9	-2.04	115.77	120.24
3	E	301[B]	ZY7	C12-C11-N10	-2.04	107.31	113.34
3	A	301[B]	ZY7	C23-O20-C1	2.02	121.89	117.51

There are no chirality outliers.

All (42) torsion outliers are listed below:

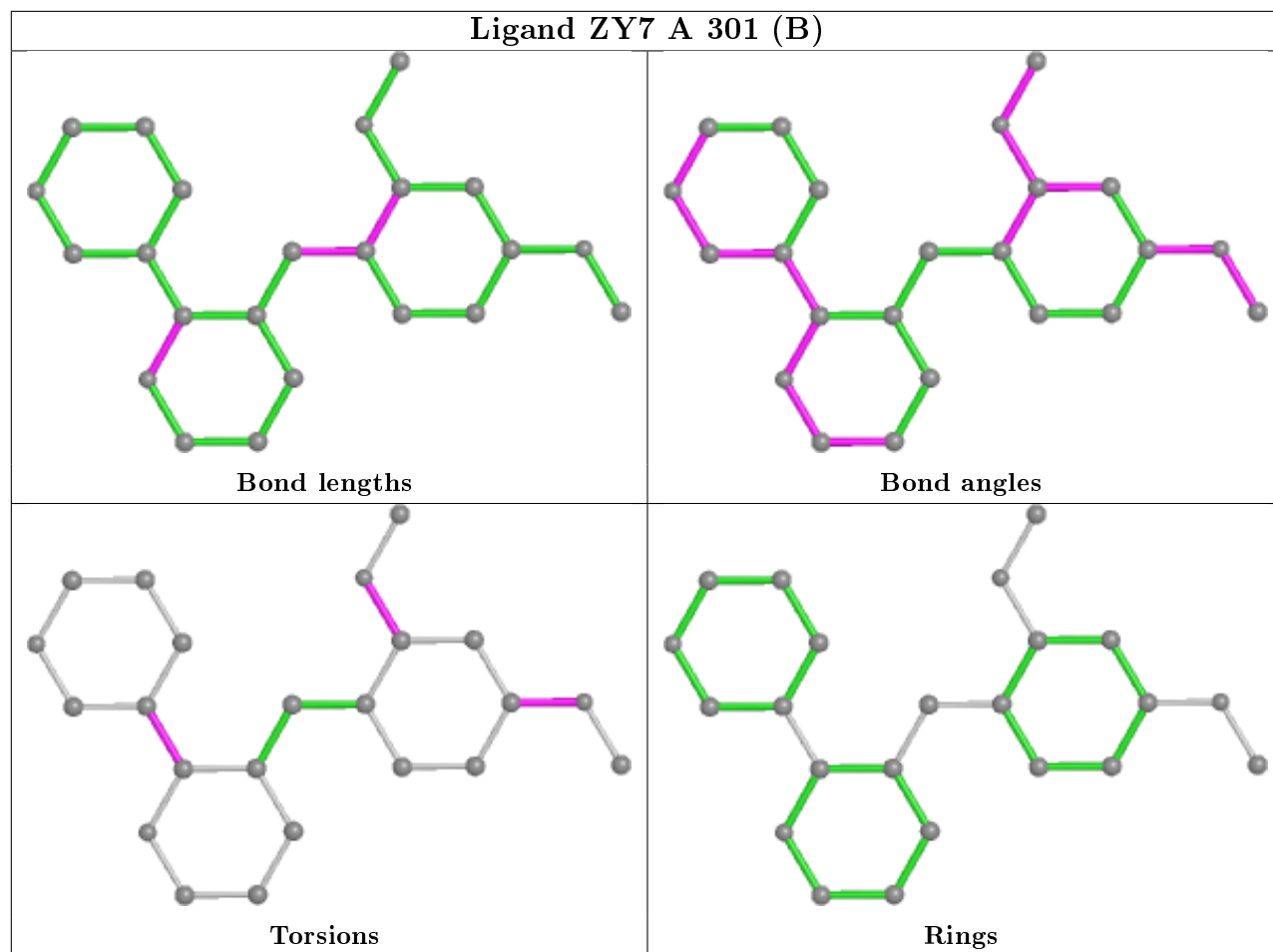
Mol	Chain	Res	Type	Atoms
3	A	301[B]	ZY7	C19-C14-C9-C8
3	A	301[B]	ZY7	C15-C14-C9-C8
3	A	301[B]	ZY7	C19-C14-C9-N10
3	D	301[B]	ZY7	C19-C14-C9-C8
3	D	301[B]	ZY7	C15-C14-C9-C8
3	E	301[B]	ZY7	C19-C14-C9-C8
3	E	301[B]	ZY7	C15-C14-C9-C8
3	B	301	ZY7	C15-C14-C9-C8
3	C	301	ZY7	C19-C14-C9-C8
3	C	301	ZY7	C19-C14-C9-N10
3	A	301[B]	ZY7	C2-C1-O20-C23
3	A	301[B]	ZY7	C6-C1-O20-C23
3	D	301[B]	ZY7	C6-C1-O20-C23
3	D	301[B]	ZY7	C2-C1-O20-C23
4	B	401	NAG	O5-C5-C6-O6
3	B	301	ZY7	C4-C3-O21-C22
4	B	401	NAG	C4-C5-C6-O6
3	C	301	ZY7	C2-C3-O21-C22
3	E	301[B]	ZY7	C6-C1-O20-C23
3	E	301[B]	ZY7	C2-C1-O20-C23
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2
3	D	301[B]	ZY7	C15-C14-C9-N10
3	E	301[B]	ZY7	C15-C14-C9-N10
3	A	301[B]	ZY7	C2-C3-O21-C22
3	B	301	ZY7	C2-C3-O21-C22
3	B	301	ZY7	C19-C14-C9-C8
3	C	301	ZY7	C15-C14-C9-C8
3	C	301	ZY7	C4-C3-O21-C22
3	A	301[B]	ZY7	C4-C3-O21-C22
3	A	301[B]	ZY7	C15-C14-C9-N10
3	C	301	ZY7	C15-C14-C9-N10
3	A	301[A]	ZY7	C2-C1-O20-C23
3	A	301[A]	ZY7	C6-C1-O20-C23
3	D	301[B]	ZY7	C19-C14-C9-N10
3	E	301[B]	ZY7	C19-C14-C9-N10
3	C	301	ZY7	C2-C1-O20-C23
3	C	301	ZY7	C6-C1-O20-C23
3	B	301	ZY7	C15-C14-C9-N10
3	D	301[A]	ZY7	C15-C14-C9-N10
3	E	301[A]	ZY7	C15-C14-C9-N10
3	B	301	ZY7	C19-C14-C9-N10

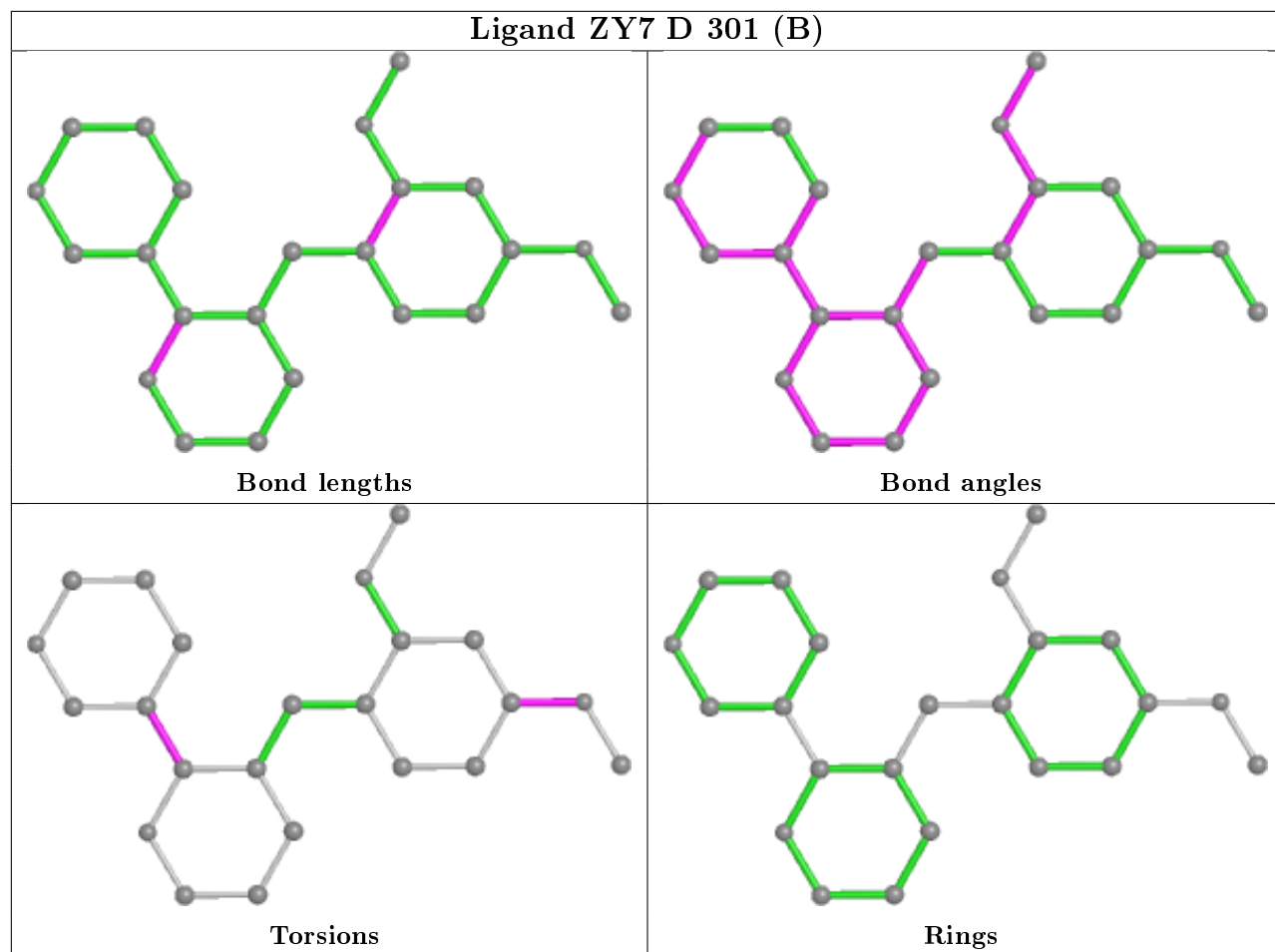
There are no ring outliers.

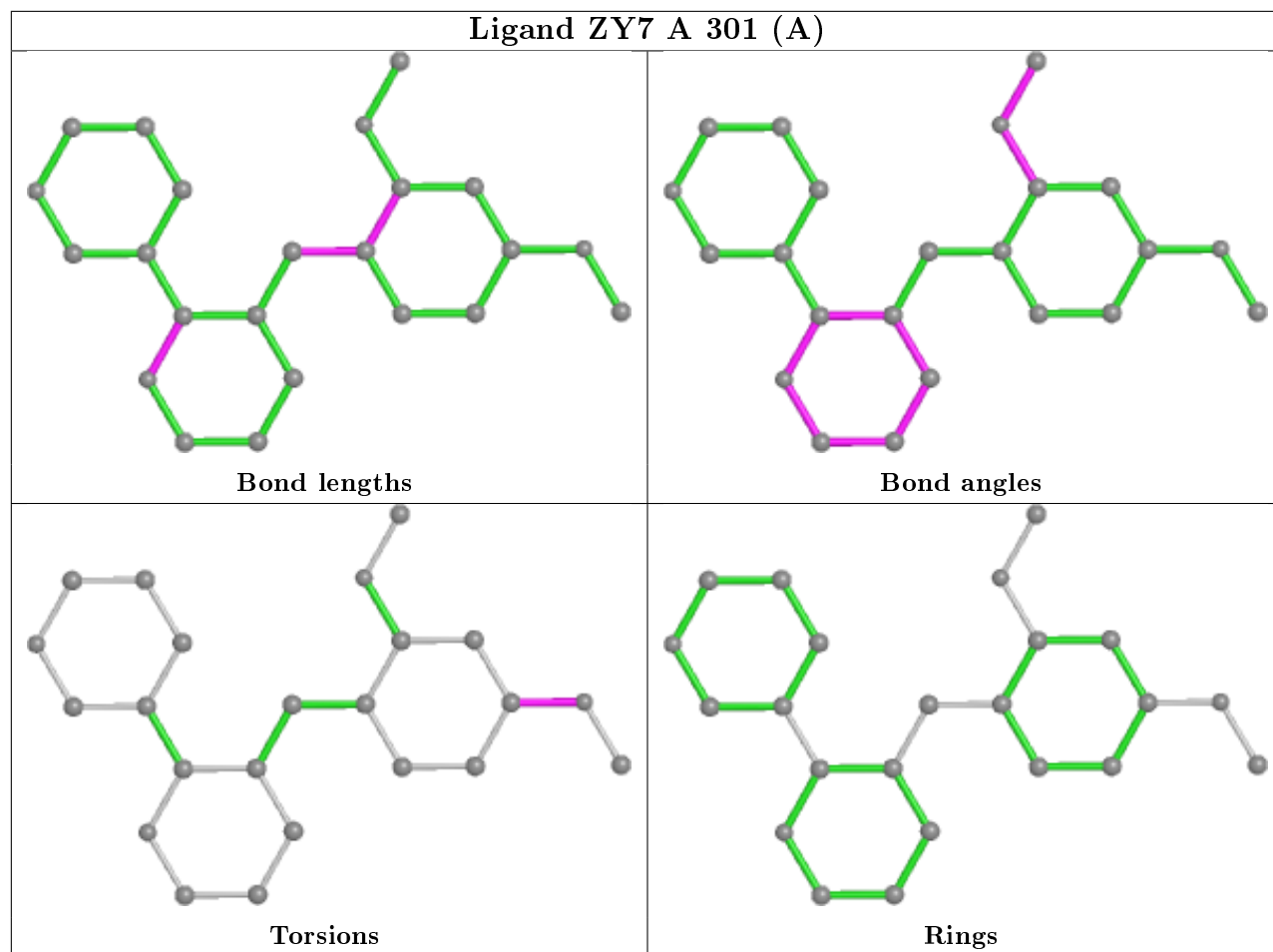
8 monomers are involved in 77 short contacts:

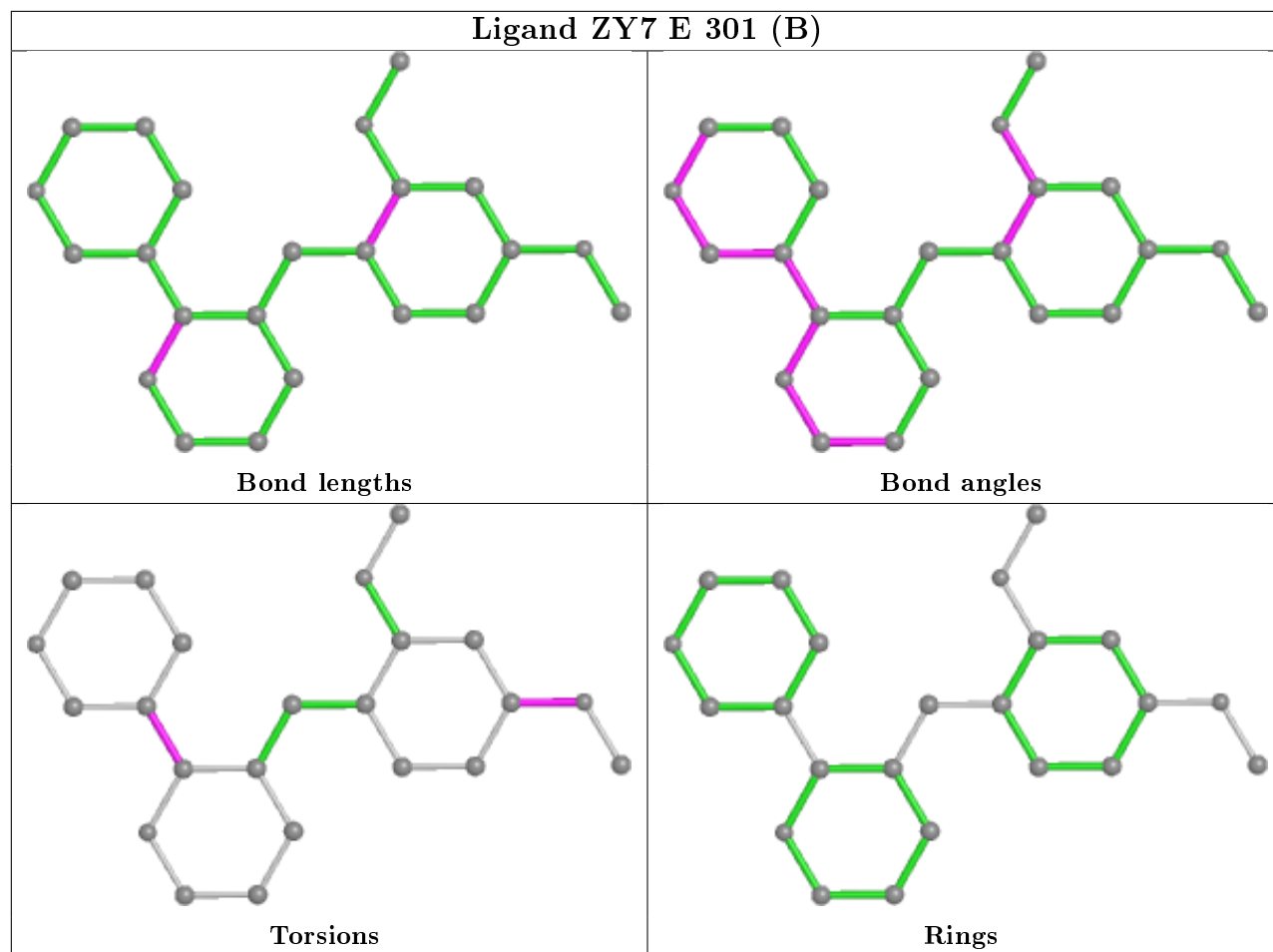
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301[B]	ZY7	10	0
3	D	301[B]	ZY7	17	0
3	A	301[A]	ZY7	5	0
3	E	301[B]	ZY7	7	0
3	E	301[A]	ZY7	19	0
3	D	301[A]	ZY7	7	0
3	B	301	ZY7	8	0
3	C	301	ZY7	4	0

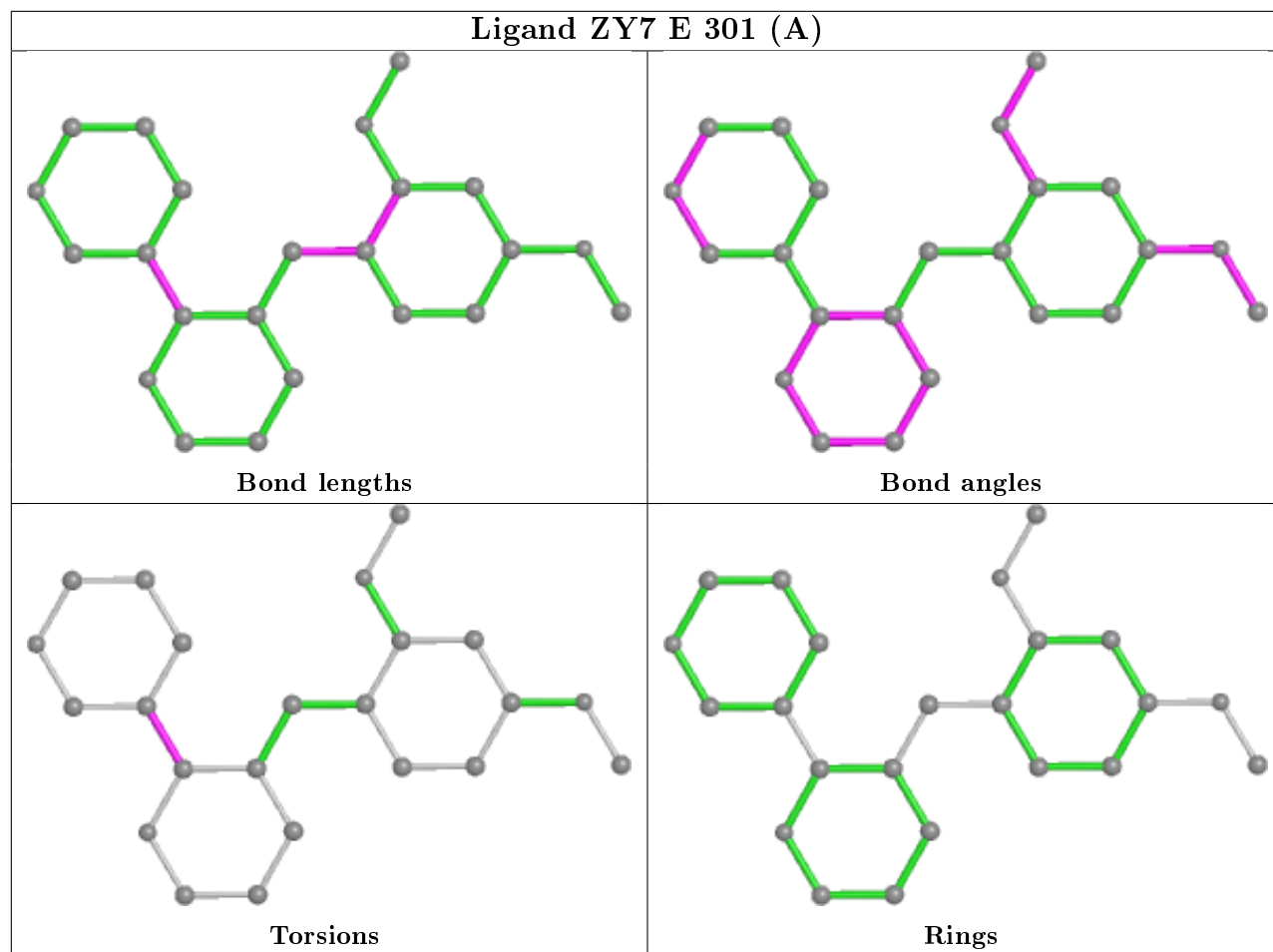
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

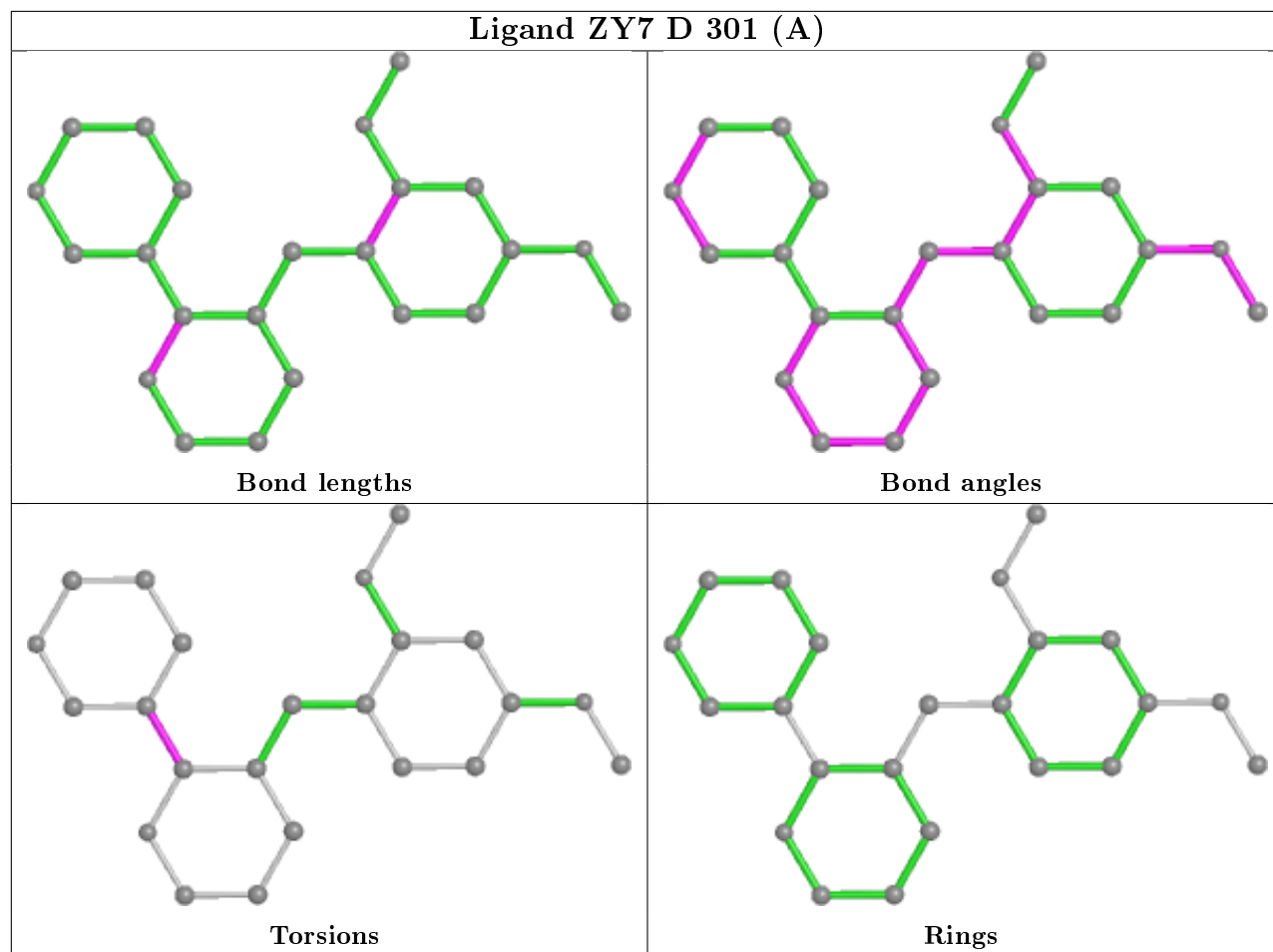


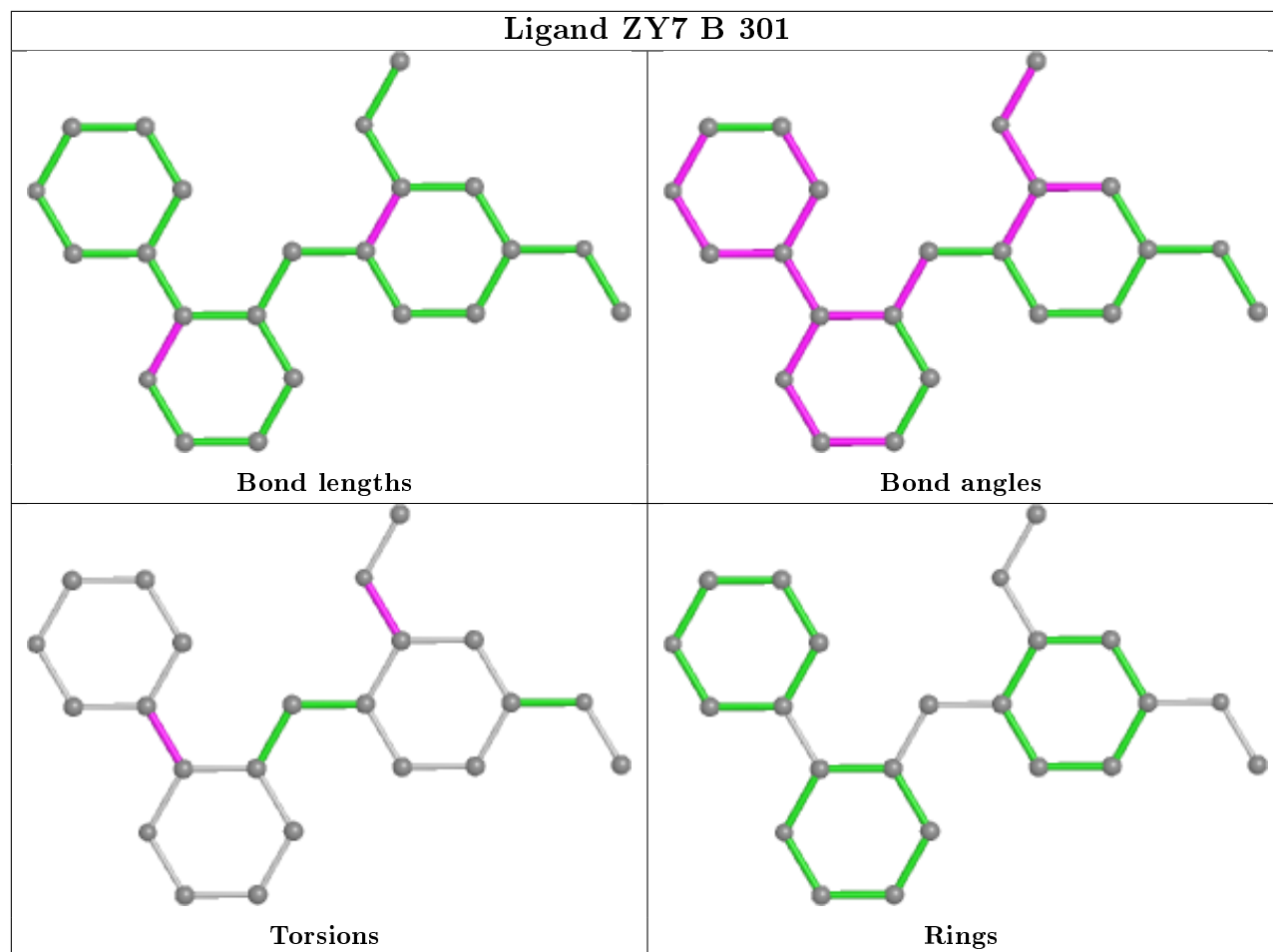


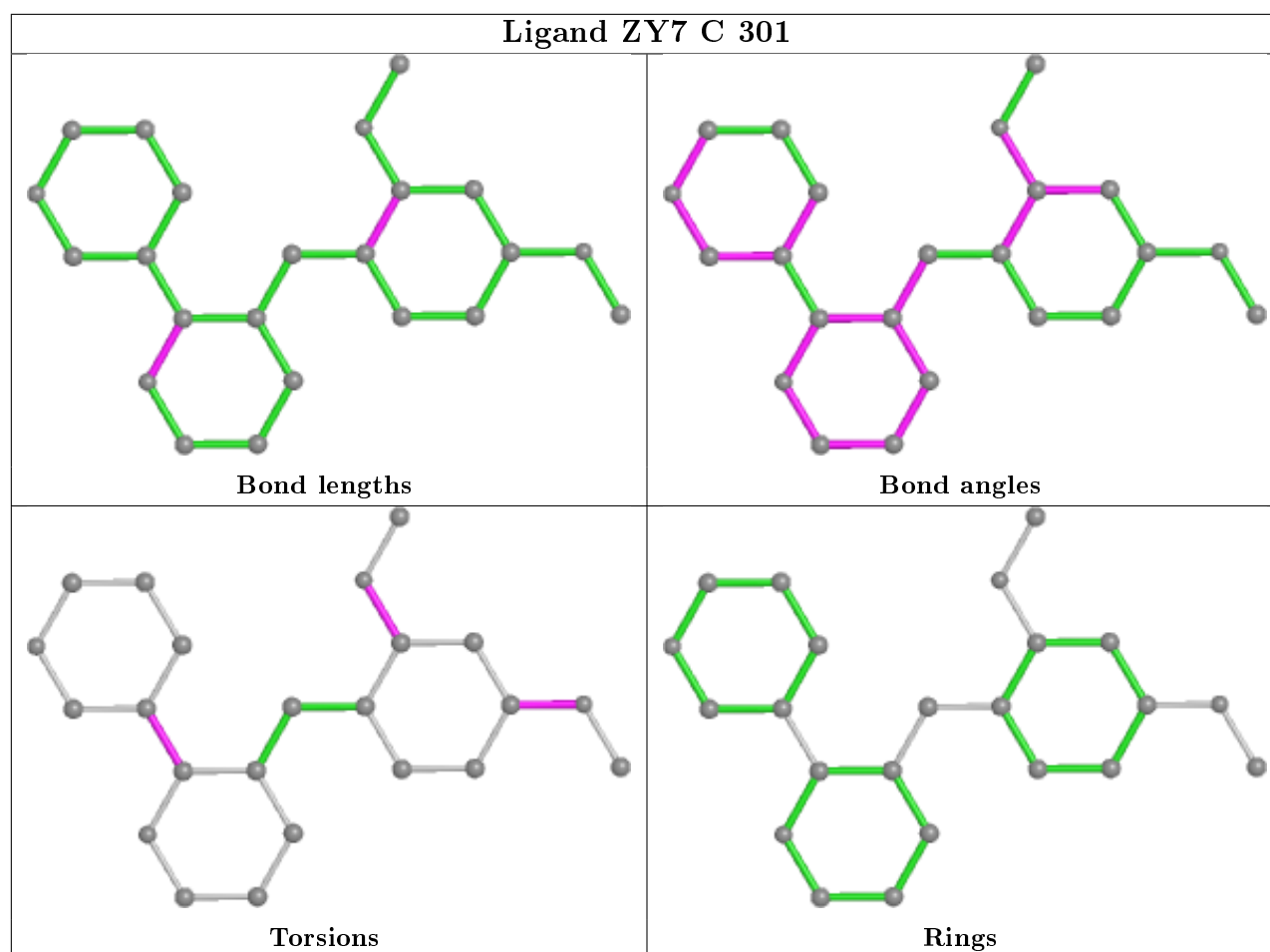












## 5.7 Other polymers [i](#)

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 ⓘ

### 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, 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	209/228 (91%)	0.16	9 (4%) 35 29	20, 31, 57, 71	2 (0%)
1	B	212/228 (92%)	0.45	16 (7%) 14 11	20, 33, 58, 83	0
1	C	214/228 (93%)	0.26	12 (5%) 24 19	21, 32, 59, 79	0
1	D	211/228 (92%)	0.34	14 (6%) 18 14	19, 29, 62, 82	0
1	E	217/228 (95%)	0.25	11 (5%) 28 22	19, 29, 51, 75	0
All	All	1063/1140 (93%)	0.29	62 (5%) 23 18	19, 31, 59, 83	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	PRO	7.9
1	A	18	PRO	7.0
1	C	19	MET	6.8
1	D	18	PRO	6.8
1	D	16	ARG	6.6
1	E	15	ASN	6.5
1	A	0	LEU	6.5
1	D	15	ASN	6.1
1	E	18	PRO	6.0
1	A	16	ARG	5.9
1	B	15	ASN	5.8
1	A	19	MET	5.7
1	A	15	ASN	5.6
1	B	18	PRO	5.2
1	E	19	MET	5.2
1	B	17	SER	5.1
1	D	0	LEU	5.1
1	A	189	SER	4.7
1	B	19	MET	4.7
1	D	17	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	16	ARG	4.4
1	E	17	SER	4.4
1	A	1	HIS	4.3
1	E	16	ARG	4.3
1	E	208	ARG	3.6
1	D	-2	ASP	3.6
1	D	-1	LYS	3.5
1	B	208	ARG	3.5
1	D	19	MET	3.4
1	B	1	HIS	3.4
1	C	16	ARG	3.3
1	B	0	LEU	3.3
1	B	-3	ASP	3.3
1	C	0	LEU	3.3
1	B	70	ASN	3.2
1	C	-4	ASP	3.0
1	A	191	CYS	2.9
1	C	15	ASN	2.9
1	B	-2	ASP	2.8
1	E	11	SER	2.7
1	D	11	SER	2.6
1	A	136	GLU	2.6
1	E	7	MET	2.6
1	C	17	SER	2.6
1	C	68	ASP	2.6
1	D	14	PHE	2.5
1	D	74	ASN	2.5
1	B	14	PHE	2.5
1	E	74	ASN	2.5
1	C	1	HIS	2.4
1	B	71	GLU	2.2
1	D	208	ARG	2.2
1	B	136	GLU	2.2
1	C	-3	ASP	2.1
1	B	2	SER	2.1
1	D	7	MET	2.0
1	E	72	TYR	2.0
1	C	14	PHE	2.0
1	D	1	HIS	2.0
1	E	97[A]	ARG	2.0
1	C	70	ASN	2.0
1	B	7[A]	MET	2.0

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

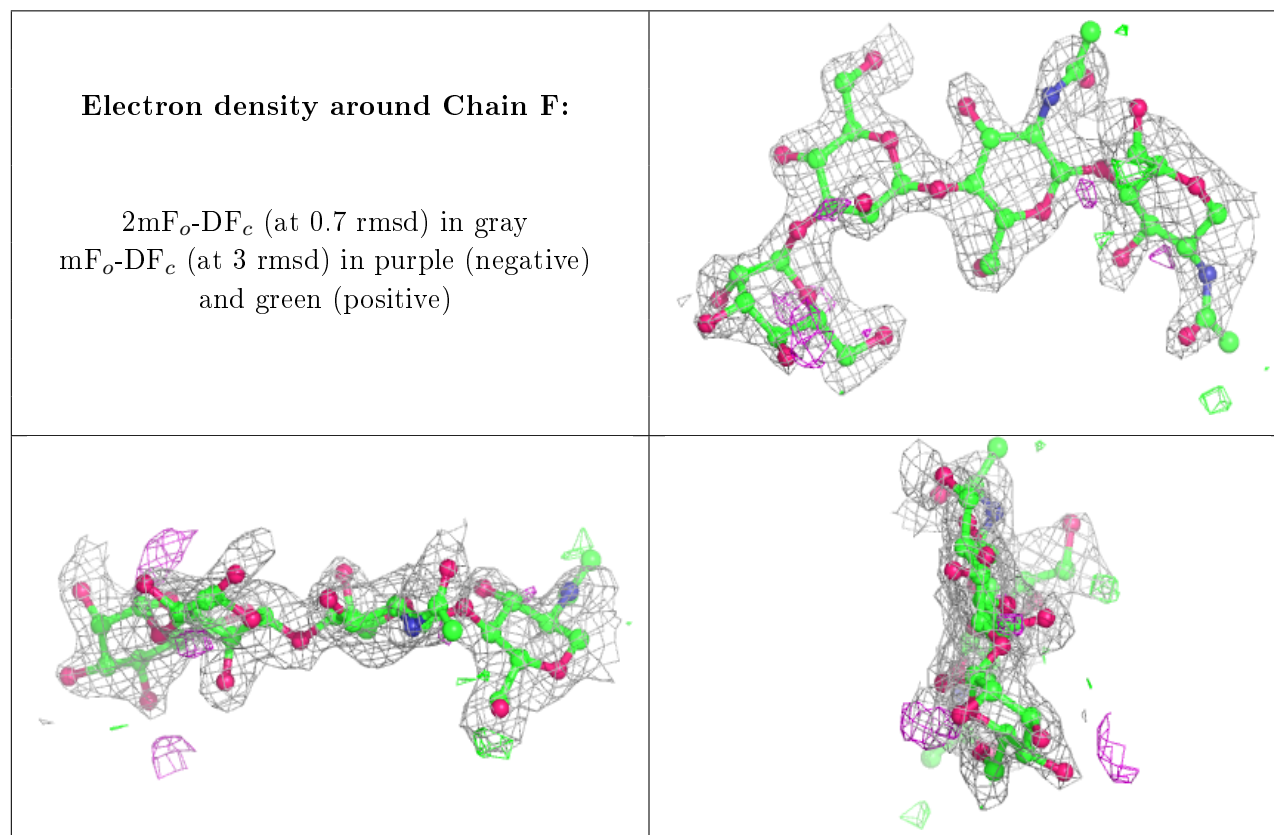
There are no non-standard protein/DNA/RNA residues in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	F	1	14/15	0.77	0.30	58,62,66,66	0
2	MAN	F	4	11/12	0.80	0.37	55,56,57,58	0
2	NAG	F	2	14/15	0.81	0.34	59,61,63,64	0
2	BMA	F	3	11/12	0.84	0.37	52,56,59,61	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

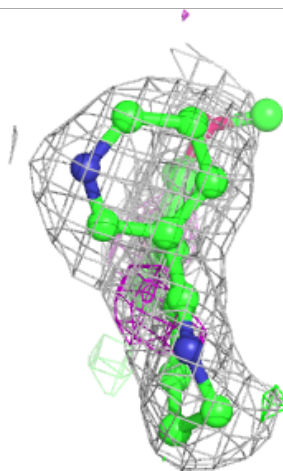
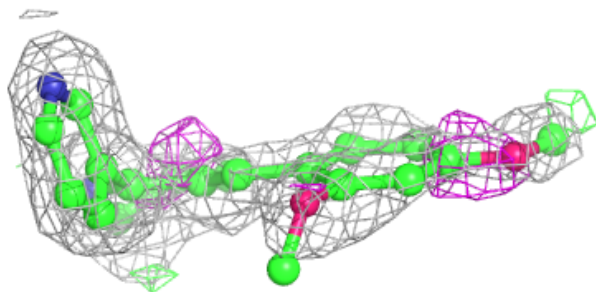
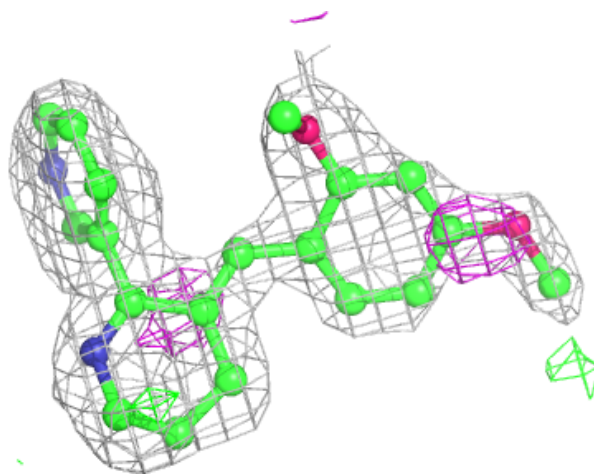
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	401	14/15	0.71	0.27	56,60,61,62	0
3	ZY7	B	301	23/23	0.80	0.20	33,42,49,52	0
3	ZY7	D	301[A]	23/23	0.90	0.20	29,34,36,37	23
3	ZY7	D	301[B]	23/23	0.90	0.20	25,31,37,38	23
3	ZY7	A	301[B]	23/23	0.91	0.19	32,37,44,45	23
3	ZY7	E	301[A]	23/23	0.91	0.18	27,30,31,32	23
3	ZY7	A	301[A]	23/23	0.91	0.19	30,35,37,37	23
3	ZY7	E	301[B]	23/23	0.91	0.18	26,30,34,37	23
3	ZY7	C	301	23/23	0.91	0.12	21,26,44,48	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.

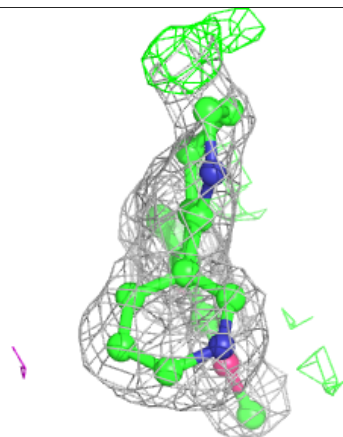
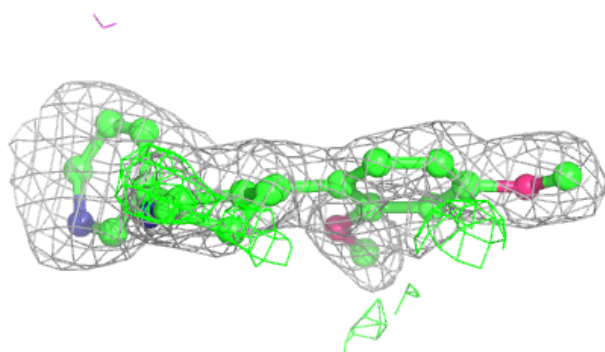
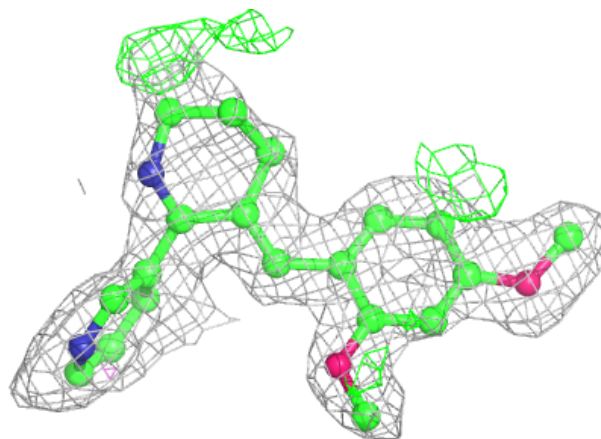
**Electron density around ZY7 B 301:**

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



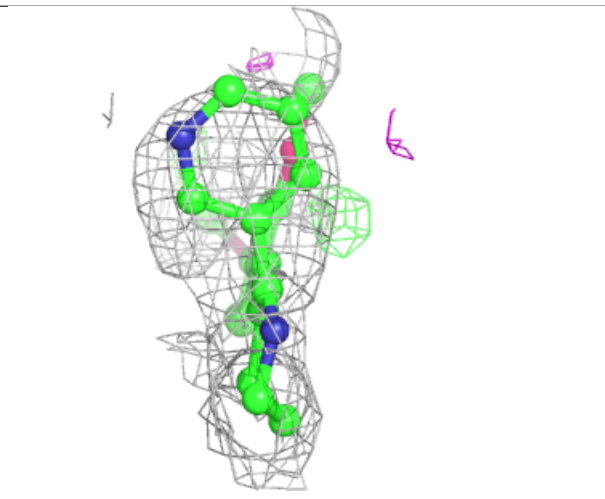
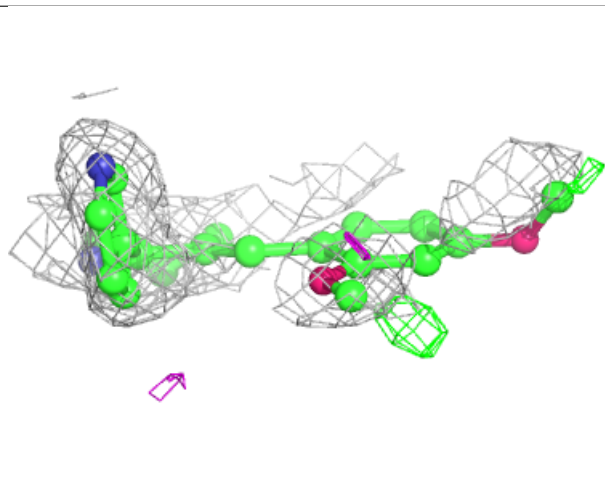
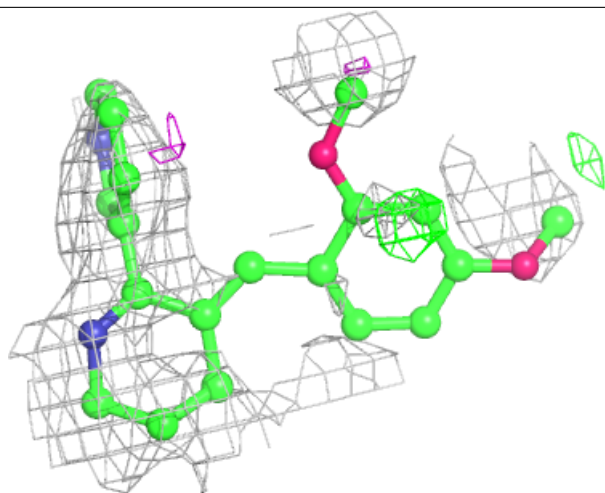
**Electron density around ZY7 D 301 (A):**

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



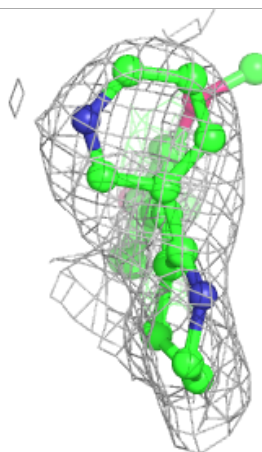
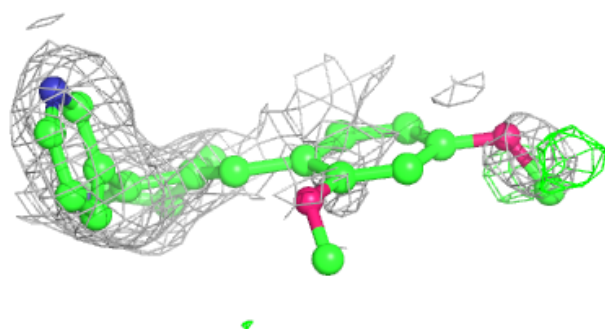
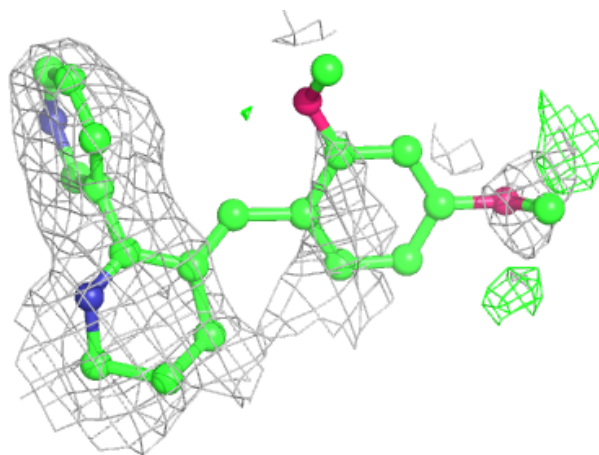
**Electron density around ZY7 D 301 (B):**

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



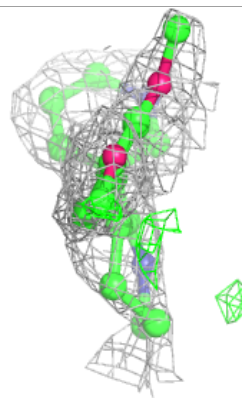
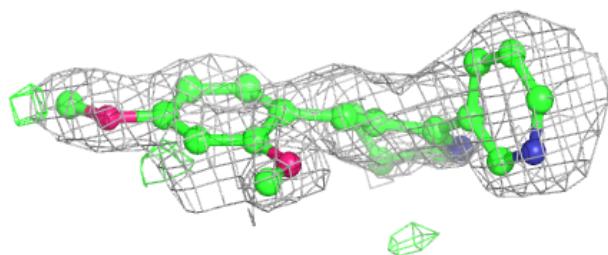
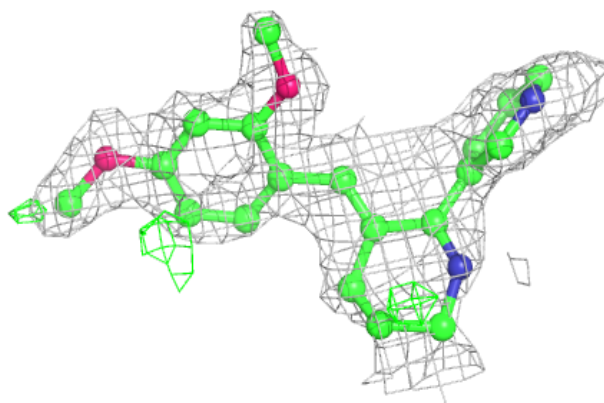
**Electron density around ZY7 A 301 (B):**

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

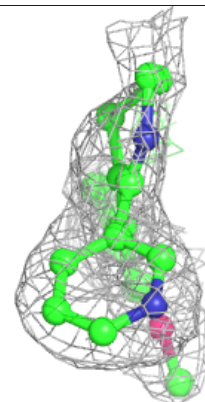
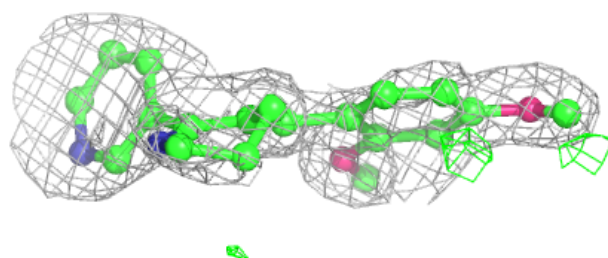
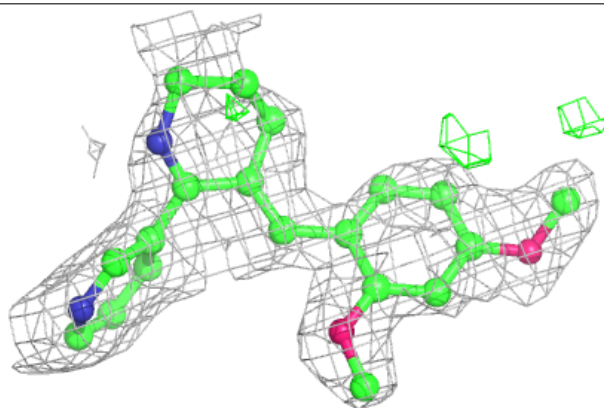


**Electron density around ZY7 E 301 (A):**

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

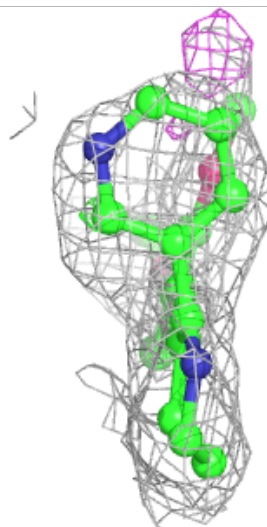
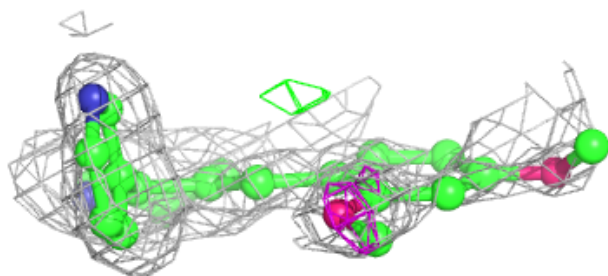
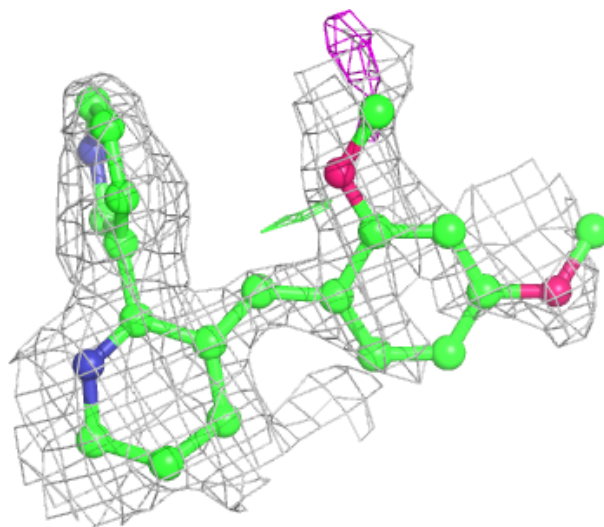
**Electron density around ZY7 A 301 (A):**

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



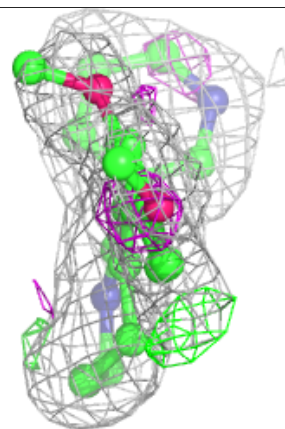
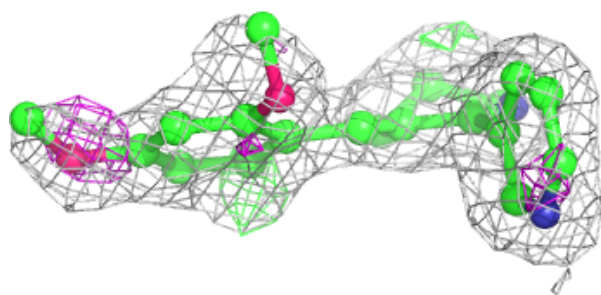
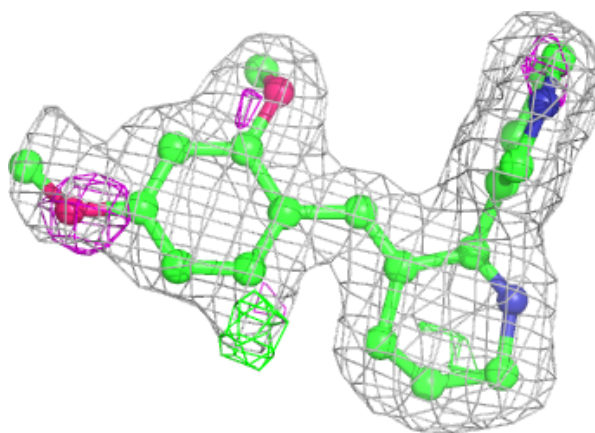
**Electron density around ZY7 E 301 (B):**

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



**Electron density around ZY7 C 301:**

$2mF_o-DF_c$  (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.