



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:24 PM BST

PDB ID : 2WN9
Title : Crystal structure of Aplysia ACHBP in complex with 4-0H-DMXBA
Authors : Sulzenbacher, G.; Hibbs, R.; Shi, J.; Talley, T.; Conrod, S.; Kem, W.; Taylor, P.; Marchot, P.; Bourne, Y.
Deposited on : 2009-07-07
Resolution : 1.75 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

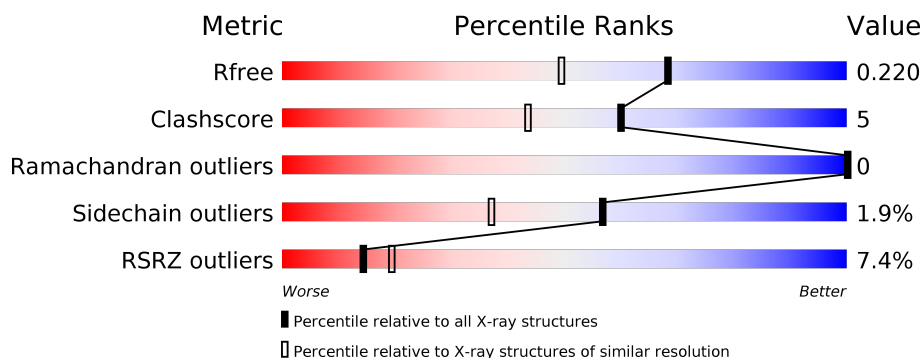
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 ≥ 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>7%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
1	B	228	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	C	228	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
1	D	228	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>
1	E	228	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>6%</div> </div> </div>
2	F	5	<div> <div></div> <div> <div>20%</div> <div>80%</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
2	MAN	F	5	-	-	-	X

2 Entry composition [i](#)

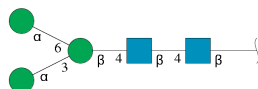
There are 5 unique types of molecules in this entry. The entry contains 9583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

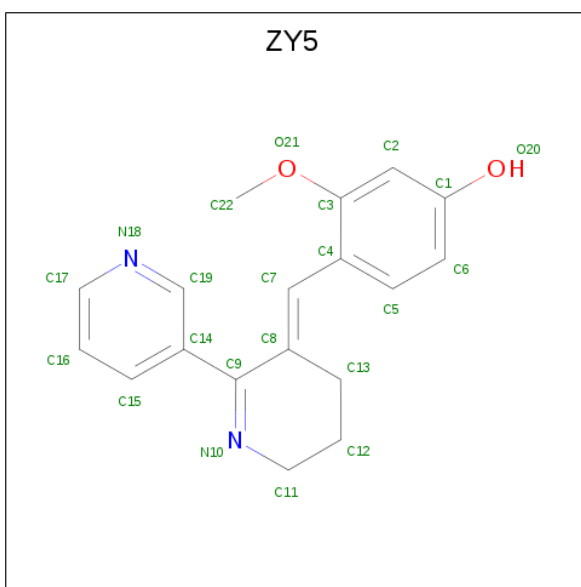
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	12	0
			1739	1105	288	336	10			
1	B	211	Total	C	N	O	S	0	6	0
			1714	1086	279	339	10			
1	C	214	Total	C	N	O	S	0	10	0
			1765	1115	292	349	9			
1	D	205	Total	C	N	O	S	0	5	0
			1671	1058	279	327	7			
1	E	214	Total	C	N	O	S	0	3	0
			1729	1092	282	346	9			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 3 is 4-[(E)-5,6-DIHYDRO-2,3'-BIPYRIDIN-3(4H)-YLIDENEMETHYL]-3-METHOXYPHENOL (three-letter code: ZY5) (formula: C₁₈H₁₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	18	2	2		
3	B	1	Total	C	N	O	0	0
			22	18	2	2		
3	C	1	Total	C	N	O	0	0
			22	18	2	2		
3	D	1	Total	C	N	O	0	0
			22	18	2	2		
3	E	1	Total	C	N	O	0	0
			22	18	2	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

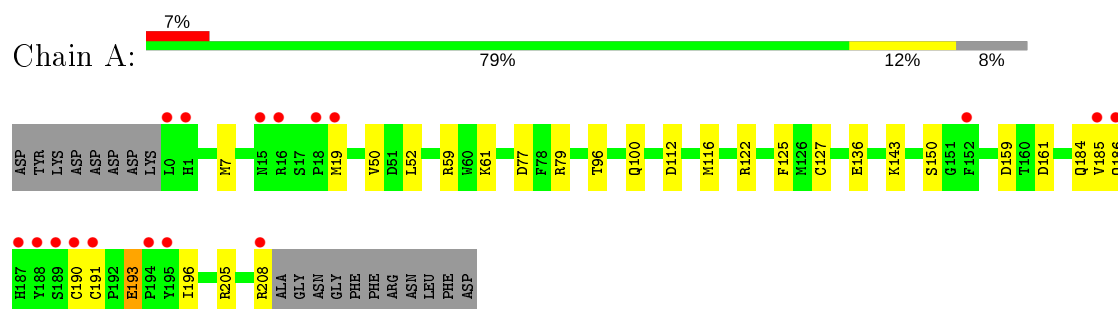
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	0
			179	179		
5	B	150	Total	O	0	0
			150	150		
5	C	148	Total	O	0	0
			148	148		
5	D	142	Total	O	0	0
			142	142		
5	E	161	Total	O	0	0
			161	161		

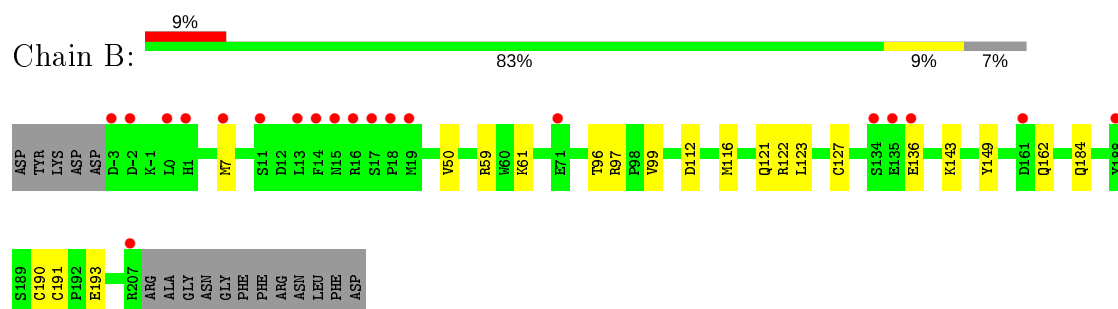
3 Residue-property plots

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.

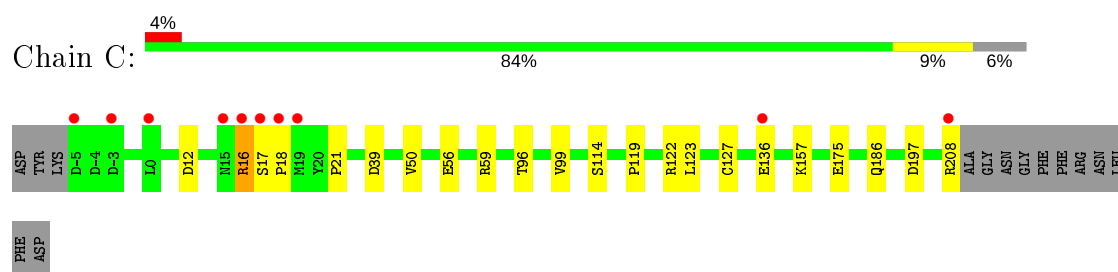
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



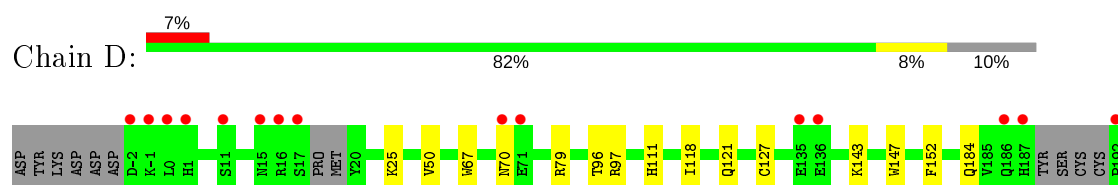
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

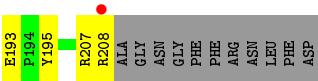


• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

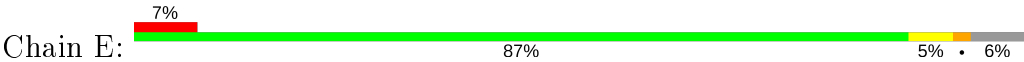


• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

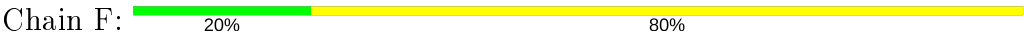




● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



● Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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, α , β , γ	86.91Å 115.39Å 130.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 43.24 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.75) 99.9 (43.24-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.170 , 0.203 0.192 , 0.220	Depositor DCC
R_{free} test set	6587 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9583	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZY5, BMA, 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	0.64	0/1816	0.78	2/2471 (0.1%)
1	B	0.69	0/1773	0.79	0/2417
1	C	0.65	0/1836	0.80	1/2501 (0.0%)
1	D	0.62	0/1723	0.79	2/2342 (0.1%)
1	E	0.66	1/1778 (0.1%)	0.75	1/2421 (0.0%)
All	All	0.65	1/8926 (0.0%)	0.78	6/12152 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	191	CYS	CB-SG	6.29	1.93	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CG-OD1	5.64	123.38	118.30
1	E	183	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	97[A]	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	97[B]	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	39	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	205	ARG	NE-CZ-NH1	-5.19	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1739	0	1716	20	0
1	B	1714	0	1660	15	0
1	C	1765	0	1720	17	0
1	D	1671	0	1632	11	0
1	E	1729	0	1658	9	0
2	F	61	0	52	0	0
3	A	22	0	18	3	0
3	B	22	0	18	3	0
3	C	22	0	18	3	0
3	D	22	0	18	4	0
3	E	22	0	18	4	0
4	B	14	0	13	0	0
5	A	179	0	0	2	0
5	B	150	0	0	3	0
5	C	148	0	0	0	0
5	D	142	0	0	2	0
5	E	161	0	0	1	0
All	All	9583	0	8541	79	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 5.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:SD	2.09	0.91
1:A:19:MET:HA	5:A:2020:HOH:O	1.77	0.83
3:C:301:ZY5:H5	3:C:301:ZY5:H131	1.63	0.81
1:E:59:ARG:HD2	1:E:116[A]:MET:SD	2.21	0.80
1:D:121:GLN:OE1	5:D:2092:HOH:O	2.03	0.74
1:A:59[B]:ARG:NH1	1:A:159:ASP:OD1	2.20	0.74
1:A:100:GLN:HE22	1:B:97[B]:ARG:HH11	1.37	0.71
1:C:59[B]:ARG:HE	1:C:114[B]:SER:HB3	1.56	0.70
3:C:301:ZY5:H5	3:C:301:ZY5:C13	2.24	0.68
1:B:97[B]:ARG:NH1	5:B:2080:HOH:O	2.23	0.67
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.37	0.65
1:C:208:ARG:N	1:C:208:ARG:HD2	2.13	0.63
3:B:301:ZY5:H5	3:B:301:ZY5:H132	1.81	0.63
1:E:185:VAL:HG13	1:E:196:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.43	0.59
3:B:301:ZY5:C5	3:B:301:ZY5:H132	2.33	0.58
1:A:52[B]:LEU:HD13	1:A:125:PHE:HE2	1.68	0.57
1:A:143:LYS:NZ	1:A:184:GLN:HE22	2.02	0.57
1:A:191:CYS:HB3	1:A:193:GLU:OE2	2.04	0.57
3:D:301:ZY5:H5	3:D:301:ZY5:H131	1.87	0.56
1:C:59[B]:ARG:CG	1:C:59[B]:ARG:HH21	2.20	0.55
1:C:59[B]:ARG:HH21	1:C:59[B]:ARG:HG2	1.71	0.55
1:E:15:ASN:HD22	1:E:15:ASN:N	2.05	0.54
1:A:7:MET:HG2	5:B:2004:HOH:O	2.07	0.54
1:A:61:LYS:HE2	1:A:112:ASP:O	2.08	0.54
3:D:301:ZY5:H5	3:D:301:ZY5:C13	2.38	0.54
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.48	0.53
1:D:143:LYS:NZ	1:D:184:GLN:HE22	2.06	0.53
1:C:122:ARG:HD2	1:D:96:THR:O	2.10	0.52
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:CE	2.39	0.52
3:B:301:ZY5:H5	3:B:301:ZY5:C13	2.40	0.51
1:A:96:THR:O	1:E:122:ARG:HD2	2.12	0.51
3:E:301:ZY5:H5	3:E:301:ZY5:C13	2.43	0.49
1:B:99[A]:VAL:HG22	1:B:123:LEU:HD13	1.95	0.49
1:B:121[A]:GLN:OE1	5:B:2101:HOH:O	2.19	0.49
1:E:50:VAL:CG2	1:E:127:CYS:SG	3.01	0.48
3:A:301:ZY5:H5	3:A:301:ZY5:C13	2.44	0.48
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.54	0.47
1:C:99[B]:VAL:HG22	1:C:123:LEU:HD13	1.97	0.47
1:C:186[A]:GLN:HG2	1:C:197:ASP:OD1	2.15	0.47
1:C:59[B]:ARG:CG	1:C:59[B]:ARG:NH2	2.78	0.46
1:A:122:ARG:HD2	1:B:96:THR:O	2.15	0.46
3:D:301:ZY5:C5	3:D:301:ZY5:C13	2.93	0.46
1:D:118:ILE:HD13	3:E:301:ZY5:H221	1.97	0.46
1:A:59[B]:ARG:HD3	1:A:116[B]:MET:HE1	1.98	0.46
1:B:61:LYS:HE3	1:B:112:ASP:O	2.15	0.46
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.55	0.45
1:D:193:GLU:HG2	1:D:195:TYR:CE2	2.51	0.45
1:B:122:ARG:HD2	1:C:96:THR:O	2.17	0.45
1:A:79:ARG:HD3	1:B:149:TYR:CE1	2.52	0.45
1:A:190:CYS:SG	1:A:191:CYS:N	2.90	0.44
3:E:301:ZY5:H132	3:E:301:ZY5:C5	2.47	0.44
1:D:147:TRP:NE1	3:D:301:ZY5:H19	2.33	0.44
5:D:2078:HOH:O	1:E:97[B]:ARG:HD3	2.17	0.44
1:C:12:ASP:OD1	1:C:16:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:HG2	1:E:148:VAL:HG23	2.00	0.44
1:A:185:VAL:HG13	1:A:196:ILE:CD1	2.48	0.44
1:C:12:ASP:HA	1:C:16:ARG:HD2	1.99	0.44
3:E:301:ZY5:H132	3:E:301:ZY5:H5	2.00	0.44
1:B:59:ARG:HD2	1:B:116[A]:MET:CE	2.49	0.43
3:A:301:ZY5:C13	3:A:301:ZY5:C5	2.96	0.43
1:C:186[A]:GLN:CG	1:C:197:ASP:OD1	2.67	0.43
1:B:191:CYS:HB3	1:B:193:GLU:OE2	2.19	0.42
1:B:143:LYS:HE2	1:B:184:GLN:HE22	1.85	0.42
3:A:301:ZY5:H5	3:A:301:ZY5:H131	2.02	0.42
1:A:50:VAL:CG2	1:A:127:CYS:SG	3.07	0.42
1:D:143:LYS:HZ2	1:D:184:GLN:HE22	1.66	0.42
3:C:301:ZY5:C13	3:C:301:ZY5:C5	2.94	0.42
1:C:17:SER:HA	1:C:18:PRO:HD3	1.89	0.41
1:B:190:CYS:SG	1:B:191:CYS:N	2.93	0.41
1:C:175:GLU:OE2	1:C:208:ARG:HD3	2.21	0.41
1:B:7:MET:CE	1:C:21:PRO:HD3	2.51	0.41
1:C:56:GLU:O	1:C:119:PRO:HD2	2.21	0.41
1:D:25:LYS:HG3	1:D:152:PHE:HB3	2.03	0.41
1:E:-6:LYS:NZ	5:E:2006:HOH:O	2.54	0.41
1:A:150:SER:CB	1:A:193:GLU:HG3	2.50	0.40
1:B:99[A]:VAL:HG22	1:B:123:LEU:CD1	2.51	0.40
1:A:161:ASP:HB3	5:A:2148:HOH:O	2.22	0.40
1:D:67:TRP:CZ3	1:D:111:HIS:HA	2.55	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	219/228 (96%)	216 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	215/228 (94%)	212 (99%)	3 (1%)	0	100	100
1	C	222/228 (97%)	219 (99%)	3 (1%)	0	100	100
1	D	204/228 (90%)	202 (99%)	2 (1%)	0	100	100
1	E	213/228 (93%)	212 (100%)	1 (0%)	0	100	100
All	All	1073/1140 (94%)	1061 (99%)	12 (1%)	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	202/206 (98%)	198 (98%)	4 (2%)	55	34
1	B	198/206 (96%)	196 (99%)	2 (1%)	76	63
1	C	205/206 (100%)	202 (98%)	3 (2%)	65	49
1	D	191/206 (93%)	188 (98%)	3 (2%)	62	45
1	E	198/206 (96%)	192 (97%)	6 (3%)	41	18
All	All	994/1030 (96%)	976 (98%)	18 (2%)	57	40

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	186	GLN
1	A	193	GLU
1	A	208	ARG
1	B	136	GLU
1	B	162	GLN
1	C	16	ARG
1	C	136	GLU
1	C	157	LYS
1	D	70	ASN

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Mol	Chain	Res	Type
1	D	207	ARG
1	D	208	ARG
1	E	15	ASN
1	E	59	ARG
1	E	185	VAL
1	E	186	GLN
1	E	190	CYS
1	E	191	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	100	GLN
1	A	184	GLN
1	B	15	ASN
1	B	57	GLN
1	B	70	ASN
1	C	184	GLN
1	D	184	GLN
1	E	15	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 ⓘ

5 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	0.25	0	17,19,21	1.40	2 (11%)
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	1.05	1 (5%)
2	BMA	F	3	2	11,11,12	0.40	0	15,15,17	0.81	0
2	MAN	F	4	2	11,11,12	0.52	0	15,15,17	1.68	4 (26%)
2	MAN	F	5	2	11,11,12	0.53	0	15,15,17	1.19	1 (6%)

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	-	1/6/23/26	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
2	MAN	F	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C4-C3-C2	-3.37	106.08	111.02
2	F	4	MAN	C1-O5-C5	3.26	116.61	112.19
2	F	5	MAN	C1-C2-C3	3.04	113.40	109.67
2	F	4	MAN	C1-C2-C3	2.85	113.17	109.67
2	F	1	NAG	O5-C1-C2	-2.76	106.93	111.29
2	F	2	NAG	C2-N2-C7	-2.47	119.39	122.90
2	F	4	MAN	O3-C3-C2	2.14	114.10	109.99
2	F	4	MAN	C3-C4-C5	-2.10	106.49	110.24

There are no chirality outliers.

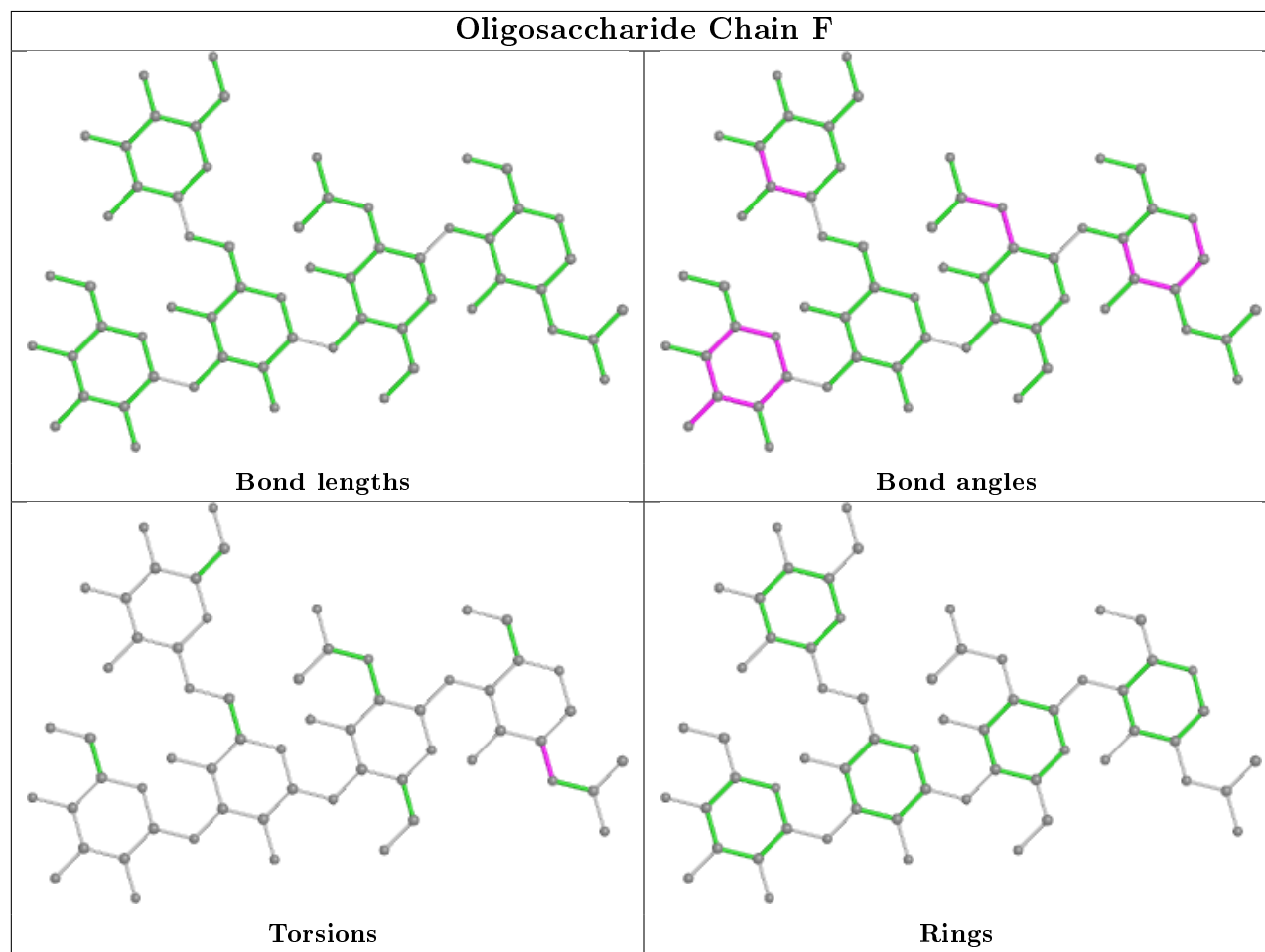
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C3-C2-N2-C7

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](#)

6 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	ZY5	C	301	-	24,24,24	0.74	0	29,32,32	2.03	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ZY5	E	301	-	24,24,24	0.95	2 (8%)	29,32,32	2.46	4 (13%)
3	ZY5	D	301	-	24,24,24	1.15	3 (12%)	29,32,32	2.13	6 (20%)
4	NAG	B	401	1	14,14,15	0.36	0	17,19,21	1.48	2 (11%)
3	ZY5	A	301	-	24,24,24	1.01	1 (4%)	29,32,32	2.58	6 (20%)
3	ZY5	B	301	-	24,24,24	1.00	1 (4%)	29,32,32	2.62	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZY5	C	301	-	-	0/10/21/21	0/3/3/3
3	ZY5	E	301	-	-	4/10/21/21	0/3/3/3
3	ZY5	D	301	-	-	0/10/21/21	0/3/3/3
4	NAG	B	401	1	-	3/6/23/26	0/1/1/1
3	ZY5	A	301	-	-	2/10/21/21	0/3/3/3
3	ZY5	B	301	-	-	0/10/21/21	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	ZY5	C4-C7	3.19	1.51	1.46
3	A	301	ZY5	C4-C7	3.05	1.51	1.46
3	D	301	ZY5	C4-C7	2.99	1.51	1.46
3	E	301	ZY5	C4-C7	2.58	1.50	1.46
3	D	301	ZY5	C9-N10	-2.43	1.27	1.28
3	D	301	ZY5	C14-C9	2.24	1.51	1.48
3	E	301	ZY5	C9-N10	-2.24	1.27	1.28

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	ZY5	C11-N10-C9	11.36	130.80	116.09
3	A	301	ZY5	C11-N10-C9	11.09	130.45	116.09
3	E	301	ZY5	C11-N10-C9	10.66	129.89	116.09
3	C	301	ZY5	C11-N10-C9	8.24	126.76	116.09
3	D	301	ZY5	C11-N10-C9	7.69	126.05	116.09
3	A	301	ZY5	C22-O21-C3	5.54	125.89	117.53
3	E	301	ZY5	C22-O21-C3	4.83	124.82	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	ZY5	C22-O21-C3	4.79	124.76	117.53
3	B	301	ZY5	C22-O21-C3	4.20	123.86	117.53
3	D	301	ZY5	C12-C11-N10	-3.62	102.64	113.34
4	B	401	NAG	C2-N2-C7	3.26	127.55	122.90
3	A	301	ZY5	C12-C11-N10	-3.16	104.02	113.34
4	B	401	NAG	C4-C3-C2	-2.86	106.82	111.02
3	D	301	ZY5	C13-C8-C7	-2.83	122.44	125.27
3	C	301	ZY5	O21-C3-C4	2.75	119.64	115.92
3	D	301	ZY5	C8-C9-N10	-2.68	115.32	124.57
3	B	301	ZY5	C4-C7-C8	-2.61	123.98	128.45
3	E	301	ZY5	C16-C15-C14	-2.51	117.37	120.34
3	C	301	ZY5	C12-C11-N10	-2.50	105.96	113.34
3	A	301	ZY5	C4-C7-C8	-2.48	124.20	128.45
3	C	301	ZY5	C22-O21-C3	2.39	121.14	117.53
3	B	301	ZY5	C12-C11-N10	-2.37	106.33	113.34
3	E	301	ZY5	C12-C11-N10	-2.36	106.39	113.34
3	D	301	ZY5	C4-C7-C8	-2.26	124.57	128.45
3	C	301	ZY5	O21-C3-C2	-2.25	120.25	124.12
3	A	301	ZY5	C17-N18-C19	2.24	120.72	116.85
3	B	301	ZY5	C16-C15-C14	-2.23	117.71	120.34
3	B	301	ZY5	C17-N18-C19	2.15	120.58	116.85
3	C	301	ZY5	C14-C9-N10	-2.14	115.94	118.04
3	C	301	ZY5	C17-N18-C19	2.11	120.49	116.85
3	A	301	ZY5	C8-C9-N10	-2.05	117.50	124.57

There are no chirality outliers.

All (9) torsion outliers are listed below:

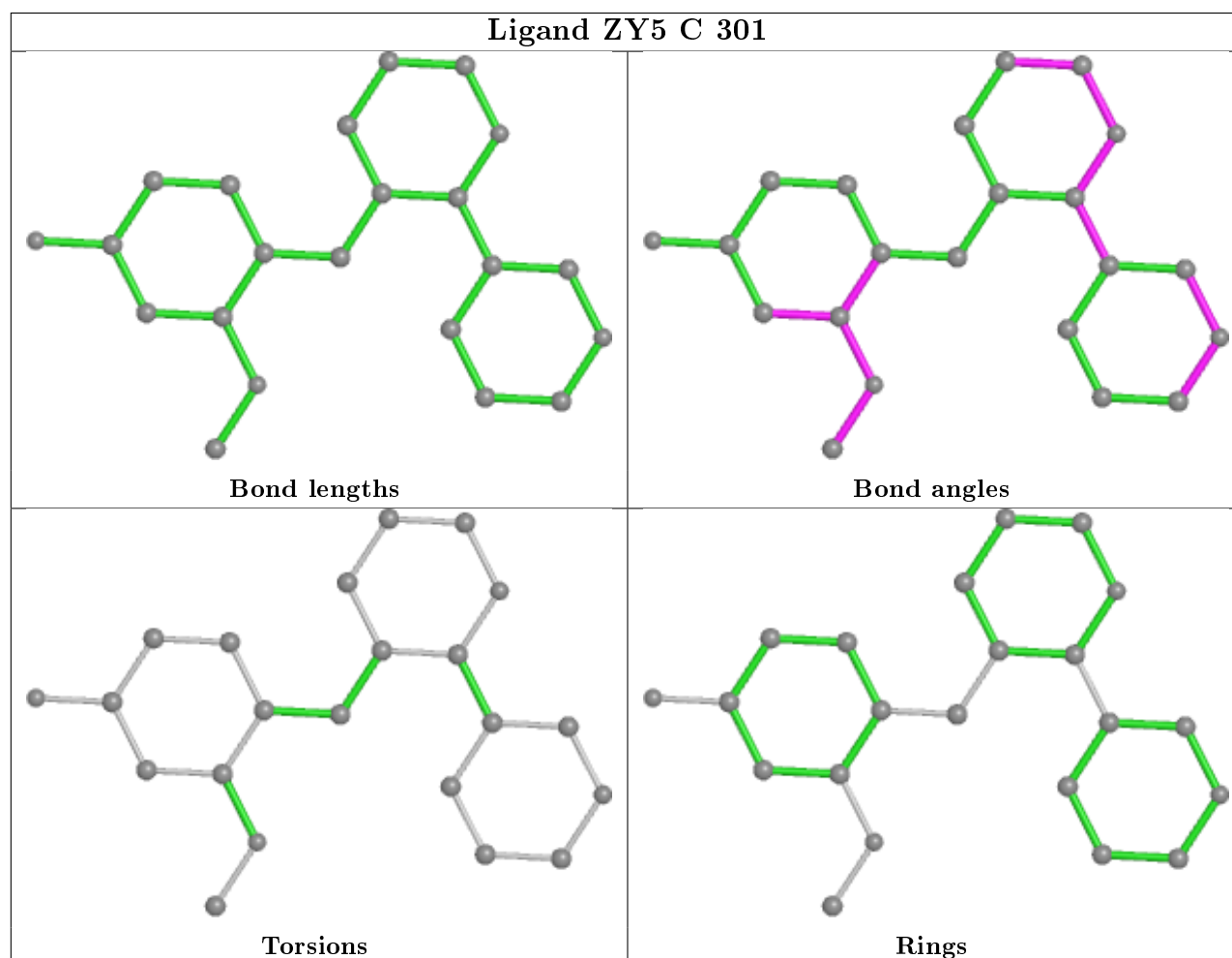
Mol	Chain	Res	Type	Atoms
4	B	401	NAG	O5-C5-C6-O6
4	B	401	NAG	C4-C5-C6-O6
3	E	301	ZY5	C15-C14-C9-N10
3	E	301	ZY5	C15-C14-C9-C8
3	E	301	ZY5	C19-C14-C9-C8
3	A	301	ZY5	C15-C14-C9-N10
4	B	401	NAG	C3-C2-N2-C7
3	E	301	ZY5	C19-C14-C9-N10
3	A	301	ZY5	C19-C14-C9-N10

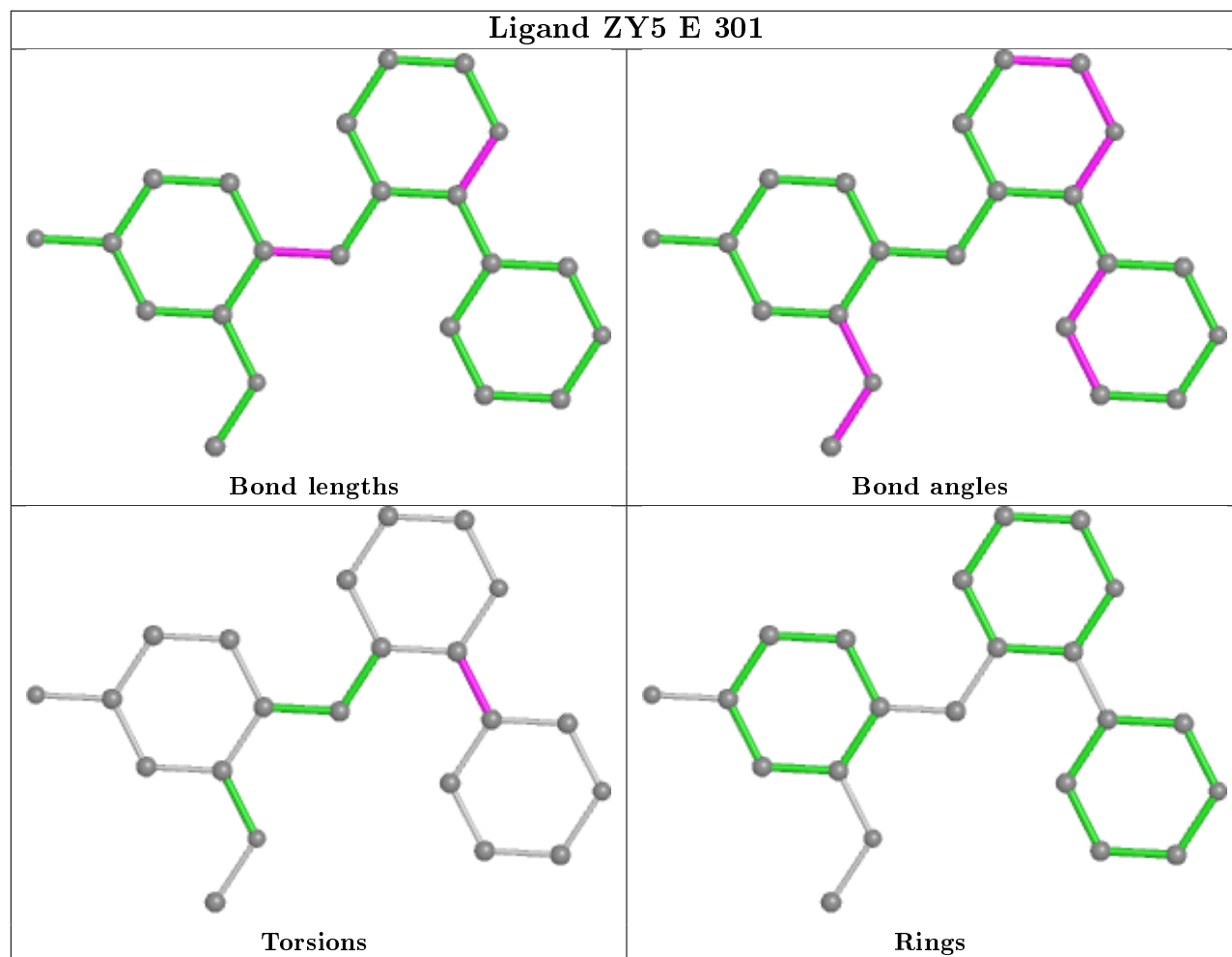
There are no ring outliers.

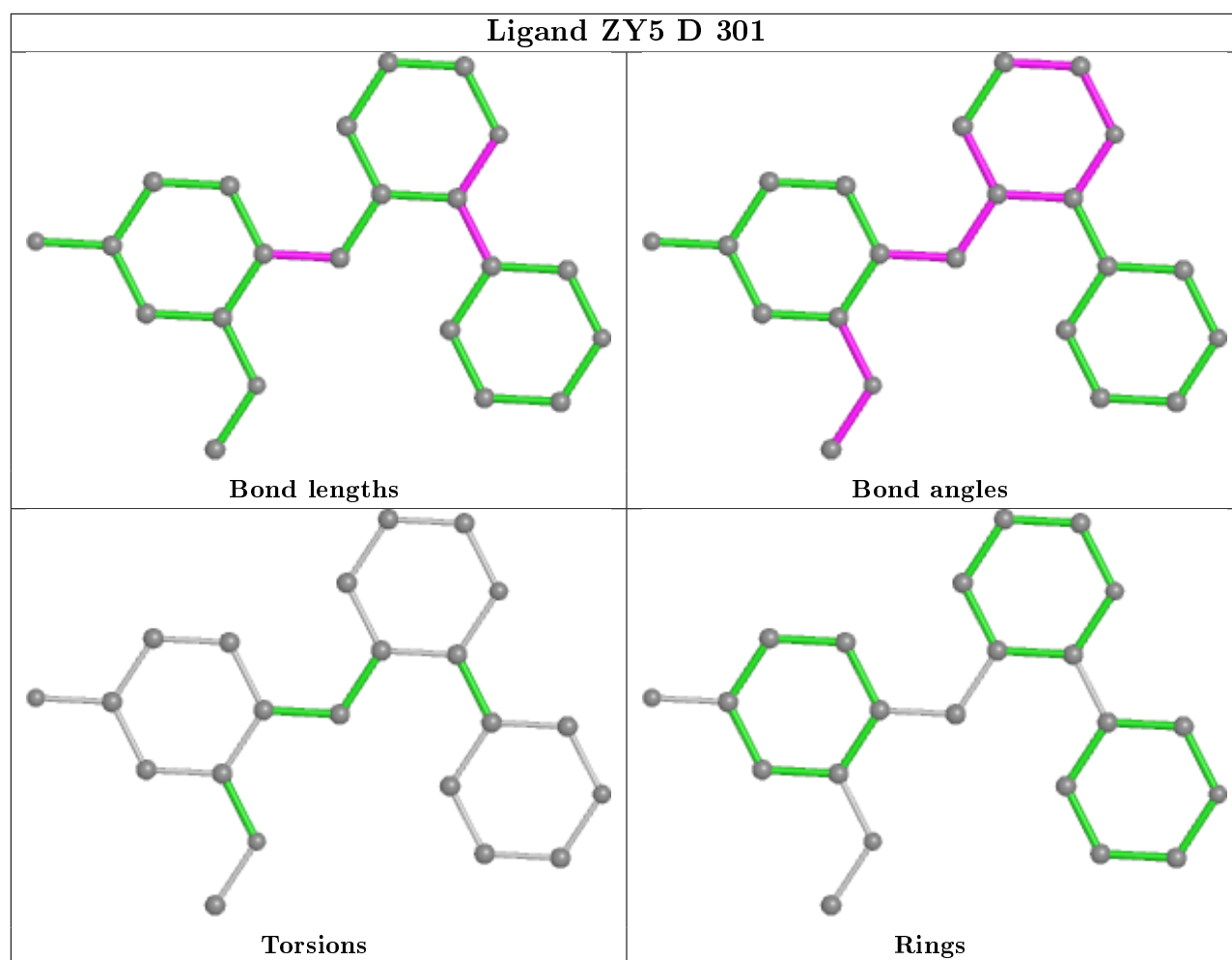
5 monomers are involved in 17 short contacts:

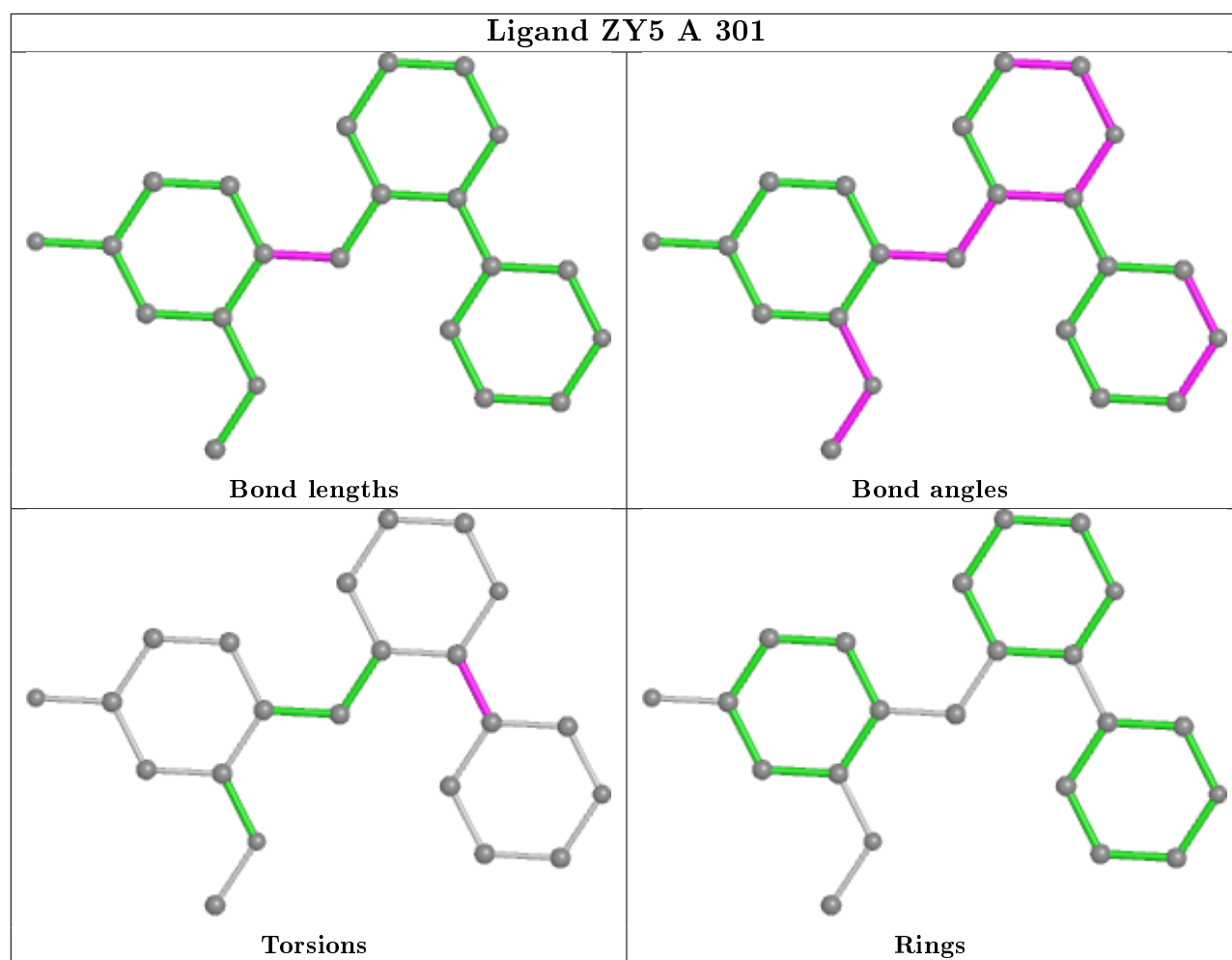
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	ZY5	3	0
3	E	301	ZY5	4	0
3	D	301	ZY5	4	0
3	A	301	ZY5	3	0
3	B	301	ZY5	3	0

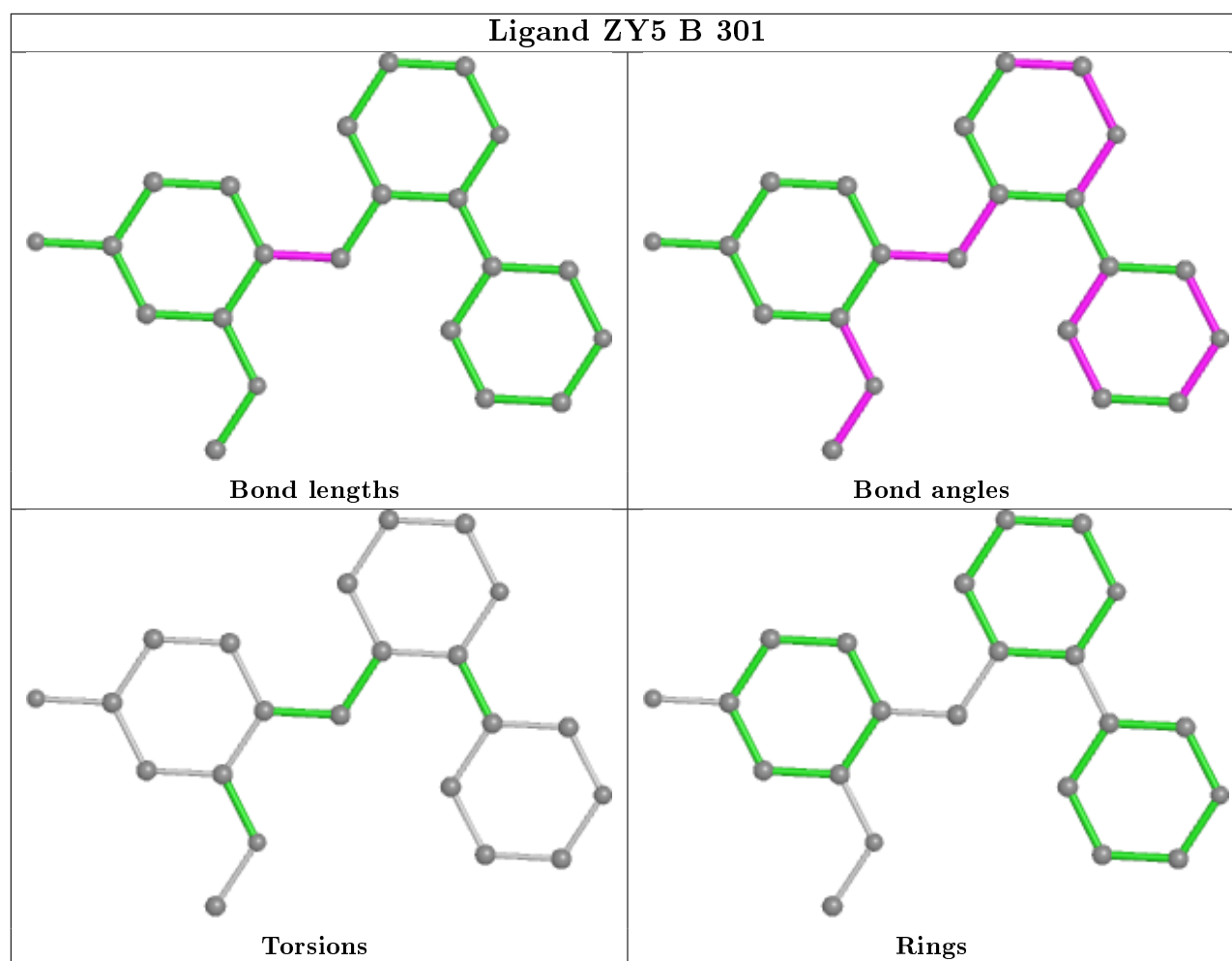
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/228 (91%)	0.37	17 (8%) 12 16	16, 27, 60, 83	0
1	B	211/228 (92%)	0.42	20 (9%) 8 11	15, 29, 58, 80	0
1	C	214/228 (93%)	0.26	10 (4%) 31 37	16, 28, 53, 71	0
1	D	205/228 (89%)	0.23	16 (7%) 13 17	17, 28, 61, 93	0
1	E	214/228 (93%)	0.46	15 (7%) 16 21	17, 29, 52, 80	0
All	All	1053/1140 (92%)	0.35	78 (7%) 14 19	15, 28, 58, 93	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ARG	9.5
1	B	18	PRO	8.6
1	E	189	SER	8.6
1	C	19	MET	8.5
1	A	190	CYS	8.4
1	B	16	ARG	8.0
1	A	19	MET	7.7
1	A	0	LEU	6.7
1	E	16	ARG	6.6
1	B	19	MET	6.5
1	E	191	CYS	6.5
1	C	18	PRO	6.4
1	B	15	ASN	6.1
1	A	191	CYS	6.1
1	B	-3	ASP	6.0
1	A	188	TYR	6.0
1	E	190	CYS	5.5
1	A	189	SER	4.8
1	B	0	LEU	4.6
1	C	0	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	15	ASN	4.5
1	B	1	HIS	4.3
1	B	17	SER	4.2
1	B	14	PHE	4.0
1	E	152	PHE	3.9
1	D	208	ARG	3.9
1	D	1	HIS	3.8
1	C	208	ARG	3.7
1	A	187	HIS	3.6
1	D	-2	ASP	3.6
1	A	1	HIS	3.6
1	D	0	LEU	3.6
1	C	17	SER	3.4
1	D	70	ASN	3.3
1	E	15	ASN	3.2
1	E	193	GLU	3.2
1	A	195	TYR	3.2
1	D	187	HIS	3.1
1	A	15	ASN	3.1
1	B	71	GLU	3.0
1	B	13	LEU	2.9
1	C	-3	ASP	2.9
1	A	185	VAL	2.9
1	A	16	ARG	2.8
1	B	-2	ASP	2.8
1	E	192	PRO	2.8
1	D	136	GLU	2.7
1	E	188	TYR	2.6
1	D	17	SER	2.6
1	A	194	PRO	2.6
1	A	18	PRO	2.6
1	E	70	ASN	2.5
1	B	134	SER	2.5
1	D	135	GLU	2.5
1	B	207	ARG	2.4
1	C	15	ASN	2.4
1	C	16	ARG	2.4
1	C	-5	ASP	2.4
1	E	17	SER	2.3
1	B	11	SER	2.3
1	E	26	ASP	2.3
1	A	208	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	11	SER	2.3
1	D	186	GLN	2.3
1	B	135	GLU	2.3
1	C	136	GLU	2.3
1	B	7	MET	2.2
1	E	187	HIS	2.2
1	A	152	PHE	2.2
1	B	136	GLU	2.2
1	B	161	ASP	2.2
1	D	-1	LYS	2.1
1	B	188	TYR	2.1
1	D	192	PRO	2.1
1	E	186	GLN	2.1
1	A	186	GLN	2.0
1	E	25	LYS	2.0
1	D	71	GLU	2.0

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

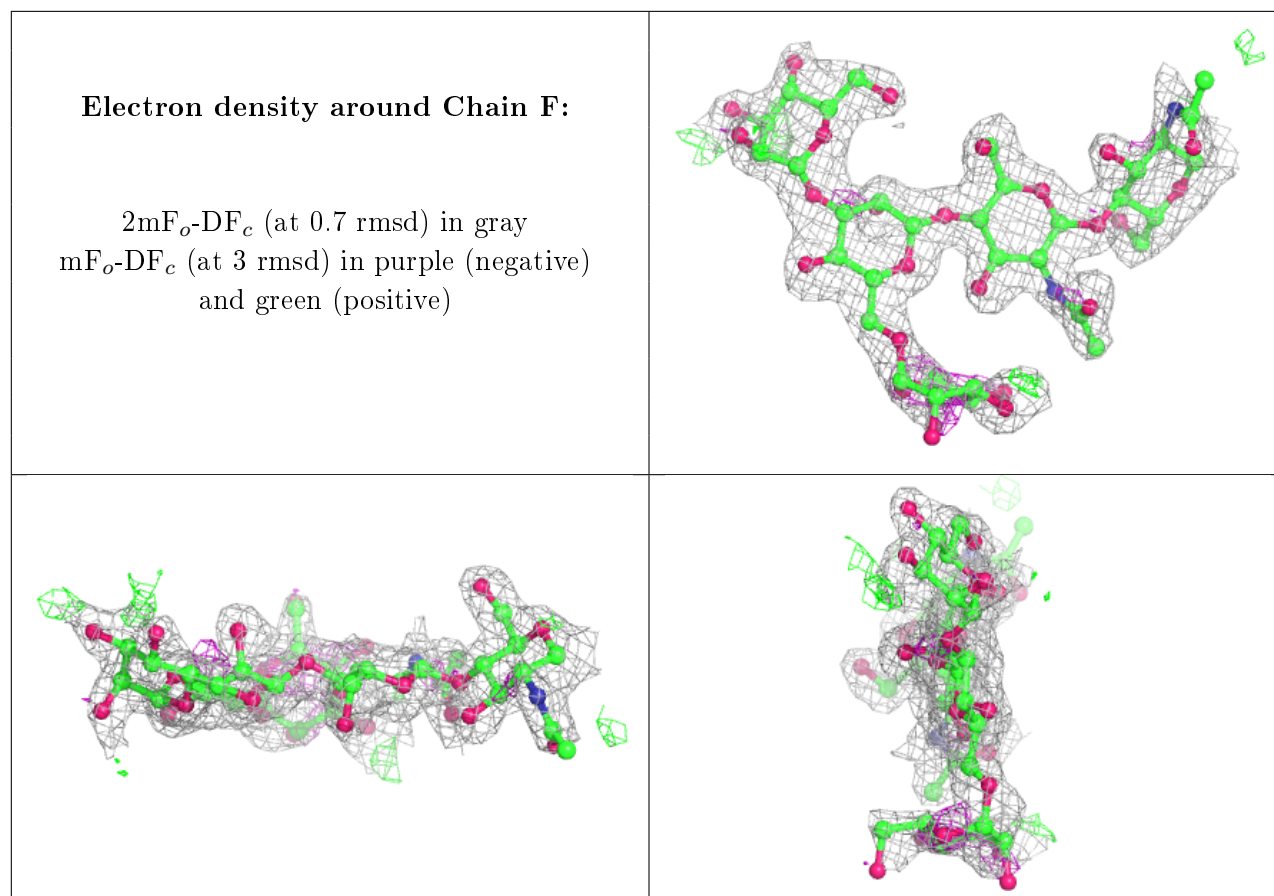
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	F	5	11/12	0.61	0.50	53,55,56,57	0
2	NAG	F	2	14/15	0.84	0.25	42,48,51,51	0
2	NAG	F	1	14/15	0.85	0.30	44,48,57,58	0
2	BMA	F	3	11/12	0.86	0.21	38,41,46,52	0
2	MAN	F	4	11/12	0.87	0.32	43,45,47,49	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 ⓘ

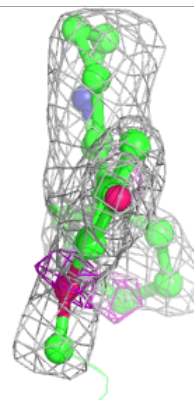
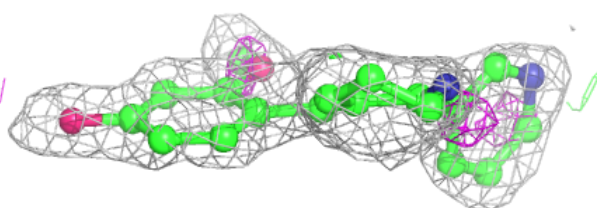
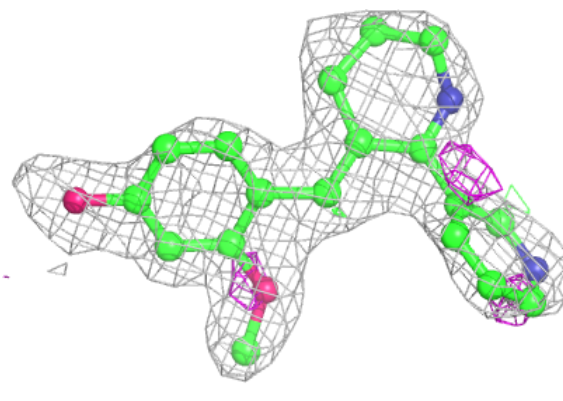
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	401	14/15	0.64	0.30	66,70,73,73	0
3	ZY5	D	301	22/22	0.80	0.23	34,40,41,42	0
3	ZY5	E	301	22/22	0.89	0.10	29,33,34,35	0
3	ZY5	A	301	22/22	0.91	0.14	30,32,35,36	0
3	ZY5	B	301	22/22	0.93	0.09	25,30,34,36	0
3	ZY5	C	301	22/22	0.94	0.09	23,29,32,32	0

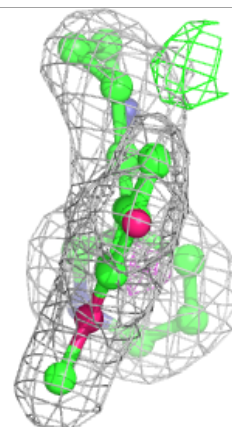
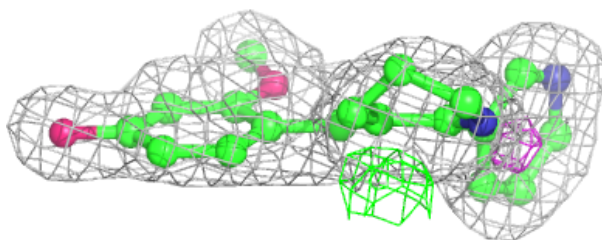
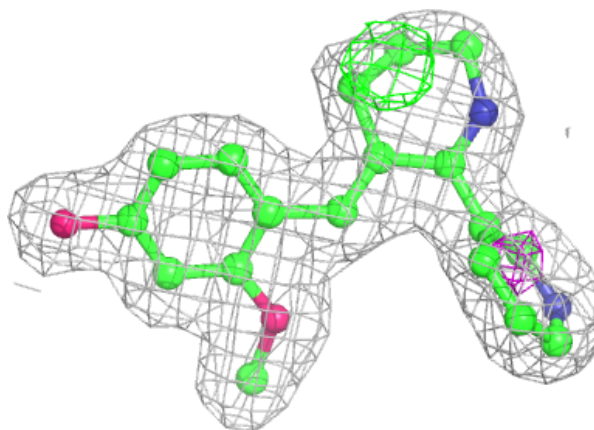
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZY5 D 301:

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

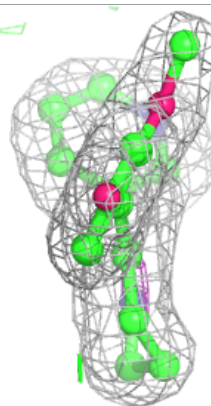
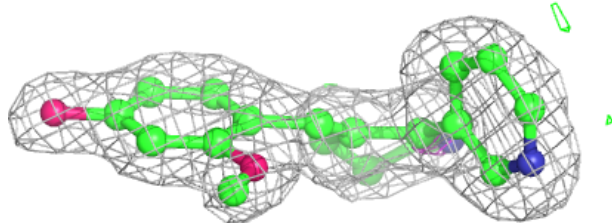
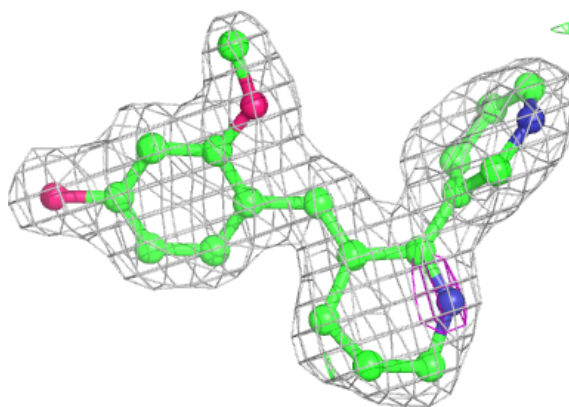
**Electron density around ZY5 E 301:**

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

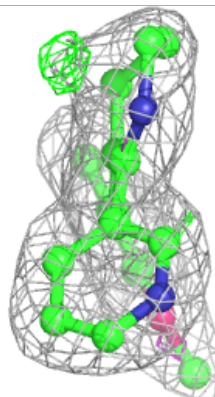
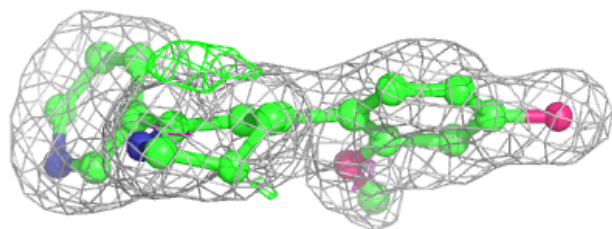
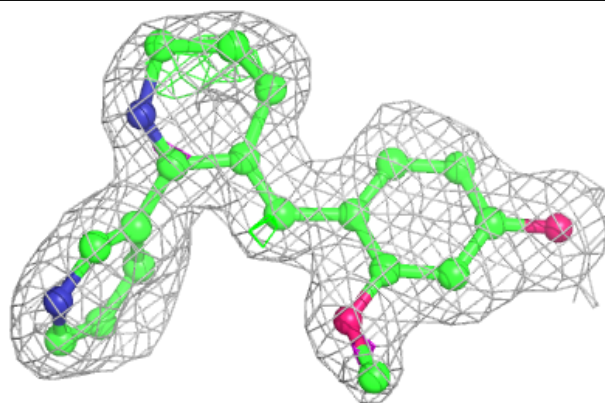


Electron density around ZY5 A 301:

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

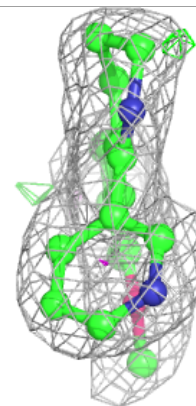
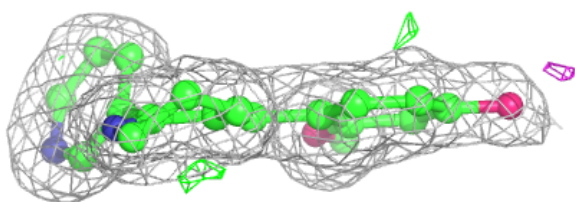
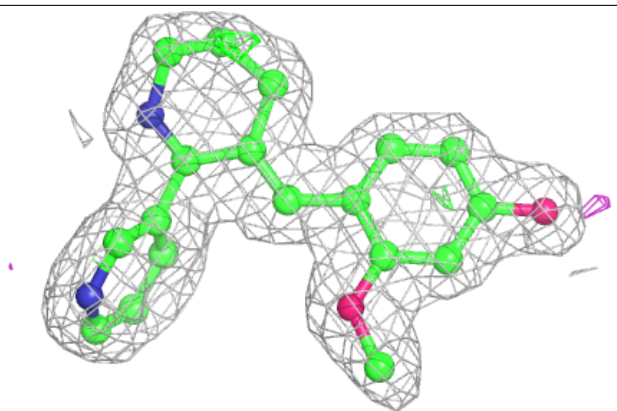
**Electron density around ZY5 B 301:**

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



Electron density around ZY5 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.